test object with the target object in each pose of a plurality of different poses, thereby creating a plurality of voxel maps. Each respective voxel map in the plurality of voxel maps comprises the test object in a respective pose in the plurality of different poses.

[0008] The at least one program further comprises instructions for unfolding each voxel map in the plurality of voxel maps into a corresponding vector, thereby creating a plurality of vectors. In some embodiments, each vector in the plurality of vectors is the same size.

[0009] The at least one program further comprises instructions for inputting each respective vector in the plurality of vectors to a network architecture that includes (i) an input layer for sequentially receiving the plurality of vectors, (ii) a plurality of convolutional layers, and (iii) a scorer. The plurality of convolutional layers includes an initial convolutional layer and a final convolutional layer. Each layer in the plurality of convolutional layers is associated with a different set of weights. Responsive to input of a respective vector in the plurality of vectors, the input layer feeds a first plurality of values into the initial convolutional layer as a first function of values in the respective vector. Each respective convolutional layer, other than the final convolutional layer, feeds intermediate values, as a respective second function of (i) the different set of weights associated with the respective convolutional layer and (ii) input values received by the respective convolutional layer, into another convolutional layer in the plurality of convolutional layers. The final convolutional layer feeds final values, as a third function of (i) the different set of weights associated with the final convolutional layer and (ii) input values received by the final convolutional layer, into the scorer.

[0010] The at least one program further comprises instructions for obtaining a plurality of scores from the scorer, where each score in the plurality of scores corresponds to the input of a vector in the plurality of vectors into the input layer. The at least one program further comprises instructions for using the plurality of scores to provide a characterization of the test object.

[0011] In some embodiments, the scorer comprises a plurality of fully-connected layers and an evaluation layer. Further, a fully-connected layer in the plurality of fully-connected layers feeds into the evaluation layer.

[0012] In some embodiments, the scorer comprises a decision tree, a multiple additive regression tree, a clustering algorithm, principal component analysis, a nearest neighbor

10. The computer system of any one of claims 1-7, wherein the target object is a polymer and the spatial coordinates are a set of three-dimensional coordinates $\{x_1, \ldots, x_N\}$ for a crystal structure of the polymer resolved at a resolution of 2.5 Å or better, or at a resolution of 3.3 Å or better.

11. The computer system of any one of claims 1-7, wherein the target object is a polymer and the spatial coordinates are an ensemble of three-dimensional coordinates for the polymer determined by nuclear magnetic resonance, neutron diffraction, or cryo-electron microscopy.

12. The computer system of any one of claims 1-11, wherein 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, wherein

when the measure of central tendency satisfies a predetermined threshold value or predetermined threshold value range, the characterization comprises deeming the test object have a first classification, and

when the measure of central tendency fails to satisfy the predetermined threshold value or predetermined threshold value range, the characterization comprises deeming the test object to have a second classification.

13. The computer system of any one of claims 1-11, wherein the using the plurality of scores to characterize the test object comprises taking a weighted average of the plurality of scores, wherein

when the weighted average satisfies a predetermined threshold value or predetermined threshold value range, the test object is deemed to have a first classification, and

when the weighted average fails to satisfy the predetermined threshold value or predetermined threshold value range, the test object is deemed to have a second classification.

14. The computer system of claim 13 wherein the weighted average is a Boltzman average of the plurality of scores.

15. The computer system of claim 13, wherein

the first classification is an IC_{50}, $EC_{50,}$ Kd, or KI for the test object with respect to the target object that is above a first binding value, and

the second classification is an IC_{50}, EC_{50}, Kd, or KI for the test object with respect to the target object that is below the first binding value.

16. The computer system of claim 15, wherein the first binding value is one micromolar or ten micromolar.

17. The computer system of claim 15, wherein the first binding value is the predicted IC50, EC50, Kd, or KI for a different test object with respect to the target object.

18. The computer system of any one of claims 1-11, wherein the using the plurality of scores to characterize the test object comprises taking a weighted average of the plurality of scores, wherein when the weighted average satisfies a respective threshold value range in a plurality of threshold value ranges, the using (F) comprises deeming the test object to have a respective classification in a plurality of a respective classifications that uniquely corresponds to the respective threshold value range.

19. The computer system of claim 18, wherein each respective classification in the plurality of classifications is an IC_{50}, $EC_{50,}$ Kd, or KI range for the test object with respect to the target object.

20. The computer system of claim 19, wherein a first classification in the plurality of classifications is between one micromolar and ten micromolar or is between one nanomolar and 100 nanomolar.

21. The computer system of any one of claims 1-7, wherein the target object is a polymer with an active site, the test object is a chemical composition, and the modeling comprises docking the test object into the active site of the polymer.

22. The computer system of any one of claims 1-21, wherein a convolutional layer in the plurality of convolutional layers has a plurality of filters and wherein each filter in the plurality of filters convolves a cubic input space of N^3 with stride Y, where N is an integer of two or greater and Y is a positive integer.

23. The computer system of claim 22, wherein the different set of weights associated with the convolutional layer are associated with respective filters in the plurality of filters.

24. The computer system of any one of claims 1-23, wherein the scorer comprises a plurality of fully-connected layers and a logistic regression cost layer wherein a fully-connected layer in the plurality of fully-connected layers feeds into the logistic regression cost layer.

25. The computer system of any one of claims 1-7, wherein

the target object is a polymer with an active site,

the test object is a chemical composition,

the modeling comprises performing a molecular dynamics run of the target object and the test object thereby forming a trajectory of the target object and the test object together over time, and

a subset of the plurality of different poses is obtained by taking snapshots of the trajectory over a period of time.

26. The computer system of claim 1, wherein the computer system further comprises a graphical processing unit having a graphical processing memory, wherein the graphical processing memory comprises the network architecture and performs the providing (D) and the at least one general processor performs the using (F).

27. The computer system of claim 1, wherein the characterization of the test object is a toxicity prediction of the test object or a prediction of the potency of the test object against a molecular disease target, wherein the potency is a binding affinity prediction of the test object against the molecular disease target.

28. The computer system of claim 1, wherein the characterization of the test object is a prediction of the selectivity of the test object against a first molecular target versus a second molecular target, wherein the first molecular target is linked to a disease.

29. The computer system of claim 12, wherein

the first classification is a determination that the test object is not toxic to a host organism, and

the second classification is a determination that the test object is toxic to the host organism.

30. The computer system of claim 12, wherein

the first classification is a prediction that the test object binds to a molecular disease target with an IC_{50}, $EC_{50,}$ Kd, or KI that is below a first binding value, and

the second classification is a prediction that the test object binds to a molecular disease target with an IC_{50}, $EC_{50,}$ Kd, or KI that is above the first binding value.

31. The computer system of claim 12, wherein

the first classification is a prediction that the test object binds to a first molecular disease target with an IC_{50}, $EC_{50,}$ Kd, or KI that is below a first binding value and that the test object binds to a second molecular disease target with an IC_{50}, $EC_{50,}$ Kd, or KI that is above the first binding value, and

the second classification is a prediction that the test object binds to a first molecular disease target with an IC_{50}, $EC_{50,}$ Kd, or KI that is below a first binding value and that the test object binds to a second molecular disease target with an IC_{50}, $EC_{50,}$ Kd, or KI that is below the first binding value.

32. The computer system of claim 30 or 31, wherein the first binding value is one micromolar or ten micromolar.

33. The computer system of claim 13 or 14, wherein

the first classification is a determination that the test object is not toxic to a host organism, and

the second classification is a determination that the test object is toxic to the host organism.

34. The computer system of claim 13 or 14, wherein

the first classification is a prediction that the test object binds to a first molecular disease target with an IC_{50}, $EC_{50,}$ Kd, or KI that is below a first binding value and that the test object binds to a second molecular disease target with an IC_{50}, $EC_{50,}$ Kd, or KI that is above the first binding value, and

the second classification is a prediction that the test object binds to a first molecular disease target with an IC_{50}, $EC_{50,}$ Kd, or KI that is below a first binding value and that the test object binds to a second molecular disease target with an IC_{50}, $EC_{50,}$ Kd, or KI that is below the first binding value.

35. The computer system of claim 34, wherein the first binding value is one micromolar or ten micomolar.

36. The computer system of claim 19 or 20, wherein the target object is linked with a disease and inhibition of the target object by binding of the test object to the target object is predicted to alleviate the disease.