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(71) Applicant: **FLAGSHIP PIONEERING INNOVATIONS VI, LLC** [US/US]; 55 Cambridge Parkway, Suite 800E, Cambridge, MA 02142 (US).

(72) Inventors: **WOLF, Fabian Alexander**; Flagship Pioneering Innovations VI, LLC, 55 Cambridge Parkway, 8th Floor, Cambridge, MA 02142 (US). **HADDAD, Ragy**; Flagship Pioneering Innovations VI, LLC, 55 Cambridge Parkway, 8th Floor, Cambridge, MA 02142 (US). **PLUGIS, Nicholas McCartney**; Flagship Pioneering Innovations VI, LLC, 55 Cambridge Parkway, 8th Floor, Cambridge, MA 02142 (US).

(74) Agent: **ALTIERI, Stephen L.** et al.; Morgan, Lewis & Bockius LLP, 1111 Pennsylvania Avenue, NW, Washington, DC 20004 (US).

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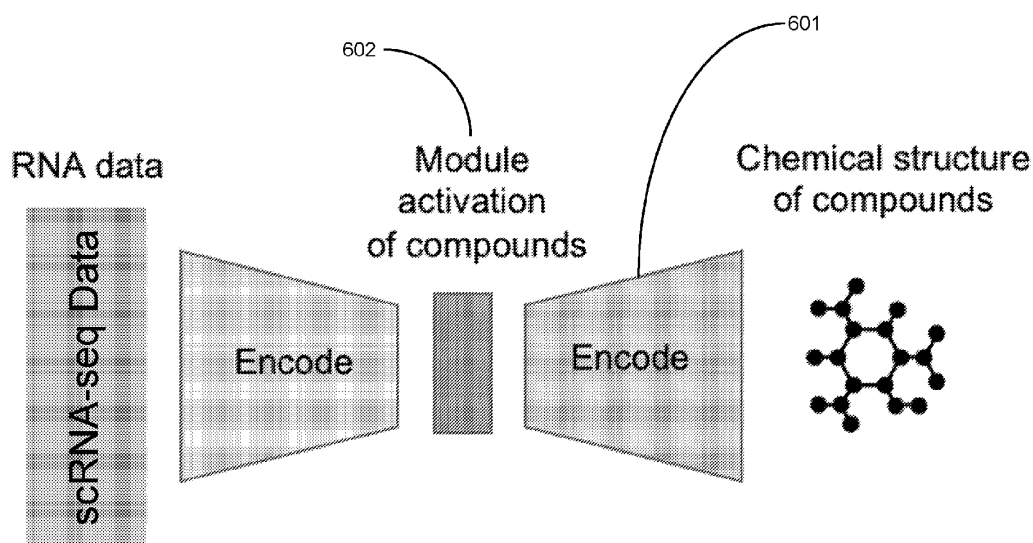


Figure 10A

(57) Abstract: Systems and methods for associating a compound with physiological conditions are provided. A fingerprint of a compound chemical structure is obtained and inputted to a model that outputs one or more calculated activation scores. Each activation score represents a cellular constituent module in a set of modules, where each module includes a subset of cellular constituents and a first module in the set of modules is associated with the physiological condition. When the activation score for the first module satisfies a threshold criterion, the compound is identified as associated with the physiological condition. In some aspects, each activation score represents a perturbation signature associated with the physiological condition and the compound is identified when the activation score for a first perturbation signature satisfies a threshold criterion. Systems and methods for training a model that associates compounds with physiological conditions are also provided.

[Continued on next page]

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