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(54) Title: COLLISION ENERGY SPECIFIC TANDEM MASS SPECTRAL PREDICTION

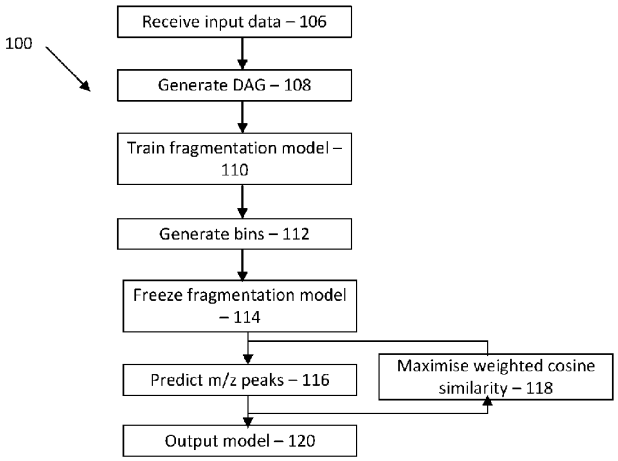

Figure 1B

(57) Abstract: A model is trained to predict collision-energy specific tandem mass spectra (MS/MS) for molecules. Directed acyclic graphs (DAG) are generated, that structurally relates predicted fragments for each molecule. A fragmentation model is then trained based on the DAGs and respective molecular inputs, to generate most probable fragments based on molecular inputs. The input data is then binned, with each bin corresponding to a non-overlapping collision energy range. The trained fragmentation model is frozen and intensity models (one for each bin) are trained to predict MS/MS spectra for molecules based on fragments generated by the fragmentation model.

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