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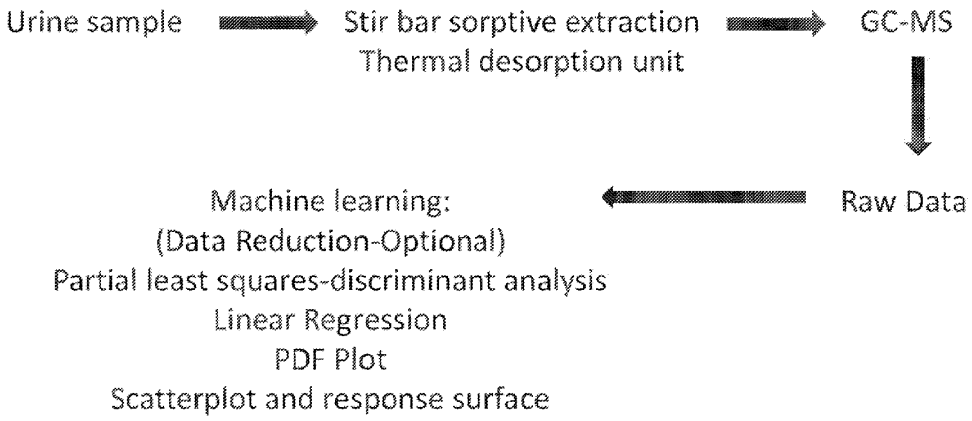
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(54) Title: TRAINING AND USE OF MACHINE-LEARNING MODELS FOR PREDICTING BIOLOGICAL CONDITIONS USING VOLATILE ORGANIC COMPOUNDS

Figure 1



(57) Abstract: Provided herein are methods and systems for diagnosing pathological conditions using machine learning and artificial intelligence models. An exemplary method can include loading an abundance matrix that represents mass spectrometry reads of a sample of a plurality of volatile organic compounds (VOCs) extracted from a biological sample. The abundance matrix can represent each of the plurality of VOCs in a mass-to-charge ratio dimension, an abundance dimension, and a retention time dimension. The method can include providing the abundance matrix to a machine-learning model. The machine- learning model can be trained on abundance matrixes of biomarkers of VOCs collected from healthy and diseased subjects. The method can include receiving, from the machine-learning model, a prediction of a state of a disease state.

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