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(54) Title: SYSTEMS AND METHODS FOR IDENTIFYING COMPOUNDS IN COMBINATORIAL LIBRARIES HAVING SPECIFIC MOLECULAR PROPERTIES

(57) Abstract: Systems and methods for identifying compounds in a combinatorial synthesis library (CSL) having specific molecular properties is provided. The CSL is accessed using an auto-encoder comprising an encoder and a decoder. The encoder maps compounds in the CSL into latent codes in a learned latent space. The decoder retrieves molecular structures of compounds using such codes. A policy selects a batch of latent codes, from which a plurality of compounds is identified using the decoder. Molecular properties of these compounds are determined and used to determine a reward function value for each compound. A probability density, under a target distribution in which latent codes are sampled through the auto-encoder from the CSL with probability proportional to tempered reward function values, is determined using the reward function values. Policy parameters are updated using at least a difference between the probability density and the target distribution, using an a-divergence based objective function.

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