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- (71) **Applicant:** **RECURSION PHARMACEUTICALS, INC.** [US/US]; 41 S. Rio Grande St., Salt Lake City, Utah 84101 (US).
- (72) **Inventors:** **BLEVINS, Andrew**; 41 S. Rio Grande St., Salt Lake City, Utah 84101 (US). **AGUILERA-IPAR-RAGUIRRE, Jorge**; 41 S. Rio Grande St., Salt Lake City, Utah 84101 (US). **LINDVALL, Mika**; 41 S. Rio Grande St., Salt Lake City, Utah 84101 (US).
- (74) **Agent:** **CAREY, John C.** et al.; ARTEGIS LAW GROUP, LLP, 7710 Cherry Park Drive, Suite T104, Houston, Texas 77095 (US).
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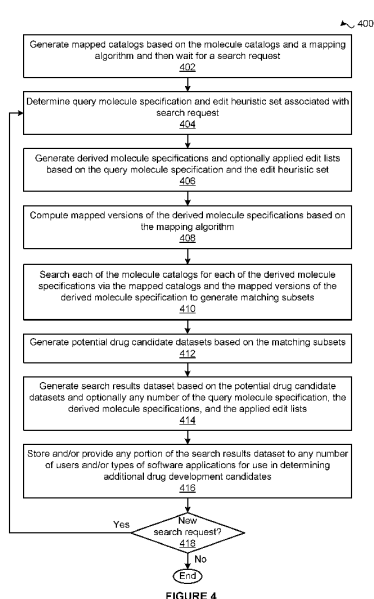


FIGURE 4

(57) **Abstract:** In various embodiments, a molecule exploration application determines one or more potential drug candidates during a drug discovery process. The molecule exploration application generates derived molecule specifications based on a query molecule specification and edit heuristics. Subsequently, the molecule exploration application performs, via a mapping algorithm, one or more mapping operations on the derived molecule specifications to generate mapped molecule specifications. The molecule exploration application then performs one or more search operations on a mapped catalog of molecules based on the mapped molecule specifications to determine the one or more potential drug candidates. Advantageously, the molecule exploration application can be used to efficiently determine additional drug development candidates during a drug discovery process.

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