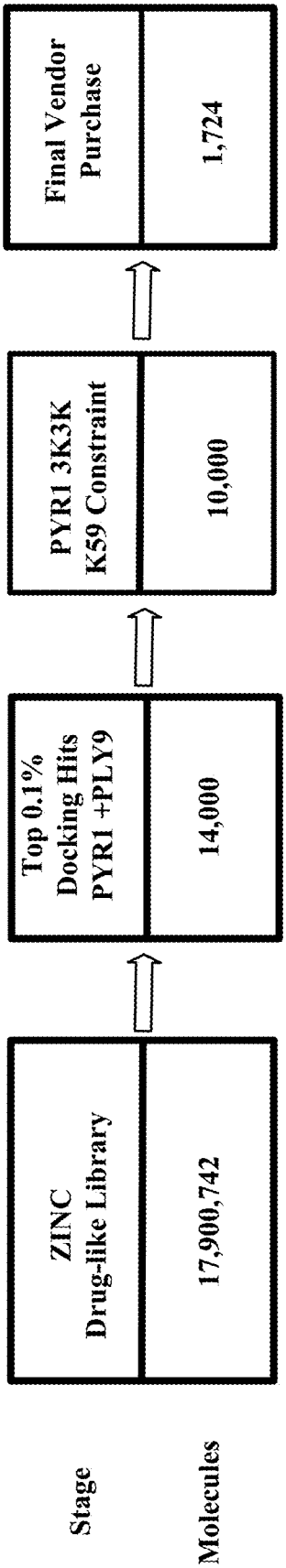
Stage
Molecules
ZINC
Drug-like Library
17,900,742
Top 0.1%
Docking Hits
PYR1 +PLY9
14,000
PYR1 3K3K
K59 Constraint
10,000
Final Vendor
Purchase
1,724

FIG. 1