Penerapan Optimasi Portfolio Untuk Pemilihan Kandidat Molekul Dalam Menghambat Ptp1b Pada Penyakit Diabetes Melitus Menggunakan Non-dominated Sorting Genetic Algorithm

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Abstract

PTP1B or Protein Tyrosine Phosphatase 1B is a protein that is one of the causes of Diabetes Mellitus. One way to handle it is by inhibiting PTP1B. There are many candidate molecules that have the potential to inhibit the growth of this protein. For make selection easier, these large numbers of molecules are chosen based on a high probability of success. This selection problem is similar to the issue of stock selection for an optimal portfolio in finance. This problem can be solved by using NSGA-ii based on the principle of Multi-Objective Optimization. In this algorithm, each generation is evaluated based on non-dominted sorting of individuals in the population to get the best individual that will be the parent of the next generation. The parent will then be used to produce offsprings. At the end of the generation, it will be obtained the best set of individuals that are depicted with efficient frontier graphs. A total of 3715 data used in this study were taken from www.ebi.ac.uk. After preprocessing there are 1452 data that meet the classification to be used. Tests carried out on a dataset of 10 times testing for 5 molecules in 1 portfolio. For each increase in the number of generations a graph with a higher level of confidence in convergence is also obtained. An increase in the number of molecules in a portfolio influences the expected return and diversity.

Keywords: multi-objective optimization, NSGA-II, expected return, diversity, efficient frontier