# INTISARI

Covid-19 telah dideklarasi sebagai pandemi global dan pencarian senyawa untuk obat masih sangat diperlukan. Jumlah kluster gen penghasil metabolit sekunder yang dimiliki *Streptomyces* sp. GMR22 merupakan jumlah paling tinggi diantara sesama *Streptomyces*, sehingga strain GMR22 berpotensi untuk menghasilkan kandidat senyawa metabolit sekunder baru. Tujuan penelitian ini, yaitu mendapatkan informasi senyawa metabolit sekunder yang berpotensi menjadi senyawa baru dari *Streptomyces* sp. GMR22 serta aplikasinya untuk menghambat SARS-CoV-2 sebagai virus penyebab Covid-19 maupun potensi lainnya di bidang bioteknologi. Metode yang dilakukan pada penelitian ini meliputi, analisis bioinformatik dengan AntiSMASH 5.0 dan BAGEL4, produksi metabolit sekunder, ekstraksi metabolit sekunder dengan pelarut metanol, etil asetat dan n-heksana, karakterisasi metabolit sekunder menggunakan LC-HRMS (*Liquid Chromatography-High Resolution Mass Spectrometry*) mode *targeted* dan *untargeted* dan GC-MS (*Gas Chromatography-Mass Spectrometry)*. Senyawa dalam mode *targeted* LC-HRMS didasarkan pada hasil prediksi AntiSMASH 5.0. Selanjutnya senyawa yang dihasilkan dari *targeted mode*, disimulasi *docking* terhadap protein target SARS-CoV-2, antara lain *Protease* (PDB ID: 6LU7), *Spike protein* (PDB ID: 6LXT), dan *receptors binding domain* (RBD)-ACE2 (PDB ID: 6VW1). Hasil penelitian ditemukan 65 kluster gen yang didominasi oleh senyawa poliketida. Beberapa senyawa yang sebelumnya sudah diprediksi oleh AntiSMASH 5.0 terdeteksi oleh LC-HRMS dengan mode *targeted*, sedangkan pada mode *untargeted*, senyawa dominan yang terdeteksi adalah *diketopiperazines*. Hasil GC-MS menunjukkan senyawa alkena dan alkana mendominasi senyawa dalam ekstrak etil asetat dan n-heksana. Berdasarkan studi komparatif pendekatan genomik dan metabolomik, senyawa baru yang berpotensi adalah *kedarcidin-like* (*cluster* 11), *natamycin-like* (*cluster* 22), dan *daptomycin–like* (*cluster* 13). Ketiganya berpotensi menghambat masuknya SARS-CoV-2 ke sel inang, sedangkan senyawa alkana dan alkena yang dihasilkan GMR22 dapat menjadi sumber alternatif bahan bakar.

Kata kunci: genomik, metabolomik, *Streptomyces* sp. GMR22, metabolit sekunder, SARS-CoV-2.

## *Abstract*

Covid-19 has been declared as a global pandemic and searching for possible compounds as drug is urgently needed. Among its genus, *Streptomyces* sp. GMR22 GMR22 was found to possess the greatest number of BGCs (Biosynthetic Gene Clusters), indicating that strain GMR22 was a promising source for producing new compounds. This study aimed to obtain information on secondary metabolites that have the potential to become new compounds from *Streptomyces* sp. GMR22 and its application as inhibitor of SARS-CoV-2 that is the causal agent of Covid-19 as well as other possible application in biotechnology. The methods used were bioinformatics analysis using AntiSMASH 5.0 and BAGEL4, secondary metabolite production, extraction of secondary metabolites with methanol, ethyl acetate, and n-hexane, and metabolome characterization using LC-HRMS (Liquid Chromatography-High Resolution Mass Spectrometry) targeted and untargeted modes, and GC-MS (Gas Chromatography-Mass Spectrometry). The compound in targeted LC-HRMS mode is based on the prediction of AntiSMASH 5.0 prediction. Then, the compounds resulted from LC-HRMS targeted mode was subjected to docking simulation against SARS-CoV-2 protein targets, i.e., Protease (PDB ID: 6LU7), Spike protein (PDB ID: 6LXT), receptors binding domain (RBD)-ACE2 (PDB ID: 6VW1). The result showed 65 gene cluster and dominated by polyketide compounds. Some compounds which have been predicted by AntiSMASH 5.0 were detected by LC-HRMS with targeted mode, whereas in untargeted mode, the dominant compound detected was diketopiperazines. GC-MMS results showed that alkenes and alkanes dominated the compounds in ethyl acetate and n-hexane extracts. Based on the comparative study between genomic and metabolomics approaches, three potential new compounds were identified, i.e., kedarcidin-like (cluster 11), natamycin-like (cluster 22), and daptomycin-like (cluster 13). These compounds were potential as SARS-CoV-2 blocking agents, while alkanes and alkenes compounds by GMR22 could be used as an alternative fossil fuel source.

Keywords: genomics, metabolomics, *Streptomyces* sp. GMR22, secondary metabolite, SARS-CoV-2.