Studi teofilin dan dexamethason sebagai agen pendeteksi virus SARS-CoV 2 = Study of theophylline and dexamethasone as detecting agents of the SARS-CoV 2 virus

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Abstrak

Penyakit coronavirus 2019 (COVID-19) merupakan penyakit yang disebabkan oleh severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). Penyakit ini dapat menular melalui cairan yang berasal dari hidung atau mulut penderita. Simulasi penambatan molekul dengan PyRx memprediksi senyawa Teofilin dan Dexamethason dapat berinteraksi baik dengan spike glikoprotein S2 SARS-CoV 2, dengan Gbinding yang diperoleh adalah berturut-turut sebesar -6,3; -7,8; -8,1 kcal/mol melalui nteraksi pada residu Ala348, Arg357 dan Val341. Sehingga dapat disimpulkan bahwa Teofilin dan Dexamethason memiliki potensi untuk dijadikan agen pengenal SARS-CoV 2. Namun simulasi dengan penambatan molekul juga menunjukan bahwa hemagglutinin (HA) H1N1 berpotensi menganggu pengukuran spike glikoprotein SARS-CoV 2. Hasil studi komputasi ini menjadi acuan untuk pengujian potensi Teofilin dan Dexamethason sebagai agen pengenal SARS-CoV 2 dengan HA H1N1 sebagai uji interferensi. Selanjutnya Studi elektrokimia dengan teknik voltametri siklik menggunakan elektroda boron-doped diamond (BDD) pada Teofilin menunjukkan puncak arus oksidasi pada potensial +0,506 V dan puncak arus reduksi pada potensial -0,5 V. Arus yang dihasilkan linear pada rentang konsentrasi 10 M sampai 100 M. Deteksi spike glikoprotein S2 SARS-CoV 2 dilakukan dengan melihat penurunan arus oksidasi Teofilin dengan kehadiran spike glikoprotein S2 SARS-CoV 2 dan virus kultur SARS- CoV 2 pada waktu optimum 10 menit. Penurunan arus linier pada rentang konsentrasi 1 ng/mL sampai 200 ng/mL. Sedangkan Dexamethason tidak elektroaktif namun pengukuran dengan spektrofotometri UV-Vis menunjukkan puncak absorbansi pada bilangan gelombang 241 nm. .....Coronavirus disease 2019 (COVID-19) is a disease caused by severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). This disease can be transmitted through droplets from the nose or mouth of the patient. Molecular docking simulation with PyRx predicts Theophylline and Dexamethason compounds can interact well with the spike glycoprotein S2 SARS-CoV 2, with G_{bindings} obtained are -6.3, respectively; -7.8; -8.1 kcal/mol via interaction with residues Ala348, Arg357 and Val341. So that theophylline and dexamethason have the potential to be used as SARS-CoV 2 identification agents. However, simulations with molecular docking also show that hemagglutinin (HA) H1N1 has the potential to interfere with the measurement of the SARS-CoV 2 spike glycoprotein with bioactive compounds. The results of this computational study serve as a reference for testing potential Theophylline and Dexamethasone as identification agents for SARS-CoV 2 and HA H1N1 as an interference compound. Furthermore, electrochemical studies using cyclic voltammetry techniques using boron-doped diamond (BDD) electrodes on theophylline showed peak oxidation currents at +0.548 V potential and peak reduction currents at -0.5 V potentials. The resulting currents were linear in the concentration range of 10 M to 100 M. Detection of spike glycoprotein S2 SARS-CoV 2 was carried out by observing a decrease in the oxidation current of Theophylline in the presence of spike glycoprotein S2 SARS-CoV 2 and cultured virus SARS-CoV 2 at the optimum time of 10 minutes. Linearity current decrease in the concentration range of 1 ng/mL to 200 ng/mL. Meanwhile, Dexamethasone is not electroactive, but measurements using UV-Vis

spectrophotometry show the absorbance peak at a wave number of 241 nm. This absorbance is linear in the concentration range of 10 M to 200 M. Detection of spike glycoprotein S2 SARS-CoV 2 with Dexamethasone was carried out by decreasing absorbance in the presence of spike glycoprotein S2 SARS-CoV 2. at the optimum time of 10 minutes. Linearity current decrease in the concentration range of 1 ng/mL to 200 ng/mL. Furthermore, the interference test performed with HA-H1N1 and spike glycoprotein S2 SARS-CoV 2 showed that neither the current in theophylline nor the peak absorption of Dexamethasone changed significantly. These results indicate Theophylline and Dexamethasone are selective against the SARS-CoV 2 spike glycoprotein S2 and can be applied as identification agents on the SARS-CoV 2 spike glycoprotein S2 sensor.