

Penapisan virtual senyawa peptida siklis komersial terhadap protein papain like protease (PL PRO) sebagai kandidat obat terbaru MERS-CoV = Virtual screening commercial cyclic peptide against MERS-CoV papain like protease (PL PRO) as novel drug candidate of MERS-CoV

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Abstrak

Middle east respiratory syndrome coronavirus (MERS-CoV) telah menjadi wabah saat ini, infeksi MERS-CoV menyebabkan gangguan pada sistem pernapasan, pencernaan, bahkan menyebabkan kematian dengan rata-rata kematian yang disebabkan infeksi MERS-CoV mencapai 50%. Sampai saat ini belum ditemukannya vaksin atau obat yang efektif untuk mengurangi infeksi MERS-CoV. papain-like protease (PLpro) bertanggung jawab untuk melepaskan protein nonstruktural yang berperan penting dalam proses pematangan virus. Dengan menginhibisi papain-like protease (PLpro) dengan suatu ligan, akan menghambat proses pelepasan protein nonstruktural, sehingga mengurangi infeksi yang diakibatkan oleh virus MERS-CoV.

Melalui studi bioinformatika dengan metode molecular docking dan melalui analisis drug scan, didapatkan inhibitor berbasis senyawa peptida siklis komersial yang dapat berikatan dengan PLpro dan mengurangi proses infeksi yaitu Aldosterone Secretion Inhibiting Factor (1-35) (bovine). Melalui analisis molecular dynamics, inhibitor ini stabil dalam tubuh baik dalam keadaan normal (310 K) dan keadaan demam (312 K), sehingga senyawa Aldosterone Secretion Inhibiting Factor (1-35) (bovine) berpotensi untuk dikembangkan menjadi obat terbaru MERS-CoV.

Middle east respiratory syndrome (MERS-CoV) has become the current outbreak, MERS-CoV infection results in illness in respiratory system, digestive, and even led to death with an average mortality caused by MERS-CoV infection reaches 50%. Until now no effective vaccine or drug to ward off MERS-CoV infection. Papain-like protease (PLpro), is responsible for cleavage of nonstructural protein that is important for viral maturation. Inhibition the papain-like protease (PLpro) with a ligand will block the cleavage process of nonstructural protein, thus reduce the infection of MERS-CoV.

Through of bioinformatics study with molecular docking, molecular dynamics and drug scan analysis, Aldosterone Secretion Inhibiting Factor (1-35) (bovine) was obtained as a inhibitor of commercial cyclic peptide, it can inhibit the papain-like protease (PLpro) and reduce infection process. With molecular dynamics analysis, this inhibitor was stable at normal body temperature (310 K) and fever temperature (312 K), with the result that Aldosterone Secretion Inhibiting Factor (1-35) (bovine) has a potential as novel candidate drug.