

Ultrasound-Assisted Enzymatic Aqueous Two-Phase Extraction Sebagai Metode Pemurnian Senyawa Flavonoid Daun Keji Beling dan Seleksi Awal Kandidat Obat Antikanker Serviks = Ultrasound-Assisted Enzymatic Aqueous Two-Phase Extraction as a Purification Method for Keji Beling Leaves of Flavonoid Compounds and Initial Selection for Cervical Anticancer Drug Candidates

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Abstrak

VHR (Vaccinia H1-related phosphatase) adalah protein yang terlibat dalam kanker serviks. Dengan obat-obatan saat ini yang mahal dan menimbulkan efek samping, sehingga diperlukan pengobatan alternatif. Daun keji beling mengandung senyawa flavonoid yang merupakan senyawa fenolik alami yang berpotensi sebagai antikanker. Untuk mendapatkan senyawa aktif, metode ekstraksi yang digunakan adalah Aqueous two-phase system (ATPS) dan Ultrasound-assisted enzymatic extraction (UAEE), dimana keduanya merupakan kombinasi metode ekstraksi hijau dan pemurnian. Kondisi operasi optimal metode ATPS yang digunakan dalam penelitian ini adalah rasio etanol 33wt% dan ammonium sulfat 14wt% yang menghasilkan nilai recovery 98,043%, nilai K 31,179, yield kuersetin 3,504mg/g, dan konsentrasi kuersetin 44,717 mg/L. Ekstrak daun keji beling diuji dengan metode shinoda, spektrofotometri UV-Vis juga Gas Chromatography and Mass Spectrometry (GC-MS), kemudian senyawa yang teridentifikasi memiliki aktivitas antikanker yaitu kuersetin, n-hexadenoic acid dan 9-dodecenoic acid, methyl ester, (E)-. Hasil uji docking molekuler memberikan docking score terbaik untuk kuersetin yaitu -6,7, diikuti oleh asam n-heksadekanoat bernilai -5,1 dan terakhir adalah asam 9-dodekanoat, metil ester, (E) - bernilai -4,2 terhadap protein 1J4X. Kuersetin merupakan senyawa dengan potensi inhibisi terbaik terhadap VHR yang ditunjukkan dengan nilai docking score terendah.

.....VHR (Vaccinia H1-related phosphatase) is a protein involved in cervical cancer. With current drugs which are expensive and cause side effects, an alternative treatment is needed. Keji beling leaves contain flavonoid compounds which are natural phenolic compounds that have the potential as anticancer. To obtain active compounds, the extraction methods used are Aqueous two-phase system (ATPS) and Ultrasound-assisted enzymatic extraction (UAEE), both of which are a combination of green extraction and purification methods. Optimal operating conditions for the ATPS method used in this study were 33wt% ethanol ratio and 14wt% ammonium sulfate which resulted in 98,043% recovery value, K value 31,179, quercetin yield 3.504 mg/g, and quercetin concentration 44.717 mg/L. Keji beling leaf extract was tested by the shinoda method, UV-Vis spectrophotometry as well as Gas Chromatography and Mass Spectrometry (GC-MS), then the compounds identified as having anticancer activity were quercetin, n-hexadenoic acid and 9-dodecenoic acid, methyl ester, (E-). Molecular docking test results give the best docking score for quercetin which is -6.7, followed by n-hexadecanoic acid -5.1 and finally is 9-dodecenoic acid, methyl ester, (E) - value -4.2 to 1J4X protein. Quercetin is a compound with the best inhibition potential against VHR which is shown by the lowest docking score.