SINTESIS TURUNAN N-BENZOTHIAZOLE PIRAZOLINA DARI 2-ASETIL-5-KLOROTIOFENA DAN UJI AKTIVITASNYA
SEBAGAI SENYAWA ANTIKANKER DAN KEMOFLUOROSENSOR
Bhagavad Gita, Prof. Dra. Tutik Dwi Wahyuningsih, M.Si., Ph.D. ; Dr. Deni Pranowo, S.Si., M.Si.
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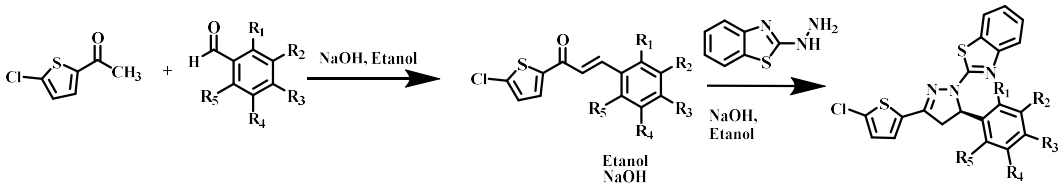
23/525042/PPA/06587

INTISARI

Sintesis turunan pirazolina berbasis N-benzotiazol dari 2-asetil-5-klorotiofena berhasil dilakukan melalui dua tahap reaksi. Tahap pertama yaitu kondensasi *Claisen–Schmidt* dengan berbagai turunan benzaldehida menggunakan NaOH 40% untuk menghasilkan kalkon **K1–K8**, selanjutnya reaksi siklisasi kalkon dengan 2-hidrazinolbenzotiazol dan NaOH 40% menghasilkan pirazolina **P1–P8**. Semua kalkon **K1-K8** dan pirazolina **P1-P8** dikarakterisasi menggunakan FTIR, GC-MS, ^{1}H- dan ^{13}C-NMR. Aktivitas antikanker semua kalkon dan pirazolina dievaluasi secara *in vitro* menggunakan metode MTT terhadap sel HeLa, T47D, MCF7, WiDr dan Vero, sedangkan kemampuan kemofluorosensor pirazolina **P1-P8** dilakukan melalui proses skrining kation, penentuan LoD, LoQ, *binding constant* dan uji interferensi.

Kalkon **K1-K8** diperoleh sebagai padatan dengan persen hasil berkisar 47–97%, sedangkan pirazolina **P1-P8** dihasilkan dengan persen hasil berkisar 47–95%. Uji antikanker menunjukkan bahwa semua kalkon berikut memiliki indeks selektivitas yang tinggi yaitu kalkon **K1** aktif terhadap sel T47D (IC_{50} = 1,43 µg/mL) dan sel WiDr (IC_{50} = 1,60 µg/mL), **K2** aktif terhadap sel MCF-7 (IC_{50} = 2,26 µg/mL), **K7** aktif terhadap sel T47D (IC_{50} 4,96 µg/mL) dan **K8** aktif terhadap sel MCF7 (IC_{50} 1,08 µg/mL), sedangkan pirazolina **P1-P8** bersifat tidak aktif sebagai antikanker. Uji kemosensor fluoresensi menunjukkan bahwa pirazolina **P3** memiliki respon *turn-off* yang sangat selektif terhadap ion Hg^{2+} dengan nilai LoD 1,91 µM dan LoQ 6,35 µM serta interferensi minimal.

Kata kunci: benzotiazol, kalkon, kemofluorosensor, pirazolina,



	1	2	3	4	5	6	7	8
R1	OCH_3	H	OCH_3	OCH_3	OCH_3	H	H	H
R2	H	OCH_3	H	H	OCH_3	OCH_3	H	Cl
R3	H	H	OCH_3	H	OCH_3	OCH_3	$N(CH_3)_2$	H
R4	H	H	H	OCH_3	H	OCH_3	H	H
R5	H	H	H	H	H	H	H	H

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SYNTHESIS OF N-BENZOTHIAZOLE PYRAZOLINE DERIVATIVES FROM 2-ACETYL-5-CHLOROTHIOPHENE AND THEIR ACTIVITY ASSAY AS ANTICANCER AND CHEMOFLUOROSENSOR COMPOUNDS

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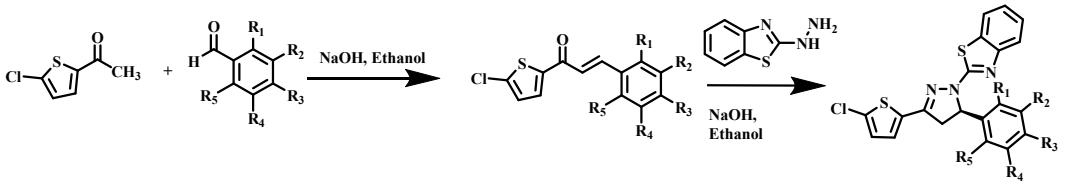
ABSTRACT

The synthesis of *N*-benzothiazole-based pyrazoline derivatives from 2-acetyl-5-chlorothiophene was successfully carried out through two reaction steps. The first step was the Claisen–Schmidt condensation with various benzaldehyde derivatives using 40% NaOH to yield chalcones **K1–K8**, followed by cyclization reaction of chalcones with 2-hydrazinobenzothiazole and 40% NaOH to produce pyrazolines **P1–P8**. All chalcones and pyrazolines were characterized using FTIR, GC-MS, ^{1}H- and ^{13}C-NMR. The anticancer activity of all chalcones and pyrazolines was evaluated *in vitro* using the MTT method against HeLa, T47D, MCF7, WiDr, and Vero cells, while the chemofluorescent ability of pyrazolines **P1-P8** was carried out through a cation screening process, determination of LoD, LoQ, binding constant, and interference test.

Chalcones **K1-K8** were obtained as solids with yields ranging from 47–97%, while pyrazolines **P1-P8** were produced with yields ranging from 47–95%. Anticancer tests showed that all of the following chalcones had high selectivity indices, namely chalcone **K1** was active against T47D cells (IC_{50} = 1.43 µg/mL) and WiDr cells (IC_{50} = 1.60 µg/mL), **K2** was active against MCF-7 cells (IC_{50} = 2.26 µg/mL), K7 was active against T47D cells (IC_{50} 4.96 µg/mL) and **K8** was active against MCF7 cells (IC_{50} 1.08 µg/mL), while pyrazolines **P1-P8** were inactive as anticancer agents. Fluorescence chemosensor testing showed that pyrazoline **P3** has a highly selective turn-off response to Hg^{2+} ions with a LoD of 1,91 µM and a LoQ of 6,35 µM, along with minimal interference.

Keywords: benzothiazole, chalcones, chemofluorosensor, pyrazoline



	1	2	3	4	5	6	7	8
R1	OCH_3	H	OCH_3	OCH_3	OCH_3	H	H	H
R2	H	OCH_3	H	H	OCH_3	OCH_3	H	Cl
R3	H	H	OCH_3	H	OCH_3	OCH_3	$N(CH_3)_2$	H
R4	H	H	H	OCH_3	H	OCH_3	H	H
R5	H	H	H	H	H	H	H	H