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Judul Jurnal Ilmiah (Artikel) : Correlation Between Number of Leucocyte and CRP Levels with Infarct Volume of Acute Ischaemic Stroke

Jumlah Penulis : 3 orang

Status Pengusul : Dwi Pudjonarko (penulis pertama)

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3D QSAR Studies of 2-Arylpyrimidines and S-Triazines as Selective PDE4B Inhibitors

ANAND GAURAV, DHARMENDRA KUMAR

ABSTRACT

Background: Phosphodiesterase 4B (PDE4B) has emerged as important target for design of anti-inflammatory drugs for respiratory tract. Several selective PDE4B inhibitors are under various stages of development, among them 2-arylpyrimidines and s-triazines have been identified as inhibitors with high degree of selectivity for PDE4B. However, the structural features responsible for the PDE4B selectivity of these molecules have not been identified and explored so far.

Method: 3D QSAR studies were performed for the series of 2-arylpyrimidines and s-triazines using Accelrys Discovery Studio 3.5. The IC_{50} values were transformed to PDE4B selectivity by taking the ratio of IC_{50} values i.e. $PDE4D(IC_{50})/PDE4B(IC_{50})$ for all the molecules in the series, and used as the dependent variable. The dataset was divided into training and test set of 45 and 10 compounds respectively and 3D QSAR was performed using the default parameters. Test set prediction and Fischer statistic was used for validation of the developed model.

Results: Statistically robust and predictive 3D QSAR models with high r^2_{cv} value of 0.9794 were obtained. The contour maps revealed the sterically and electronically favourable and unfavourable regions around the 2-arylpyrimidines and s-triazines scaffolds.

Conclusion: 3D QSAR model for 2-arylpyrimidines and s-triazines as selective PDE4B inhibitors were developed and validated. The models were highly predictive and provided vital structural information for the design of newer and more selective PDE4B inhibitors having the 2-arylpyrimidine and s-triazines scaffold. The results of the present study will be followed up by the design, synthesis and experimental evaluation of newer selective PDE4B inhibitors.

Keywords: Cyclic Nucleotide Phosphodiesterases, Type 4B; 3D Quantitative Structure-Activity Relationship; Fischer statistic; 2-arylpyrimidines; s-triazines

INTRODUCTION

Prevalence of Inflammatory diseases of respiratory tract i.e., asthma and COPD has increased in recent years, with more than 200 million people affected by it worldwide. Most of the mortality related to these inflammatory disorders occurs in low- and low middle income countries¹.

Phosphodiesterase 4 (PDE4) is a major family of enzymes that selectively hydrolyze 3',5'-cyclic adenosine monophosphate (cAMP) and are involved in regulating the release of anti-inflammatory and pro-inflammatory cytokines within cells^{2,3,4}. Even though PDE4s are widely expressed in immune and inflammatory cells, levels of different PDE4 subtypes (PDE4A, PDE4B, PDE4C and PDE4D) vary in a specific cell. PDE4B is abundant in monocytes and neutrophils, while PDE4A is expressed to very low levels and PDE4C is absent in inflammatory cells^{5,6,7,8,9}. This makes PDE4B an interesting and

promising targets for anti-inflammatory drugs meant to be used in respiratory inflammatory diseases such as asthma and chronic obstructive pulmonary disease (COPD). Inhibition of PDE4 has been shown to suppress a diverse spectrum of inflammatory responses *in vitro* and *in vivo*.¹⁰⁻¹³ More importantly, many PDE4 inhibitors in development are efficacious in animal models of various inflammatory disorders, such as asthma, COPD, psoriasis, inflammatory bowel diseases, and rheumatoid arthritis^{11,14,15}, as well as in clinical trials for asthma and COPD^{16,17,18}. However the development of PDE4 inhibitors has been slowed down due to narrow therapeutic window of most of the compounds. A major reason for their poor clinical results is the consequence of dosing limitation caused by side effects such as nausea and emesis.¹⁹ Recent findings in PDE4 knockout mice suggest that an inhibitor with PDE4B selectivity should retain many beneficial anti-inflammatory effects without the unwanted side effects^{20,21}.

The highly conserved catalytic domain of PDE4 isozymes makes the generation of inhibitors with PDE4 subtype selectivity a challenging task. However, residues in regulatory domain such as control region 3 (CR3) vary among subfamilies, which has proved to be responsible for PDE4B selectivity.²²

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Insufficient Implementation of Tuberculosis Screening and Prophylaxis in Child Contacts: a Situational Analysis

J KROTZEK-SEAH¹, AB HIMAWAN², A RONDAGS^{1,3}, JF METSEMAKERS¹, TRI NUR KRISTINA^{2*}

ABSTRACT

Background: Contact investigations and chemoprophylaxis are proven cost-effective and safe means to reduce TB-related morbidity and mortality in children living with pulmonary tuberculosis (PTB) cases.

Aim: To evaluate the implementation of tuberculosis (TB) screening and chemoprophylaxis in child contacts of smear-positive adult TB cases, and to identify practical barriers experienced by the staff of community health centers (CHCs) in a rural area in Central Java, Indonesia.

Methods: Firstly, a short questionnaire was used to collect information on whether children in the household were screened and received chemoprophylaxis through home visits or at the CHC. Secondly, semi-structured interviews and an FGD were performed with the TB officer, a nurse responsible for the TB program activities, the assistant of the TB officer, a medical doctor from the outpatient clinic, and the head of the CHC. The data was then independently analyzed using the theoretical thematic analysis, then the findings were compared and integrated into one set of themes.

Results: Out of 67 child contacts, determined through record reviews and visits of smear-positive TB patients, only 5(7.5%) were screened. None was started on chemoprophylaxis. In-depth interviews and a focus group discussion with CHCs' staff identified shortcomings in organization and management of care, lack of awareness and knowledge among staff, limited understanding of caregivers, and practical obstacles related to the rural setting.

Conclusions: A comprehensive approach is needed that matches these site-specific practical barriers and might require a redistribution of organizational power from health authorities to the CHCs.

Keywords: TB contact, children, screening, chemoprophylaxis

INTRODUCTION

It is only in recent years that more attention is drawn on the burden and impact of childhood tuberculosis (TB). Children usually get infected with the *Mycobacterium tuberculosis* by adult pulmonary TB (PTB) cases in their closest surroundings, i.e., parents or other household members. Particularly in children under 5 years of age (under-fives), bearing an underdeveloped immune system, the risk of progression to active disease after primary infection is high^{1,2}. Contact investigations and chemoprophylaxis with isoniazid preventive therapy (IPT), are proven cost-effective and safe means to reduce TB-related morbidity and mortality in children living with PTB cases³. IPT can reduce the risk of developing active disease from primary (asymptomatic) infection by 60-65% over 2 years or longer³.

In Indonesia, where TB remains a major public health challenge, 8.47% of the 328.824 newly

diagnosed patients in 2012 were under the age of 15 years, exceeding the global average of 6% of TB cases that occur in children⁴. The Indonesian national TB control program (NTP) recommends screening of all child household contacts (in particular under-fives) of smear-positive PTB cases using the Indonesian scoring system for TB diagnosis in children⁵.

Different from the WHO recommendations (Fig. 1), this scoring system requires tuberculin skin test (TST) and chest-X-ray (CXR). If TB disease is excluded (i.e. score <6), under-fives should receive a 6-month IPT (5-10 mg/kg bodyweight daily),⁵ which in line with the present WHO recommendations⁶ (Fig. 1). Current recommendations recommend 10mg/kg per day for 6 months⁷.

A systematic review showed an overall prevalence of TB infection ranging from 24.4 to 69.2% in children (<15 years) living with a smear-positive TB case in South East Asia⁸. Despite the benefits of screening and chemoprophylaxis in child contacts, numerous studies from high TB burden countries indicated that these measures are often poorly implemented⁹⁻¹¹. A cross-sectional study in 4 TB units in South India, for example, showed that only 14% of 84 child contacts under 5 years had been screened for TB disease, and only 19% had been initiated on IPT with no follow-up. Focus group

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