Synthesis of new isoquinoline-base-oxadiazole derivatives as potent inhibitors of thymidine phosphorylase and molecular docking study

By: Zaman, K (Zaman, Khalid)[1] ; Rahim, F (Rahim, Fazal)[1] ; Taha, M (Taha, Muhammad)[2] ; Wadood, A (Wadood, Abdul)[3] ; Shah, SAA (Shah, Syed Adnan Ali)[4,5] ; Ahmed, QU (Ahmed, Qamar Uddin)[6] ; Zakaria, ZA (Zakaria, Zainul Amiruddin)[7,8]

View Web of Science ResearcherID and ORCID

SCIENTIFIC REPORTS
Volume: 9
Article Number: 16015
DOI: 10.1038/s41598-019-52100-0
Published: NOV 5 2019
Document Type: Article
View Journal Impact

Abstract

Here in this study regarding the over expression of TP, which causes some physical, mental and socio problems like psoriasis, chronic inflammatory disease, tumor angiogenesis and rheumatoid arthritis etc. By this consideration, the inhibition of this enzyme is vital to secure life from serious threats. In connection with this, we have synthesized twenty derivatives of isoquinoline bearing oxadiazole (1-20), characterized through different spectroscopic techniques such as HREI-MS, H-1-NMR and C-13-NMR and evaluated for thymidine phosphorylase inhibition. All analogues showed outstanding inhibitory potential ranging in between 1.10 +/- 0.05 to 54.60 +/- 1.50 mu M. 7-Deazaxanthine (IC50 = 38.68 +/- 1.12 mu M) was used as a positive control. Through limited structure activity relationships study, it has been observed that the difference in inhibitory activities of screened analogs are mainly affected by different substitutions on phenyl ring. The effective binding interactions of the most active analogs were confirmed through docking study.

Keywords

KeyWords Plus: ALPHA-GLUCOSIDASE SYNTHESIS; IN-VITRO EVALUATION; CELL GROWTH-FACTOR; BETA-GLUCURONIDASE; BIOLOGICAL EVALUATION; ANALOGS; ACETYLCHOLINESTERASE; THIOSEMICARBAZIDES

Author Information

Reprint Address: Taha, M (reprint author)

Imam Abdulrahman Bin Faisal Univ, Inst Res & Med Consultat, Dept Clin Pharm, POB 1982, Dammam 31441, Saudi Arabia.

Reprint Address: Zakaria, ZA (reprint author)

Univ Putra Malaysia, Fac Med & Hlth Sci, Dept Biomed Sci, Serdang 43400, Selangor, Malaysia.

Reprint Address: Zakaria, ZA (reprint author)

Univ Putra Malaysia, Halal Inst Res Inst, Serdang 43400, Selangor, Malaysia.

Addresses:

[1] Hazara Univ, Dept Chem, Mansehra 21300, Khyber Pakhtunk, Pakistan

[2] Imam Abdulrahman Bin Faisal Univ, Inst Res & Med Consultat, Dept Clin Pharm, POB 1982, Dammam 31441, Saudi Arabia

[3] Abdul Wali Khan Univ Mardan, Dept Biochem, Mardan 23200, Pakistan

[4] Univ Teknol MARA, Fac Pharm, Cawangan Selangor Kampus, Selangor 42300, DE, Malaysia

[5] Univ Teknol MARA, Atta Ur Rahman Inst Nat Prod Discovery AuRIns, Cawangan Selangor Kampus PuncakAlam, Selangor 42300, DE, Malaysia

[6] Int Islamic Univ Malaysia, Kulliyyah Pharm, Dept Pharmaceut Chem, Pahang Dm 25200, Kuantan, Malaysia

[7] Univ Putra Malaysia, Fac Med & Hlth Sci, Dept Biomed Sci, Serdang 43400, Selangor, Malaysia

[8] Univ Putra Malaysia, Halal Inst Res Inst, Serdang 43400, Selangor, Malaysia

E-mail Addresses: mtaha@iau.edu.sa; zaz@upm.edu.my

Funding

Funding Agency	Grant Number
Higher Education Commission (HEC) Pakistan under the National Research Program for Universities	5721 5092

View funding text

Publisher

NATURE PUBLISHING GROUP, MACMILLAN BUILDING, 4 CRINAN ST, LONDON N1 9XW, ENGLAND

Journal Information

Impact Factor: Journal Citation Reports

Categories / Classification

Research Areas: Science & Technology - Other Topics

Web of Science Categories: Multidisciplinary Sciences

See more data fields

Cited References: 48

Showing 30 of 48 **View All in Cited References page** *(from Web of Science Core Collection)*

1. **Synthesis of Thymidine Phosphorylase Inhibitor Based on Quinoxaline Derivatives and Their Molecular Docking Study** — Times Cited: 2
By: Almandil, Noor Barak; Taha, Muhammad; Farooq, Rai Khalid; et al.
MOLECULES Volume: 24 Issue: 6 Article Number: 1002 Published: MAR 2 2019

2. **Toward the Development of a Potent and Selective Organoruthenium Mammalian Sterile 20 Kinase Inhibitor** — Times Cited: 55
By: Anand, Ruchi; Maksimoska, Jasna; Pagano, Nicholas; et al.
JOURNAL OF MEDICINAL CHEMISTRY Volume: 52 Issue: 6 Pages: 1602-1611 Published: MAR 26 2009

3. **Evolving strategies for enzyme engineering** — Times Cited: 233
By: Bloom, JD; Meyer, MM; Meinhold, P; et al.
CURRENT OPINION IN STRUCTURAL BIOLOGY Volume: 15 Issue: 4 Pages: 447-452 Published: AUG 2005

4. **5 '-O-tritylinosine and analogues as allosteric inhibitors of human thymidine phosphorylase** — Times Cited: 28
By: Casanova, Elena; Hernandez, Ana-Isabel; Priego, Eva-Maria; et al.
JOURNAL OF MEDICINAL CHEMISTRY Volume: 49 Issue: 18 Pages: 5562-5570 Published: SEP 7 2006

5. **Overexpression of the angiogenic factor platelet-derived endothelial cell growth factor thymidine phosphorylase in psoriatic epidermis** — Times Cited: 50
By: Creamer, D; Jaggar, R; Allen, M; et al.
BRITISH JOURNAL OF DERMATOLOGY Volume: 137 Issue: 6 Pages: 851-855 Published: DEC 1997

6. **Thymidine Phosphorylase: A Two-Face Janus in Anticancer Chemotherapy** — Times Cited: 55
By: Focher, F.; Spadari, S.
CURRENT CANCER DRUG TARGETS Volume: 1 Issue: 2 Pages: 141-153 Published: 2001

7. **THE ENZYMATIC SYNTHESIS OF NUCLEOSIDES .1. THYMIDINE PHOSPHORYLASE IN MAMMALIAN TISSUE** — Times Cited: 304
By: FRIEDKIN, M; ROBERTS, D
JOURNAL OF BIOLOGICAL CHEMISTRY Volume: 207 Issue: 1 Pages: 245-256 Published: 1954

8. **Thymidine phosphorylase from Escherichia coli: Tight-binding inhibitors as enzyme active-site titrants** — Times Cited: 14
By: Gbaj, A; Edwards, PN; Reigan, P; et al.
JOURNAL OF ENZYME INHIBITION AND MEDICINAL CHEMISTRY Volume: 21 Issue: 1 Pages: 69-73 Published: FEB 2006

9. **Synthesis of Bis-indolylmethane sulfonohydrazides derivatives as potent alpha-Glucosidase inhibitors** — Times Cited: 14
By: Gollapalli, Mohammed; Taha, Muhammad; Ullah, Hayat; et al.
BIOORGANIC CHEMISTRY Volume: 80 Pages: 112-120 Published: OCT 2018

10. **Antifolate Inhibitors of Thymidylate Synthase as Anticancer Drugs** — Times Cited: 29
By: Jarmula, A.
MINI-REVIEWS IN MEDICINAL CHEMISTRY Volume: 10 Issue: 13 Pages: 1211-1222 Published: NOV 2010

11. **Novel purine nucleoside analogues for hematological malignancies** — Times Cited: 24
By: Korycka, Anna; Lech-Maranda, Ewa; Robak, Tadeusz
RECENT PATENTS ON ANTI-CANCER DRUG DISCOVERY Volume: 3 Issue: 2 Pages: 123-136 Published: JUN 2008

12. **Bush by SRM Enzymatic assay of thymidine phosphorylase (EC 2.4. 2.4)** — Times Cited: 1
Patent Number: 212.1
Inventor/Assignee: Krenitsky, T. A.
US. Pat Published: 1979

13. **SPECIFICITY OF MOUSE URIDINE PHOSPHORYLASE - CHROMATOGRAPHY PURIFICATION + PROPERTIES** — Times Cited: 108
By: KRENITSKY, TA; JACQUEZ, JA; BARCLAY, M
JOURNAL OF BIOLOGICAL CHEMISTRY Volume: 239 Issue: 3 Pages: 805-+ Published: 1964

14. **Prediction of protein-ligand interactions. Docking and scoring: Successes and gaps** — Times Cited: 464
By: Leach, Andrew R.; Shoichet, Brian K.; Peishoff, Catherine E.
JOURNAL OF MEDICINAL CHEMISTRY Volume: 49 Issue: 20 Pages: 5851-5855 Published: OCT 5 2006

15. **Global, local and novel consensus quantitative structure-activity relationship studies of 4-(Phenylaminomethylene) isoquinoline-1, 3 (2H, 4H)-diones as potent inhibitors of the cyclin-dependent kinase 4** Times Cited: 24
By: Lei, Beilei; Xi, Lili; Li, Jiazhong; et al.
ANALYTICA CHIMICA ACTA Volume: 644 Issue: 1-2 Pages: 17-24 Published: JUN 30 2009

16. **Thymidine phosphorylase is noncompetitively inhibited by 5 '-O-trityl-inosine (KIN59) and related compounds** Times Cited: 9
By: Liekens, S.; Balzarini, J.; Hernandez, A. I.; et al.
NUCLEOSIDES NUCLEOTIDES & NUCLEIC ACIDS Volume: 25 Issue: 9-11 Pages: 975-980 Published: 2006

17. **Derivatives of 7-amino-1,2,3,4-tetrahydroisoquinoline and isophthalic acids as novel fibrinogen receptor antagonists** Times Cited: 15
By: Malovichko, Olga L.; Petrus, Anna S.; Krysko, Andrei A.; et al.
BIOORGANIC & MEDICINAL CHEMISTRY LETTERS Volume: 16 Issue: 20 Pages: 5294-5297 Published: OCT 15 2006

18. **The effect of a thymidine phosphorylase inhibitor on angiogenesis and apoptosis in tumors** Times Cited: 178
By: Matsushita, S; Nitanda, T; Furukawa, T; et al.
CANCER RESEARCH Volume: 59 Issue: 8 Pages: 1911-1916 Published: APR 15 1999

19. **Novel functional antitumor nucleoside TAS-102, combined form of F3dThd adn its modulator: 2. Inhibitory effect of TPI on tumor-derived angiogenesis and metastasis** Times Cited: 12
By: Miyadera, K.; Emura, T.; Suzuki, N.; et al.
Proceedings of the American Association for Cancer Research Annual Meeting Volume: 39 Pages: 609 Published: March, 1998

20. **THYMIDINE PHOSPHORYLASE IS ANGIOGENIC AND PROMOTES TUMOR-GROWTH** Times Cited: 384
By: MOGHADDAM, A; ZHANG, HT; FAN, TPD; et al.
PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA Volume: 92 Issue: 4 Pages: 998-1002 Published: FEB 14 1995

21. **Investigation of the lactam side chain length necessary for optimal indenoisoquinoline topoisomerase i inhibition and cytotoxicity in human cancer cell cultures** Times Cited: 51
By: Morrell, Andrew; Placzek, Michael S.; Steffen, Jamin D.; et al.
JOURNAL OF MEDICINAL CHEMISTRY Volume: 50 Issue: 9 Pages: 2040-2048 Published: MAY 3 2007

22. **Discovery of 5-substituted-6-chlorouracils as efficient inhibitors of human thymidine phosphorylase** Times Cited: 36
By: Nencka, Radim; Votruba, Ivan; Hrebabecky, Hubert; et al.
JOURNAL OF MEDICINAL CHEMISTRY Volume: 50 Issue: 24 Pages: 6016-6023 Published: NOV 29 2007

23. **Synthesis of alpha amylase inhibitors based on privileged indole scaffold** Times Cited: 22
By: Noreen, Tayyaba; Taha, Muhammad; Imran, Syahrul; et al.
BIOORGANIC CHEMISTRY Volume: 72 Pages: 248-255 Published: JUN 2017

24. **Thymidine phosphorylase inhibitors: Recent developments and potential therapeutic applications** Times Cited: 43
By: Perez-Perez, MJ; Priego, EM; Hernandez, AI; et al.
MINI-REVIEWS IN MEDICINAL CHEMISTRY Volume: 5 Issue: 12 Pages: 1113-1123 Published: DEC 2005

25. **Identification of Novel and Potent Isoquinoline** Times Cited: 1
By: Ping, C.
Bioorg. Med. Chem. Lett. Volume: 13 Pages: 1345-1348 Published: 2003

26. **Syntheses of pyrimidine acyclic nucleoside phosphonates as potent inhibitors of thymidine phosphorylase (PD-ECGF) from SD-lymphoma** Times Cited: 14
By: Pomeisl, Karel; Votruba, Ivan; Holy, Antonin; et al.
NUCLEOSIDES NUCLEOTIDES & NUCLEIC ACIDS Volume: 26 Issue: 8-9 Pages: 1025-1028 Published: 2007

27. **Effects of higenamine and its 1-naphthyl analogs, YS-49 and YS-51, on platelet TXA(2) synthesis and aggregation** Times Cited: 25
By: Pyo, Mi Kyung; Kim, Jeong Mi; Jin, Jing-Ling; et al.
THROMBOSIS RESEARCH Volume: 120 Issue: 1 Pages: 81-86 Published: 2007

28. **Synthesis and in vitro acetylcholinesterase and butyrylcholinesterase inhibitory potential of hydrazide based Schiff bases** Times Cited: 19
By: Rahim, Fazal; Ullah, Hayat; Taha, Muhammad; et al.
BIOORGANIC CHEMISTRY Volume: 68 Pages: 30-40 Published: OCT 2016

29. **Synthesis, in vitro evaluation and molecular docking studies of thiazole derivatives as new inhibitors of alpha-glucosidase** Times Cited: 51
By: Rahim, Fazal; Ullah, Hayat; Javid, Muhammad Tariq; et al.
BIOORGANIC CHEMISTRY Volume: 62 Pages: 15-21 Published: OCT 2015

30. **Synthesis, molecular docking, acetylcholinesterase and butyrylcholinesterase inhibitory potential of thiazole analogs as new inhibitors for Alzheimer disease** Times Cited: 33
By: Rahim, Fazal; Javed, Muhammad Tariq; Ullah, Hayat; et al.
BIOORGANIC CHEMISTRY Volume: 62 Pages: 106-116 Published: OCT 2015

Showing 30 of 48 **View All in Cited References page**