

# Synthesis of novel ricinoleic acid-based 1,2,3-triazoles and their anticancer activity

Y Mohini<sup>a#</sup>, K R Kunduru<sup>a</sup>, Madiga HariKrishna<sup>a</sup>, M S L Karuna<sup>\*a</sup>, Y Poornachandra<sup>b</sup>, C Chandrasekhar<sup>c</sup> & Podha Sudhakar<sup>d</sup>

<sup>a</sup> Centre for Lipid Science and Technology, <sup>b</sup> Medicinal Chemistry and Pharmacology Division,

<sup>c</sup> Organic Synthesis and Process Chemistry Division, CSIR-Indian Institute of Chemical Technology, Uppal Road, Hyderabad 500 007, India

<sup>d</sup> Department of Biotechnology, Acharya Nagarjuna University, Guntur 522 510, India

E-mail: karuna@iict.res.in, karuna@csiriict.in

Received 15 October 2024; accepted (revised) 27 December 2024

A series of novel chiral 1,4-disubstituted-1*H*-1,2,3-triazole derivatives **8a-i** has been accomplished using (*Z*)-methyl-12-azidooctadec-9-enoate, which is a derivative of castor oil fatty acid ester, methyl ricinoleate. The 1,2,3-triazole analogues have been synthesized regioselectively by the Cu-catalysed azide-alkyne cycloaddition (CUAAC) *via* Huisgen "Click Chemistry". The target 1,2,3-triazole derivatives' structure has been characterized by FT-IR, <sup>1</sup>H and <sup>13</sup>C NMR, and mass spectroscopy. The dipole moment of the triazole derivatives are in the range of 4.8 –5.6 Debye units, indicating their stability towards different environments. The synthesized compounds **8 a-i** have been evaluated for their anticancer activity against four different cancer cell lines such as human lung cancer cell line (A549), human cervical cancer cell line (HeLa), human prostate cancer cell line (DU145), and human breast cancer cell line (MDA-MB-231) and doxorubicin is used as a standard reference drug. All the compounds exhibit moderate anticancer activity against the four cancer cell lines except compound **8g** bearing phenylalanine. Among these compounds, **8c**, *i.e.*, valine substituted-1,2,3-triazole displays superior anticancer activity against A549 (IC<sub>50</sub> 12.3 ± 0.24 μM); DU145 (IC<sub>50</sub> 15.6±0.24 μM); MDA-MB-231 (IC<sub>50</sub> 17.8±0.20 μM) cancer cell line compared to the other tested compounds. Further, the triazole derivatives are found to be quite safe towards the normal cell, as they do not exhibit any activity towards HLF-Human lung fibroblast.

**Keywords:** Castor oil, L-Amino acid, Click reaction, CUAAC, 1,2,3-Triazole, Anticancer activity