# Synthesis of novel *bis*-allyloxy and hydroxypropoxy derivatives of 4, 5-diaryl thiophene-2-carboxylic acid and their biological evaluation

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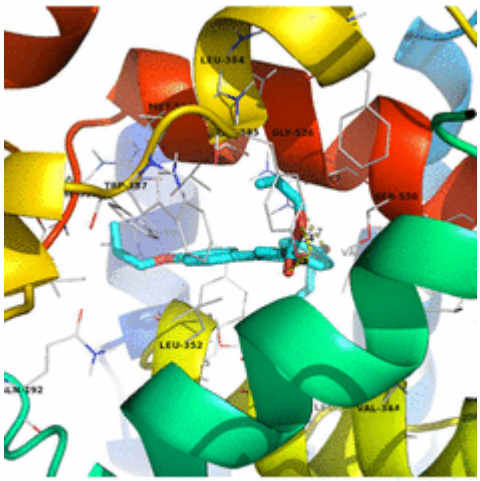
## Abstract

In our earlier studies, we have shown that the introduction of amino moieties at carboxylic acid of 4,5-diarylthiophene-2-carboxylic acid significantly improved the anti-inflammatory activity of the compound against the standard drug diclofenac sodium. In the present study, we have synthesized new derivatives of 4,5-diarylthiophene-2-carboxylic acid by modifying the hydroxyl group of the phenyl ring and carboxylic acid group of the thiophene ring. A series of novel 4,5-diarylthiophene-2-carboxylic acid derivatives containing *bis*-allyloxy and hydroxypropoxy with methyl or ethyl ester moieties were synthesized, characterized and subsequently evaluated for anti-inflammatory and antioxidant property. Among the novel compounds, the inhibition of bovine serum albumin denaturation assay revealed that the compound 4,5-*bis*(4-(3-hydroxypropoxy)phenyl)thiophene-2-carboxylic acid (**15**) and ethyl ester (**13**) having anti-inflammatory activity better than the standard drug diclofenac

sodium. The antioxidant screening showing 4,5-*bis*(4-(allyloxy)phenyl)thiophene-2-carboxylic acid (**10**), 4,5-*bis*(4-(3-hydroxypropoxy)phenyl)thiophene-2-carboxylic acid methyl ester (**11**) and 4,5-*bis*(4-(3-hydroxypropoxy)phenyl)thiophene-2-carboxylic acid ethyl ester (**13**) exhibited a slightly moderate antioxidant activity than standard ascorbic acid. Molecular docking analysis was performed for the synthesized compounds with the cyclooxygenase-2 (COX-2) receptor (PDB 1D: 1PXX). Docking studies revealed that all the synthesised compounds exhibit greater binding affinity than the standard drug. Particularly, the compound ethyl 4,5-*bis*(4-(allyloxy)phenyl)thiophene-2-carboxylate (**8**) and allyl 4,5-*bis*(4-(allyloxy)phenyl)thiophene-2-carboxylate (**9**) having high free energy binding of −10.40 and −10.48 Kcal/mol, respectively.

## Graphical Abstract.

Synopsis: A new series of *bis*-allyloxy and hydroxypropoxy substituted 4,5-diarylthiophene-2-carboxylic acid derivatives were synthesized, characterized, evaluated their *in vitro* anti-inflammatory and anti-oxidant activity, and performed molecular docking study.




Docking of 9 with COX-2

# Keywords

*Bis*-allyloxy derivatives hydroxypropoxy derivatives 4,5-diarylthiophene-2-carboxylic acid anti-inflammatory antioxidant molecular docking

# Electronic supplementary material

The online version of this article (doi: 10.1007/s12039-017-1274-6 (https://doi.org/10.1007/s12039-017-1274-6)) contains supplementary material, which is available to authorized users.

# Notes

# Supplementary information (SI)

The characterization of the compounds **2**–**16** using $^{1}$H NMR, $^{13}$C NMR, IR and Mass spectral data (Figures S1–S60) are given in the Supplementary Information, which is available at www.ias.ac.in/chemsci (http://www.ias.ac.in/chemsci).

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# Supplementary material

12039_2017_1274_MOESM1_ESM.docx (17.9 mb)
Supplementary material 1 (docx 18315 KB)

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