especially the properties regarding its carbohydrate recognition domain structure. As a consequence, it is absolutely essential to understand the structure of TM, in order to get into more functional details of its regulation in the aforementioned properties. Thrombomodulin (TM) forms a 1:1 complex with thrombin. Whereas thrombin alone cleaves fibrinogen to make the fibrin clot, the thrombin-TM complex cleaves protein C to initiate the anticoagulant pathway. Until present, the so-far available structures, either through NMR or through X-ray analyses, can not shed lights into the decent structural-functional interpretations for TM regulations. Crystallographic investigations of the complex between thrombin and TM-EGF456 did not show any changes in the thrombin active site. Therefore, research has focused recently on how TM may provide a docking site for the protein C substrate with different Ca^{2+} concentration. Previous work, however, showed that when the thrombin active site was occupied by substrate analogues labeled with fluorophores, the fluorophores responded differently to active (TMEGF1-6) versus inactive (TMEGF56) fragments of TM.

Keywords: Thrombomodulin, Structural analysis, Calcium-induced dimerization.

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Crystal structure of 6- Methoxy- 4-bromomethylcoumarin. Ramakrishna Gowda[a], K.V Arjuna Gowda[b], Mahantesha Basanagouda[c], Manohar V. Kulkarni[c]. [a]*Department of Physics, Govt. College for Women, Kolar - 563 101, Karnataka, India.* [b]*Department of Physics, Govt. First Grade College, K.R. Pura, Bangalore-560 036, Karnataka, India.* [c]*Department of Chemistry, Karnatak University, Dharwad-580 003, Karnataka, India.* E-mail: arjunagowda@indiainfo.com

Coumarins are a class of naturally occurring oxygen heterocycles which have been found to exhibit wide ranging biological activities [1-3] through its innumerable derivatives. Structural studies on coumarins have been focused on their solid state photochemical dimerization [4], hydrogen bonding [5], mode of packing [6], molecular self assembling [7] and photophysical properties [8]. Introduction of bromine has resulted in formation of hydrates, intermolecular hydrogen bonding, eclipsed conformation observed in 3-bromocoumarin [9], 6-bromo-3-acetylcoumarin [10] and 3-bromoacetylcoumarin [11] respectively. 3-Bromophenyl-6-acetoxymethyl-coumarin-3-carboxylates have been found to exhibit potential anticancer and antitumour activity [12].

Crystals suitable for diffraction studies were grown by slow evaporation technique using acetic acid as a solvent. The crystals of the compound crystallize in Monoclinic with space group $P2_1/n$ having 8 molecules in the unit cell of dimensions crystal system: a = 4.3573(3), b = 9.2859(6), c = 25.2677(17) Å and β = 91.927(3) ^{0}. The three dimensional intensity data was collected using a crystal of size 0.25 × 0.15 × 0.10 mm mounted on Bruker axs kappa apex2 ccd diffractiometer with Mok_α radiation. The data was collected using ω and φ scan mode. 9957 measured reflections of which 2130 independent reflections and 1502 reflections with $I > 2\sigma(I)$. With absorption correction: multi-scan.

The structure was solved using wingx software package and the model was refined by the full-matrix least-square method. The refinement was continued till the final R = 0.0449, R_w = 0.1103.

The title compound is cyclic and planar but non-aromatic in nature due to the continuous delocalization of electrons around the coumarin ring. Skeleton is not possible. There is a significance deviation in bond angle at 01-C1-C2 (117.2(3) ° due to the electronic repulsion of oxygen (02) atom which is present at C1 carbon atom.

[1]. Kulkarni MV, Kulkarni GM, Lin CH, Sun CM (2006) Curr Med Chem,13:2795.[2] Fylaktakidou KC, Hadjpavlou D, Litinas KE, Nicolaides DN (2004) Curr,Pharm Design 10:3813.[3]. Neyts J, Clercq ED, Singha R, Chang YH, Das AR, Chakraborty SK, Hong,SC, Tsay SC, Hsu MH, Hwu JR (2009) J Med Chem 52:1486. [4]. Gnanaguru K, Ramasubbu N, Venkatesan K, Ramamurthy V (1985) J Org,Chem 50:2337. [5]. Munshi P, Row T. N. G (2005) J Phys Chem A 109:659. [6]. Gavuzzo E, Mazza F (1974) Acta Cryst B30:1351,[7]. Murthy JN, Venkatakrishnan P, Singh AS (2003) CrystEngComm 5:507.[8]. Katerinopoulos HE (2004) Curr Pharm Des 10:3835.[9]. Gaultier J, Hauw C (1965) Acta Cryst C19:927, [10]. Kokila MK, Puttaraja, Kulkarni MV, Shivaprakash NC (1996) Acta Cryst, C52: 2078. [11]. Puttaraja, Vasudevan KT, Kulkarni MV (1991) Acta Cryst C47:774,[12]. Kempen I, Papapostolou D, Thierry N, Pochet L, Counerotte S, Masereel B, Foidart J-M, Reboud-Ravaux M, Noel A, Pirotte B (2003) Br J Can 88:1111.

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