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Actual Problems of the Chemistry of Natural Compounds

ABSTRACTS

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SYNTHESIS, CRYSTAL STRUCTURE AND HIRSHFELD SURFACE ANALYSIS OF NEW DERIVATIVE OF THIENO[2,3-D]PYRIMIDINE

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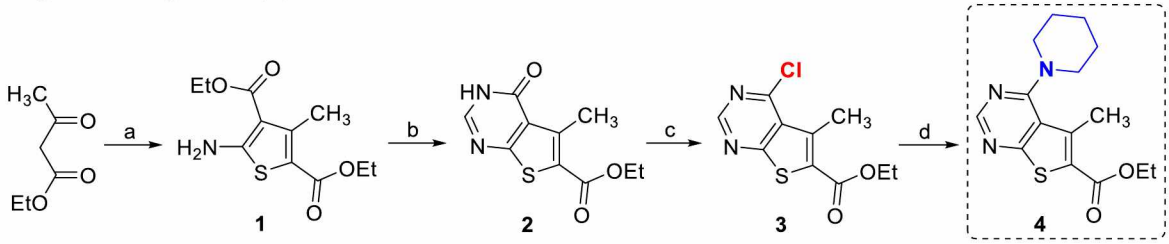
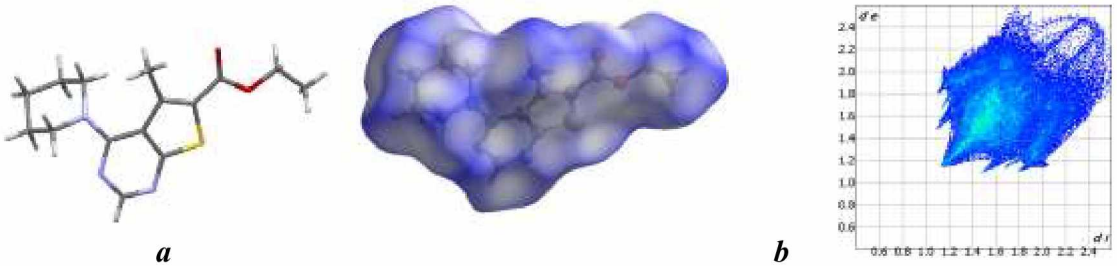
Many thieno[2,3-d]pyrimidine (TP) derivatives were reported as phosphodiesterase inhibitors, also exhibited good H_1 receptor antagonistic activities, 4-amino derivatives showed insecticidal and acaricidal activities. Numerous TPs have been proved to use in case of cerebral ischemia, malaria, tuberculosis, Alzheimer's and Parkinson's diseases.

In this context, TP containing piperidine fragment with similar structural qualities would be projected to result in newer molecular systems with increased efficacy. Definitely, piperidine template has been known to express considerable antimicrobial, antitubercular and anticancer activities. A systematic approach to the synthesis of targeted compound **(4)** was described follow:



Reagents and reaction conditions: **n**= 1,2,3 **(a)** ethyl cyanoacetate, S_8, morpholine, absolute ethanol, 40-45°C, 24 h. **(b)** formamide, 150°C, 8 h, **(c)** $POCl_3$, triethylamine (TEA), 110°C, 6 h, **(d)** piperidine, TEA, absolute ethanol, 78°C, 6 h.



a ***b***

Using modern X-ray structural analysis and the Hirshfeld surface analysis method, it is possible to identify an important hydrogen bond in molecular crystals. X-ray structural analysis of piperidin-1-yl derivative of thieno[2,3-d]pyrimidine (**4**) shows that compound was found to crystallize in the monoclinic system (P21, Z= 4). The piperidine ring adopts a chair conformation (a). Hirshfeld surface analysis of the intermolecular contacts reveal that the most important contributions for the crystal packing are from H···H (52.9%), H···C/C···H (11.2%), O···H/H···O (9.6%), H···S/S···H (9.7%) and H···N/N···H (12.5%) (b). Also, Structure of synthesized compound was confirmed by IR, ^1H and ^{13}C NMR spectroscopy.