

5,5'-Disubstituted-3,3'-Methanediyl-bis-Indoles as Potential Antitumorals

Irena Wolska^a, Dorota Maciejewska^b, ^a*Department of Crystallography, Faculty of Chemistry, Adam Mickiewicz University, Grunwaldzka 6, 60-780 Poznań, Poland.* ^b*Department of Organic Chemistry, Faculty of Pharmacy, Medical University of Warsaw, Banacha 1, 02 097 Warsaw, Poland.* E-mail: iwolska@amu.edu.pl

Certain compounds found in the diet are a potential source of new classes of chemotherapeutic and chemopreventive agents. Indole-3-carbinol, a major indole metabolite from cruciferous vegetables, and its natural condensation product 3,3'-diindolylmethane, have been found to inhibit the development of tumors in breast, uterus and liver [1-3]. However, both compounds may exhibit adverse tumor promoting activity in other organs. In search for new *anti* cancer agents we have decided to investigate 3,3'-diindolylmethane derivatives which may reduce the growth of human tumor cell lines by the inhibition of the binding of some transcription factors to the adequate sequences in DNA.

To determine structural parameters important for the biochemical activity we have performed the ¹H and ¹³C NMR data and single crystal X-ray analysis of 5,5'-disubstituted-3,3'-methanediyl-bis-indoles. The results of these studies indicate insignificantly different molecular structures of the investigated compounds but significantly different networks of intermolecular interactions in crystals. Interesting NH... π hydrogen bonds are observed which may have a functional role in biological features.

[1] Grubbs C.J., et al., *Anticancer Res.*, 1995, **15**, 709. [2] Cover C.M., et al., *J. Biol. Chem.*, 1998, **273**, 3838. [3] Hong C., et al., *Bioch. Pharmacol.*, 2002, **63**, 1085.

Keywords: anticancer compounds, 5,5'-disubstituted-3,3'-methanediyl-bis-indoles, x-ray single-crystal diffraction