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5,6-Epoxycholestanes have stimulated the interest of researchers some years after the photo-oxidation products of cholesterol were suspected to be involved in photo-carcinogenesis [1]. Because of the presence of an oxirane group, it was supposed that 5,6-epoxycholestane could be electrophilic and behave like alkylating agents with direct carcinogenic properties. Recent data from literature ruled out that 5,6-epoxycholestanes could be direct alkylating substances [2] and provides evidence that 5,6-epoxycholestanes may be involved in physiological processes that result in metabolites with tumor promoter properties as well as to the production of steroidal alkaloids which are anti-oncogenic. Ring B oxysterols were reported to stimulate cholesterol ester formation in cultured fibroblasts [3] and 5 α ,6 α -epoxy cholestane was shown to be the most potent allosteric activator for ACAT-1 (acyl-coA: cholesterol acyl transferase) where 5 β ,6 β -epoxycholestane was found to be inefficient [4]. A series of epoxycholestane derivatives have been included to predict their pharmacological effects, specific mechanisms of action, known toxicities, drug-likeness, etc, by using the statistics of multilevel neighborhoods of atoms (MNA) descriptors for active and inactive fragments. The biological activity spectra for substances have been correlated on SAR base (structure-activity relationships data and knowledge base), which provides the different Pa (possibility of activity) and Pi (possibility of inactivity). Most of the probable activities have been characterized by Pa and Pi values, which depict that all the molecules have high value of teratogen activity. Some selected bond distances and bond angles have been taken into account and deviation of bond distances/bond angles. X-H...A intra and intermolecular hydrogen bonds in the molecules have been described with the standard distance and angle cut-off criteria.

[1] Roffo, A.H. (1933). American Journal of Cancer 17, 42-57.

[2] Paillasse, M.R et. al. (2012). Journal of Lipid Research 53, 718-725.

[3] Brown, M.S. et. al. (1975). Journal of Biological Chemistry 250, 4025-4027.

[4] Zhang, Y. et.al. (2003). Journal of Biological Chemistry 278, 11642-11647.

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