

Review of: "Synthesis of 1, 2-Disubstituted Benzimidazoles at Ambient Temperature Catalyzed by 1-Methylimidazolium Tetraflouroborate ([Hmim] BF_4) and Investigating Their Anti-ovarian Cancer Properties Through Molecular Docking Studies and Calculations"

Robert Ancuceanu¹

1 Carol Davila University of Medicine and Pharmacy

Potential competing interests: No potential competing interests to declare.

"All the synthesized compounds bind to an agonist at the active site of the 6LAD protein, ...". Generally speaking, agonists or antagonists bind to different receptors or ion channels (with different affinities), but we are not aware of ligands binding to agonists. If they do (which seems rather unlikely), it is more probable that the result would be inactivation of the agonist.

"Among the heterocyclic compounds, the heterocyclic compounds containing nitrogen and sulphur are of special importance..." The repeated use of "heterocyclic compounds" in this sentence could and should be avoided for fluency and clarity.

"Ovarian cancer occurs when normal cells in the fallopian tubes turn into abnormal cells grow out of control and enter the ovaries." The origin of ovarian cancer seems actually controversial: "On the one hand, evidence suggests that this cancer arises from the ovarian surface epithelium (OSE), which is related to the mesothelium of the peritoneum [15]. It is loosely attached to the underlying ovarian stroma and separated by the tunica albuginea. The OSE harbours stem cells, which may contribute to tumor formation (Fig. 1). On the other hand, it has been suggested that HGSOC originates from the fallopian tubes, which consist of differentiated columnar epithelium composed of ciliary and secretory cells" (Klotz, D.M., Wimberger, P. Cells of origin of ovarian cancer: ovarian surface epithelium or fallopian tube?. *Arch Gynecol Obstet* 296, 1055–1062 (2017). https://doi.org/10.1007/s00404-017-4529-z).

"The effective factors of ovarian cancer include obesity, family history, endometriosis, ageing and menopause before 40 years of age." It is not clear to me what "effective factors" means in this context.

- "The mode of interaction was investigated by docking" is too vague to be of any utility. What protein was used as the target, and how was the binding pocket selected? What software was used for docking, and what were the main parameters used? What protein pre-treatment was performed? How were the docking results analyzed?
- "According to Lee Pinsky's laws, the molecular mass of the drug should not be more than 500 g/mol, because the higher the molecular mass, the lower its absorption and permeability. All synthesized compounds follow this. According to Lee



Pinsky's laws, the molecular mass of the drug should not be more than 500 g/mol, because the higher the molecular mass, the lower its absorption and permeability. Fortunately, all the synthesized compounds have a molecular mass of less than 500 g/mol." In essence, in this text the same info is repeated twice.

We are not aware of an "octanol-water dissociation coefficient," but rather of an octanol-water partition coefficient.

Figures 2 and 4 (for different reasons) seem pretty vague to be really informative.

"This procedure suffers from many advantages such as reduced reaction times, easy purification, high yields,..." This phrasing seems rather strange, as "suffers" is commonly associated with disadvantages, not with "advantages."