

Atomistic molecular dynamics simulations of cyanobiphenyl compounds

Egor Gerts, Andrei V. Komolkin

Faculty of Physics, St. Petersburg State University, 198504, Ulyanovskaya 3,

St. Petersburg, Russia

E-mail: gerts-e-d@yandex.ru

Liquid crystalline materials are very interesting objects for the researchers. They are used not only in technological devices. Some biological systems also possess sort of liquid crystallinity. Cell membranes form lamellar bi-layer mesophase, and this is the case for cancer cells as well. One of the difficulties in the development of effective anticancer drugs is the transportation of the drug inside the cell. And liquid crystals can be rather useful in solving this problem. Some recent papers [1-3] showed that certain cyanobiphenyl compounds can inhibit cell growth and even recognize normal and cancer cells. Although the anticancer activity was observed, its mechanism still stays unclear.

This work focuses on two cyanobiphenyl compounds: thermotropic nematic liquid crystal 4-cyano-4'-(6-hydroxyhexyloxy)biphenyl (HO-6OCB) and 4-methyloxy-4'-(6-hydroxyhexyloxy)biphenyl (HO-6OMeOB), that does not form mesophase. Local and conformational structures of these substances and their equimolar mixture are studied via fully atomistic molecular dynamics simulations. This information will help to investigate the mechanisms of intermolecular interactions, thus giving insights into the development of novel anticancer drugs.

Acknowledgements. It is a pleasure to thank Saint-Petersburg State University for the research grant 11.37.159.2014. Research was carried out using computational resources provided by Resource Center "Computer Center of SPbU" (<http://cc.spbu.ru>).

References.

- [1] Yoshizawa, Atsushi, et al. "Biological activity of some cyanobiphenyl derivatives." *Chemistry Letters* 38, 6 (2009): 530-531.
- [2] Takahashi, Yuuka, et al. "Supramolecular assembly composed of different mesogenic compounds possessing a ω -hydroxyalkyl unit exhibits suppressive effects on the A549 human lung cancer cell line." *MedChemComm* 2, 1 (2011): 55-59.
- [3] Ishikawa, Junya, et al. "Suppressive effects of liquid crystal compounds on the growth of U937 human leukemic monocyte lymphoma cells." *Cancer Cell Int* 12, 3 (2012).