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Nematic liquid crystals doped with resorcinol: supramolecular arrangement and potential biomedical application

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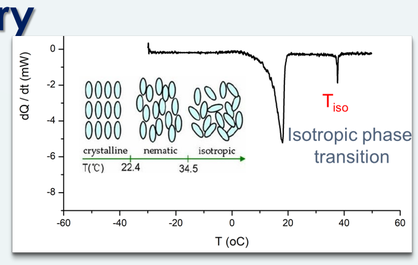
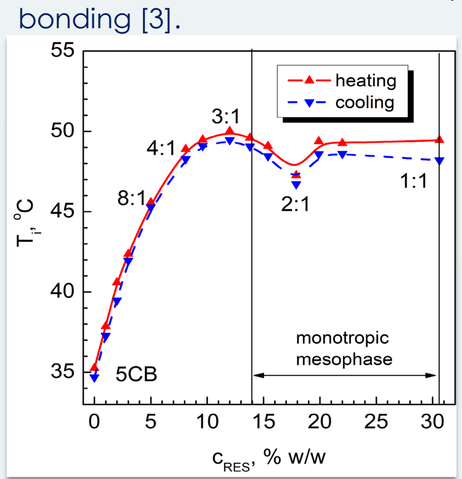
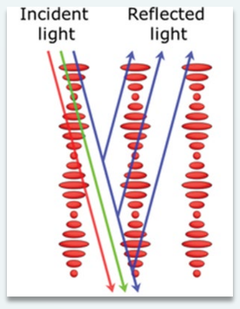
• **Topicality** • Drug delivery systems based on nanostructurized materials, such as liquid crystals (LC), possess a number of unique features and seem prospective for transdermal application [1,2]. In particular, they emerge as multifunctional anisotropic scaffolds capable of reacting to temperature, light, electric or magnetic fields [2]. These systems are mostly configured as a kind of ordered solvent for an active component (drug molecule), where no specific intermolecular interactions are anticipated. However, accounting for possibilities of such interactions paves the way for developing a novel type of LC-based drug delivery systems, where an active component itself is a structure-governing factor.

• Differential scanning calorimetry (DSC)

Anomalous increase in the nematic-to-isotropic phase transition (up to ~15 °C for **5CB:RES 3:1**), which directly pointed to specific intermolecular interactions in the system with. This finding has been strictly supported by FTIR data, which revealed 5CB-RES hydrogen bonding [3].



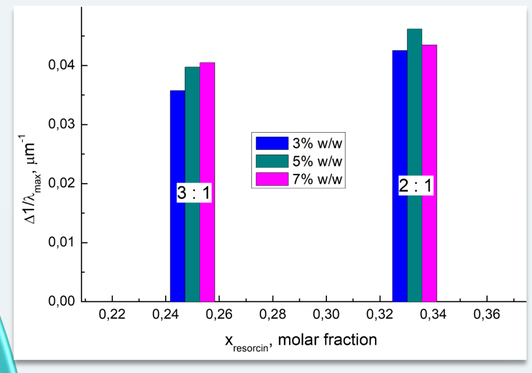




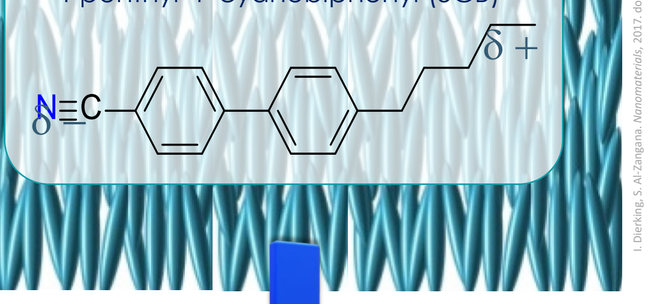
• Selective reflection spectra (SR)

M5 cholesteric matrix (cholesteric ethers composition) was used as a quasi-inert solvent to study 5CB-RES interactions

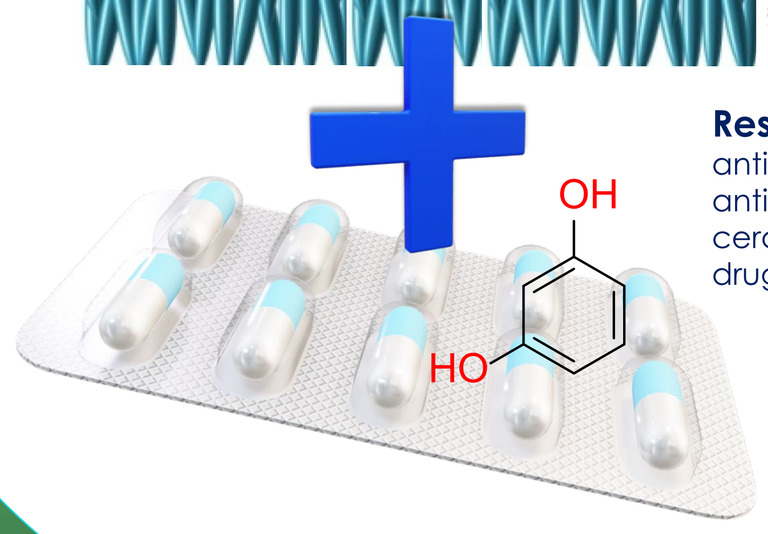
The deviation of $1/\lambda_{max}$ parameters from additivity bears witness to stoichiometric **5CB-RES 2:1** complex formation in the cholesteric matrix



Nematic LC matrix
4-penthyl-4'-cyanobiphenyl (5CB)



I. Dierking, S. Al-Zangana. *Nanomaterials*, 2017. doi:10.3390/nano7100305

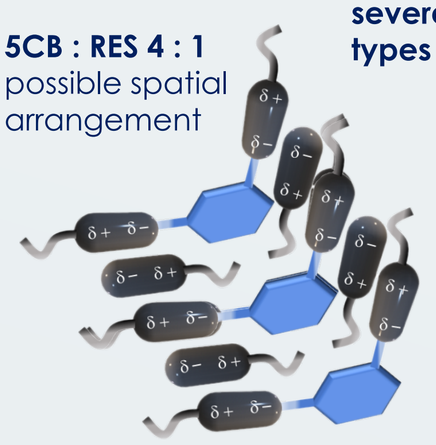


Resorcinol (RES)
antimicrobial, antifungal, ceratoplastic drug

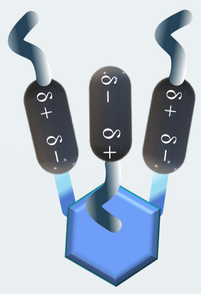
5CB : RES 2 : 1
stoichiometric complex stabilized by H-bonds

Coexistence of several complex types is supposed

5CB : RES 4 : 1
possible spatial arrangement



5CB : RES 3 : 1
alleged complex corresponding to maximal stability of the nematic phase



• Possible molecular arrangement

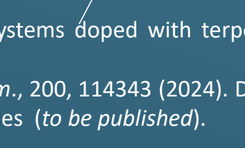
MTT-based cytotoxicity assay

Max tested concentration: 100 μM

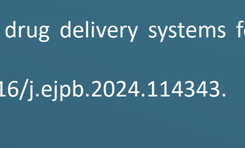
NHDF (fibroblasts):
- Resorcinol: no toxicity (cytotoxicity > 100 μM)
- 5CB: IC_{50} ≈ 20 μM

HaCaT (keratinocytes):
- Resorcinol: no toxicity (cytotoxicity > 100 μM)
- 5CB: IC_{50} ≈ 30 μM

Normal Human Dermal Fibroblasts (NHDF)



Human epidermal keratinocytes (HaCaT)



• Biological activity

• Conclusions •

- Model LC systems have been proposed to study intermolecular 'drug - carrier' interactions for testing of the developed pharmaceutical compositions for transdermal applications.
- It has been shown that emerging H-bonds can provide complex formation and efficient supramolecular structuring providing the relevant properties of the system.
- On the system studied, preliminary data on biological activity are presented.

1. M. Nesterkina, B. Veldung, O. Vashchenko, P. Vashcnenko, L. Lisetski, I. Kravchenko, A. K. H. Hirsch, C.-M. Lehr. Thermoresponsive cholesteric liquid crystal systems doped with terpenoids as drug delivery systems for skin applications. Eur. J. Pharm. Biopharm., 191, 139-149 (2023). DOI: 10.1016/j.ejpb.2023.09.002.
2. M. Nesterkina, I. Kravchenko, A.K.H. Hirsch, C.-M. Lehr. Thermotropic liquid crystals in drug delivery: A versatile carrier for controlled release. *Eur. J. Pharm. Biopharm.*, 200, 114343 (2024). DOI: 10.1016/j.ejpb.2024.114343.
3. P.V. Vashchenko, D.S. Sofronov, L.N. Lisetski. Energy gap as a physico-chemical characteristic of liquid crystal mixtures with specific interaction of component molecules (*to be published*).