

# Host-guest interactions of non-steroidal anti-inflammatory drugs on the functionalized dendronized polymeric nanocomposite, Poly(N-tris[[(cyano-ethoxy)methyl] methylacrylamide).

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The use of dendronized polymers (DP), such as

Poly(N-tris[[(cyano-ethoxy)methyl]methylacrylamide) (PATCN), as carriers models of different non-steroidal anti-inflammatory drugs (NSAIDs), such as ibuprofen (IBU), Ketoprofen (KTP), and Naproxen (NPX), is reported. DSC and TGA measurements demonstrate strong interactions between dendronized polymeric nanocomposites and these drugs. FT-IR, UV-Vis, and AFM measurements confirm that the interactions in the blend give rise to a compatible new material in only one phase. Using the Fukui Theory (FT), the interaction appears to take place through the main amide and its neighborhood. Thus, the drugs' and polymer's functional groups contribute to the strength of the interaction. The functional groups and the sizes of the drugs are the driving force for the interaction with the DP. Finally, MD calculations are carried out through DFT methods to investigate the behavior of the dendronized polymer, showing that different chain behaviors depend on the placement of the lateral chains. © 2018 Taylor & Francis Group, LLC.

Cavities

Fukui

Ibuprofen (IBU)

Ketoprofen (KTP)

Naproxen (NPX)

Poly(N-tris[[(cyano-ethoxy)methyl]methylacrylamide) (PATCN)

Polymer blends

Chains

Nanocomposites

Polymer blends

Cavities

Fukui

Ibuprofen (IBU)

Ketoprofen

Naproxens

Poly(N-tris[[(cyano-ethoxy)methyl]methylacrylamide) (PATCN)

Drug interactions