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Title:	Methyl group: A potential building block for edge-to-face interlocking of benzimidazole scaffolds in developing blue light emitting molecular aggregates
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Abstract:	Biologically active benzimidazoles are well-known for their therapeutic applications; however, the molecular systems enable their impact in various optical applications. We report a catalyst-free synthesis of methyl-substituted benzimidazole compounds. The benzimidazole derivatives, 2-(p-tolyl)-1H-benzo[d]imidazole (4-Me) and 2-mesityl-1H-benzo[d]imidazole (246-Trime) were synthesized in an oxygenated-aqueous medium through the reaction of ortho-phenylenediamine and methyl-substituted benzaldehydes at 75 °C. The photophysical properties of the benzimidazole scaffolds were investigated in the aqueous medium. 4-Me and 246-Trime derivatives in their aggregated form in solid state displayed a red shift of absorbance and fluorescence intensity relative to their molecular form in the aqueous medium. Spectroscopic, structural and morphological characteristics of the benzimidazole compounds reveal that effective supramolecular interactions are operative to decelerate the intramolecular movements of 4-Me and 246-Trime leading to J-type molecular aggregates. The supramolecular interactions and energy framework analysis of the compounds suggest that strong and short C–H···π interactions with very strong and short intermolecular N···H hydrogen bonding play important role for the development of molecular aggregates and attribute the contribution of dispersive energy to a large extent for the stabilization of 4-Me and 246-Trime molecular aggregates. The para positional effect of the methyl group in the benzimidazole derivatives marks a notable impact on the additional stability of the blue light-emitting molecular aggregates of nano-dimension.
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