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Entitled

DEVELOPMENT OF SUPRAMOLECULAR MULTICOMPONENT CHROMOPHORES TOWARDS PHOTOLUMINESCENCE SWITCHES

by

Rukayat Shola Bojesomo

Faculty Advisor

Dr. Na'il Saleh Ibrahim, Department of Chemistry

College of Science

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Abstract

A new fluorescent dye (4PBZC) comprises of coumarin, piperazine and benzimidazole (BZ) was designed, prepared and complexed to cucurbit[7]uril (CB7) to detect carnosol (CAR) anticancer drug in sub-nanomolar concentrations utilizing the supramolecular indicator displacement assay (IDA) strategy, the CB7-assisted pK_a shift and the CB7-retarded photoinduced electron transfer (PET) process. The host–guest complexation was confirmed by UV–visible absorption, fluorescence, and proton NMR spectroscopy, which confirm binding to 4PBZC via the BZ and coumarin moieties. Also, CB7 preferentially binds the indicator dye via the protonated BZ group compared to the neutral BZ group, demonstrated by a higher binding constant of the complex in its protonated form, which led to an increase in the pK_a of the BZ moiety by ca. 3.0 units after the addition of CB7. In the aqueous solution under pH of 6, switching the emission signals between 4PBZH$^+$C/CB7 (ON state) and 4PBZC (OFF state) was achieved by displacement of the protonated dye from the cavity of CB7 by the CAR analyte. An efficient sensor was fabricated for the highly sensitive detection of CAR in aqueous solution at pH 6 with a low-detection limit (LOD) of 0.39 ng/mL (1.2 nM).

Keywords: Cucurbituril, coumarin, piperazine, benzimidazole, photoinduced electron transfer, indicator displacement assay, pK_a shifts.