SUPPORTING INFORMATION

Binding of a Neutral Guest to Cucurbiturils: Photophysics, Thermodynamics and Molecular Modelling

María José González-Álvarez^a, Thais Carmona^a, Didem Evren^b and Francisco Mendicuti^{a}*

^a Departamento de Química Física, Universidad de Alcalá, E-28871 Alcalá de Henares, Madrid, Spain.

^b Istanbul Technical University, Faculty of Science and Letters, Department of Chemistry, 34469 Maslak, Istanbul, Turkey.

INDEX

Figure S1. Stern-Volmer plots of the intensity (measured as area under emission spectra) against [KBr] for 2MN in the absence and in the presence of CB6, CB7 and CB8 at 25°C. Concentrations were: for 2MN free and 2MN/CB7 water solutions, the [2MN] was 3×10^{-5} M and [CB7] was 2.11×10^{-3} M; for 2MN/CB6 and 2MN/CB8 water solutions, [2MN] was 3×10^{-6} M and the [CB6] and [CB8] were at saturation.	3
Figure S2. Histories of interaction energies for 2MN/CB6 (upper), 2MN/CB7 (middle) and 2MN/CB8 (bottom) structures obtained from the analysis 1.0 ns MD trajectories in the presence of water: E_{binding} (black), E_{binding} electrostatics (red) and E_{binding} van der Waals (blue).....	4
Figure S3. Histories of the distances between the center of mass of CB6 macroring and 2MN naphthalene and ester groups, as well as, for the interaction energy and contributions for the CB-ester group of the 2MN/CB6(3) structure obtained from the analysis 1.0 ns MD trajectories in the presence of water: E_{binding} (black) and electrostatics (red) and van der Waals (blue) contributions.....	5
Figure S4. Coordinate system used to define the 2MN/CB complexation processes.....	6

Figure S1. Stern-Volmer plots of the intensity (measured as area under emission spectra) against [KBr] for 2MN in the absence and in the presence of CB6, CB7 and CB8 at 25°C. Concentrations were: For 2MN free and 2MN/CB7 water solutions, the [2MN] was 3×10^{-5} M and [CB7] was 2.11×10^{-3} M; for 2MN/CB6 and 2MN/CB8 water solutions, [2MN] was 3×10^{-6} M and the [CB6] and [CB8] were at saturation.

Figure S2. Histories of interaction energies for 2MN/CB6 (upper), 2MN/CB7 (middle) and 2MN/CB8 (bottom) structures obtained from the analysis 1.0 ns MD trajectories in the presence of water: E_{binding} (black), E_{binding} electrostatics (red) and E_{binding} van der Waals (blue).

Figure S3. Histories of the distances between the center of mass of CB6 macroring and 2MN naphthalene (black) and ester (red) groups, as well as, for the interaction energy and contributions for the CB-ester group of the 2MN/CB6(3) structure obtained from the analysis 1.0 ns MD trajectories in the presence of water: E_{binding} (black) and electrostatics (red) and van der Waals (blue) contributions.

Figure S4. Coordinate system used to define the 2MN/CB complexation processes.