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Article

Calix[4]arene Derivative for Iodine Capture and Effect on Leaching of Iodine through Packaging

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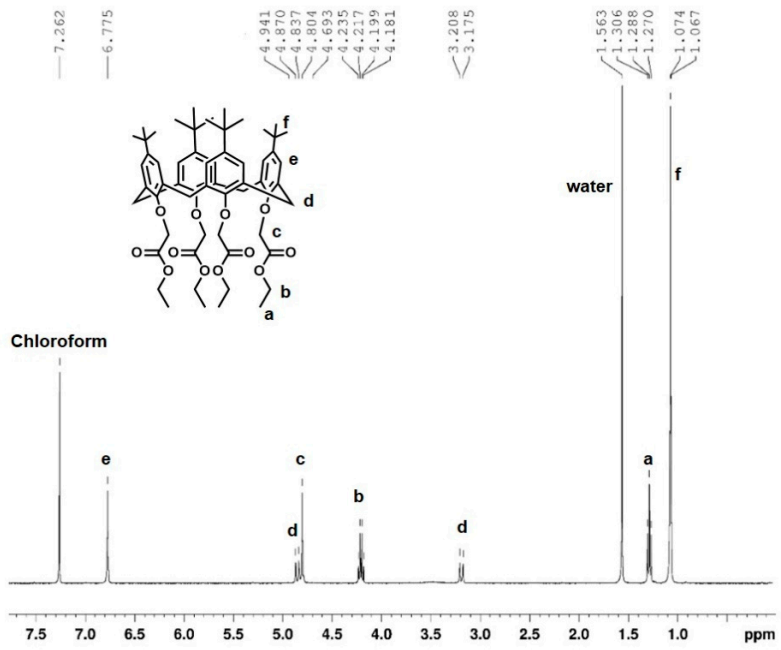

Figure S1. ^{1}H NMR spectrum of the tetra(ethoxycarbonyl-methoxy)-4-tert-butylcalix[4]arene (CX) (400 MHz, $CDCl_3$, 297 K).

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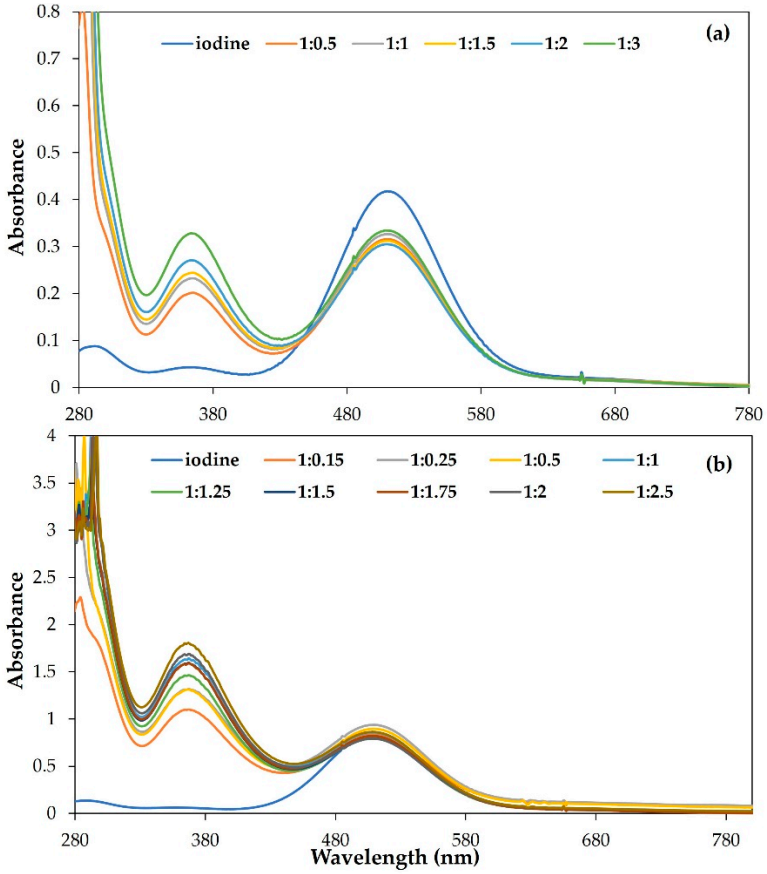

Figure S2. UV-vis spectra of iodine $CHCl_3$ solution (1.3 x 10^{-3} M) in the presence of increasing amounts of CX (from 0 to 3.9 x 10^{-3} M).

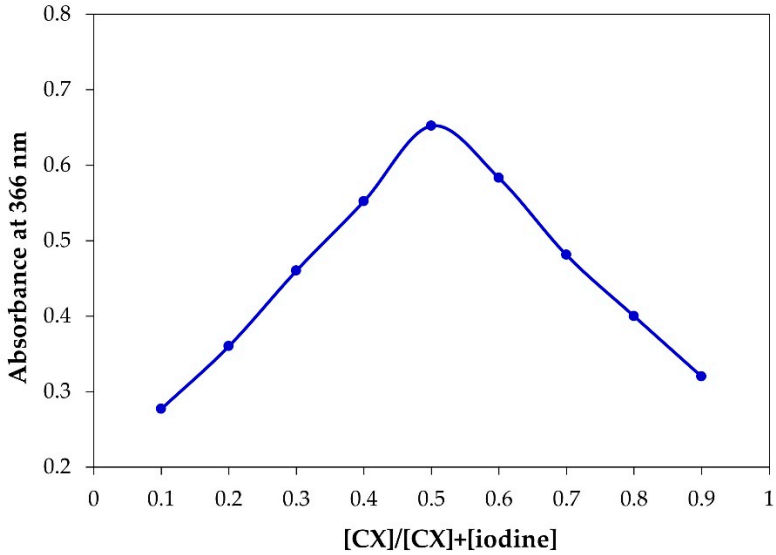

Figure S3. Job's plot for the determination of the stoichiometry of the CX/iodine complex.

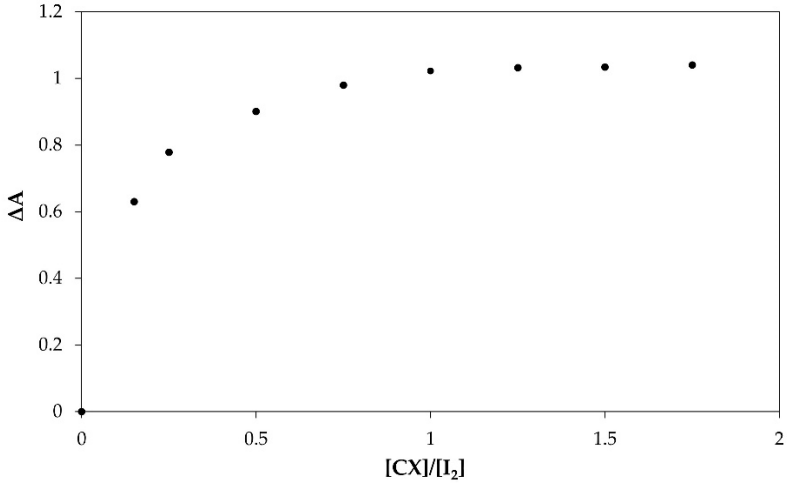

Figure S4. Plot of absorbance change versus mole ratio [CX]/[Iodine] at λ = 366 nm.

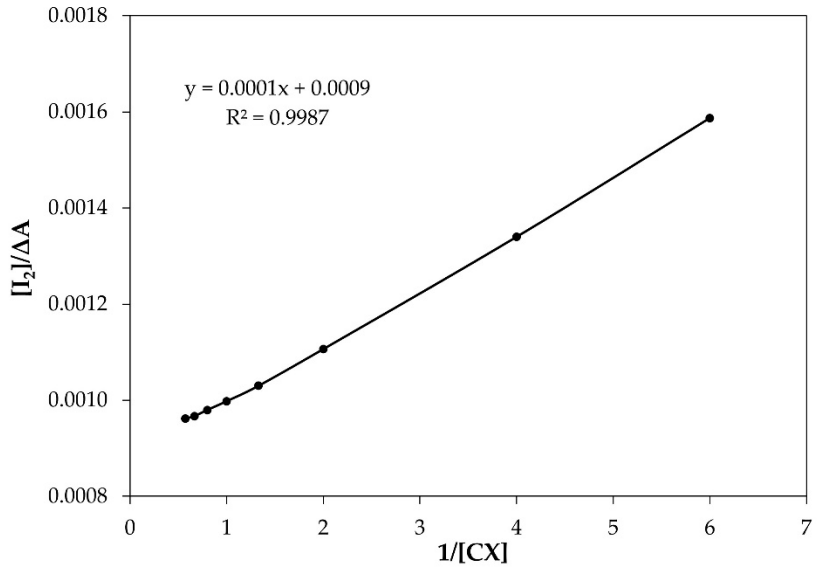

Figure S5. Benesi-Hildebrand plot of absorption data for the CX/iodine complex.

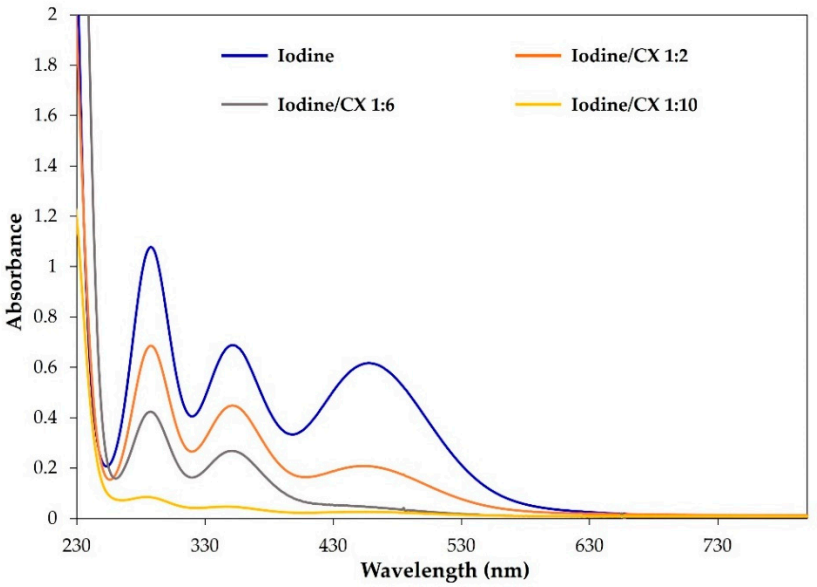

Figure S6. UV-vis spectra of iodine in water solution (1.3 x 10^{-3} M) alone and after stirring with increasing amounts of CX powder (iodine:CX 1:2, 1:6, and 1:10 molar ratio).

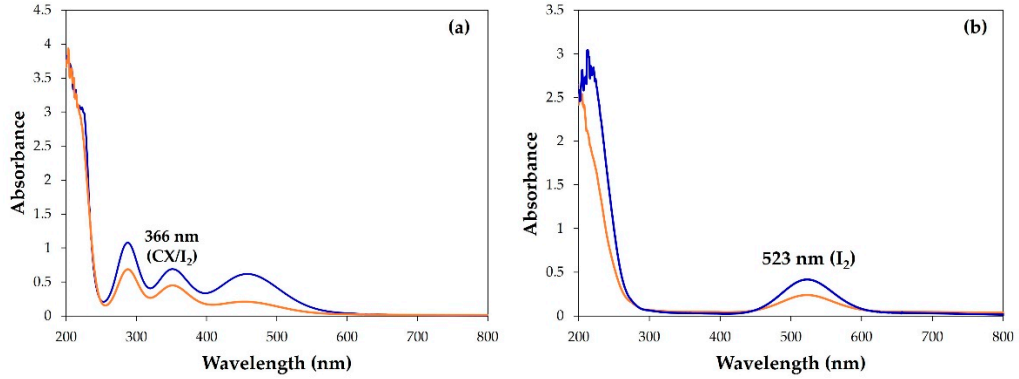

Figure S7. UV-vis spectra of (**a**) iodine in water solution (1.3 x 10^{-3} M) before (blue line) and after stirring with CX powder (iodine:CX, 2:1 molar ratio) (orange line); (**b**) iodine extracted by cyclohexane from the water solution of iodine (1.3 x 10^{-3} M) alone (blue line) and after stirring with CX powder (iodine:CX, 2:1 molar ratio) (orange line).

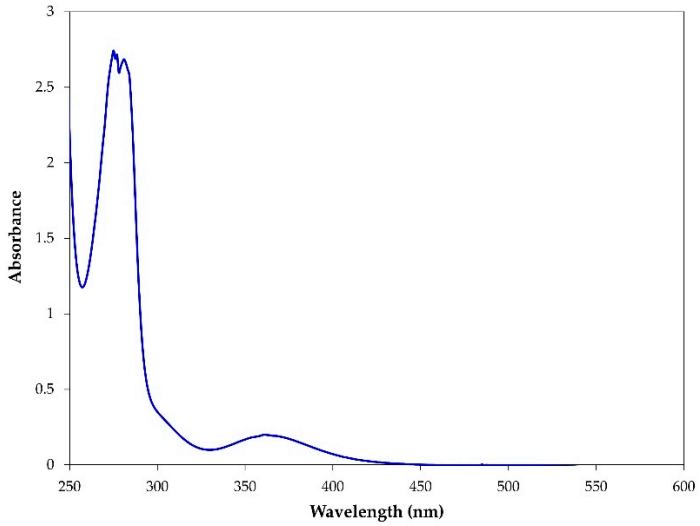

Figure S8. UV-vis spectrum in chloroform of the CX/iodine complex from solid-air method.

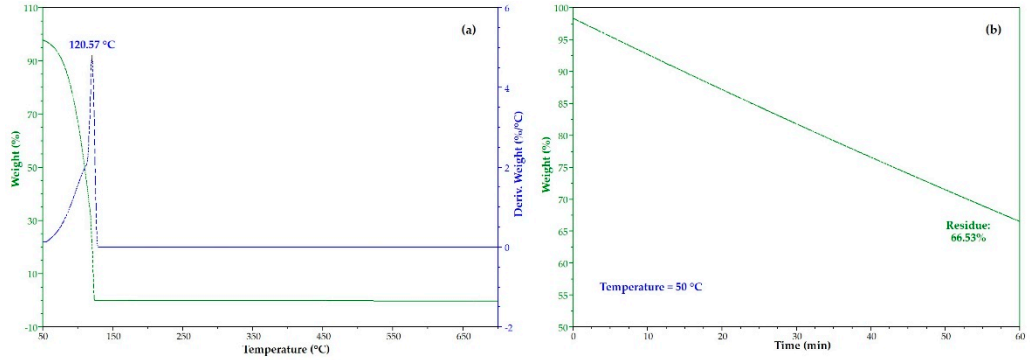

Figure S9. (**a**) TGA and (**b**) isothermal at 50 °C (60 minute) of I_2 sample.

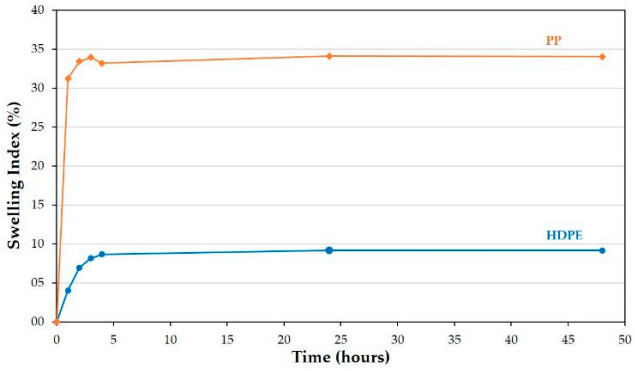

Figure S10. Swelling index in $CHCl_3$ vs time for HDPE and PP strip samples at room temperature.