Supporting information

Chiral imaging in living cells with a functionalized graphene oxide

Xiaowei Mao, and Haibing Li*

Key Laboratory of Pesticide & Chemical Biology (CCNU), Ministry of Education; College of Chemistry, Central China Normal University, Wuhan 430079, PR China Ihbing@mail.ccnu.edu.cn.

Data Analysis and Fitting

All fittings were performed in a nonlinear manner according to spectrofluorometric titrations.^[1] For the direct host-guest titrations, the complexation process of the β -CD-GO host (H) with the dye guest D/L-Phe-F (G) was expressed by *eq.1* according to a 1:1 host-guest binding stoichiometry and the complex stability constant (Ka) is given by *eq.2*

$$H + G \xrightarrow{K_a} H \cdot G \tag{1}$$

$$K_{a} = \frac{[H \cdot G]}{[H] \cdot [G]}$$
(2)

where $\triangle F$ and $\triangle \epsilon'$ denote the changes in the fluorescence intensity and molar extinction coefficient of the chromophoric β -CD-GO derivative upon inclusion complexation of the D/L-Phe-F.

$$\triangle \mathbf{F} = \ \triangle \mathbf{\epsilon}' \left[\mathbf{H} \cdot \mathbf{G} \right] \tag{3}$$

Solving the simultaneous equations, we obtained eq 4.

$$\Delta F = \frac{\Delta \varepsilon'([H]_0 + [G]_0 + \frac{1}{K_a}) \pm \sqrt{\Delta \varepsilon'^2([H]_0 + [G]_0 + \frac{1}{K_a})^2 - 4\Delta \varepsilon'^2[H]_0[G]_0}}{2}$$
(4)

The complex stability constant Ka and the sensitivity factor $\triangle \epsilon'$ were calculated by nonlinear fitting using the value of $\triangle F$ observed at each initial guest concentration [G]₀.



Figure S1. TEM images of the GO.



Figure S2. FT-IR spectra of a) GO, b) pure mono-6-amino- β -CD, and (c) β -CD-GO.



Figure S3. (A) XPS spectra of the original GO (curve black) and β -CD-GO (curve red); (B) Water drop profile changes of β -CD-GO (top), and GO (bottom) measuring on glass slides.



Figure S4. XPS C1s spectrum of A) GO; B) β-CD-GO.



FigureS5. Effect of increasing concentrations of native β -CD-GO on the fluorescence intensity of A) L-Phe-F, B) D-Phe-F (5×10⁻⁶ M). (excitation: 330 nm).

Parallel experiment with other two aromatic amino acids (tyrosine and histidine) has done to investigate the chiral sensing capacity of this platform. The chiral discrimination ratio (K_D/K_L) of β -CD-GO probe for D/L-Tyr-F and D/L-His-F is 2.18 and 1.91, respectively. Such parallel experiments indicated that this β -CD-GO sensor produced a good enantioselectivity of D-Phe-F with higher chiral discrimination ratio (K_D/K_L) toward other aromatic amino acids. Consequently, we choose D-phenylalanine as a model example for their biosensing device in the living cells.



FigureS6. Effect of increasing concentrations of β -CD-GO on the fluorescence intensity of A) L-Tyr-F, B) D-Tyr-F (10⁻⁵ M) (excitation: 330 nm); C) The increase in relative fluorescence intensity of D/L-Tyr-F at the same concentrations of β -CD-GO based on nonlinear fitting model (eq.4); The dependence of increasing β -CD-GO concentrations on the fluorescence intensity of D) L-His-F, E) D-His-F (10⁻⁵ M) (excitation: 330 nm); F) Effect of increasing concentrations of β -CD-GO on the fluorescence intensity of D/L-His-F based on nonlinear fitting model (eq.4).



Figure S7. Relative cell viability of Hela treated with β -CD-GO. Hela cells were incubated with different concentrations of β -CD-GO for 24 h in fresh medium.



FigureS8. Confocal fluorescence microscopy images of Hela cells were incubated with D/L-Phe-F (control L and D), or incubated for 2~4 h at 37 °C with D/L-Phe-F and β -CD-GO at the concentration of 0.25 µg/mL (L1 and D1), 0.50 µg/mL (L2 and D2), 0.75 µg/mL (L3 and D3) in sequence, and the images were obtained after extensive washing of cells with PBS. Bright-field (top), dark-field fluorescence (middle), and overlap of images of dark and bright field (bottom), respectively.



FigureS9. The mean fluorescence intensity of Hela cells incubated with D/L-Phe-F and without β -CD-GO (L₀ and D₀), or with β -CD-GO at the concentration of 0.25 µg/mL (L₁ and D₁), 0.50 µg/mL (L₂ and D₂), 0.75 µg/mL (L₃ and D₃) in sequence for 2-4 h at 37 °C, and the measurement were carried out after extensive washing of cells with PBS, which analyzed by flow cytometry.

 Y. J. Zhang, W. X. Cao, J. Xu, Chin. J. Chem., 2002, 20, 322; Y. Liu, B. H. Han, S. X. Sun, T. Wada, Y. Inoue, J. Org. Chem. 1999, 64, 1487; Y. Matsui, K. Mochida, Bull. Chem. Soc. Jpn., 1979, 52, 2808.