Cyclodextrin encapsulated pH sensitive dyes as fluorescent cellular probes: self-aggregation and in vitro assessments

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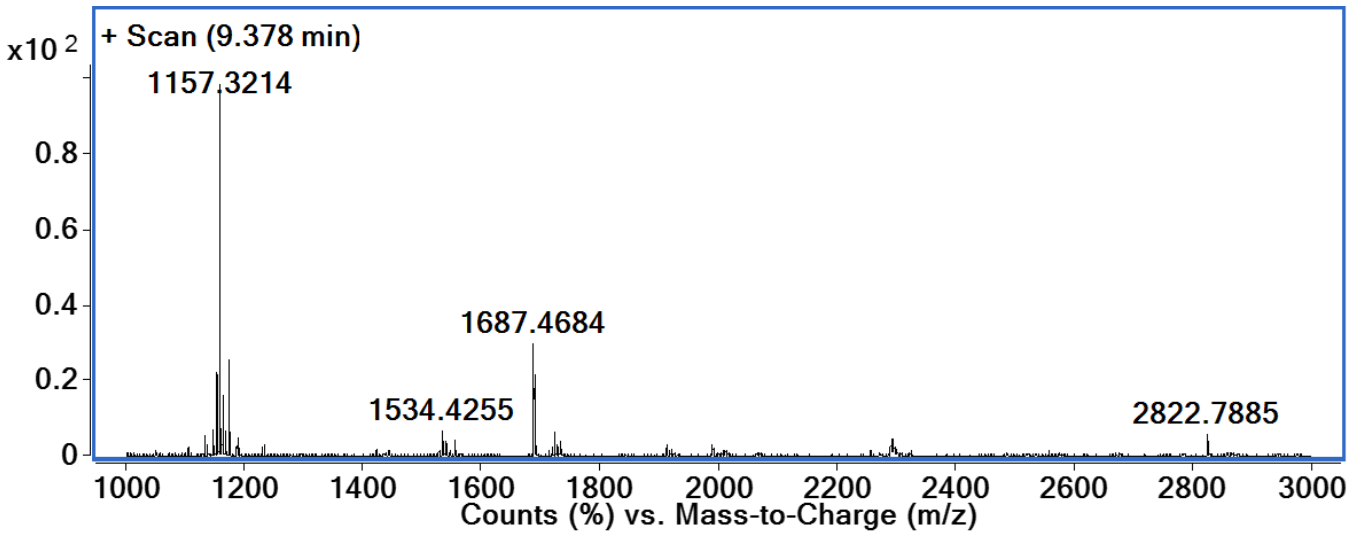
Content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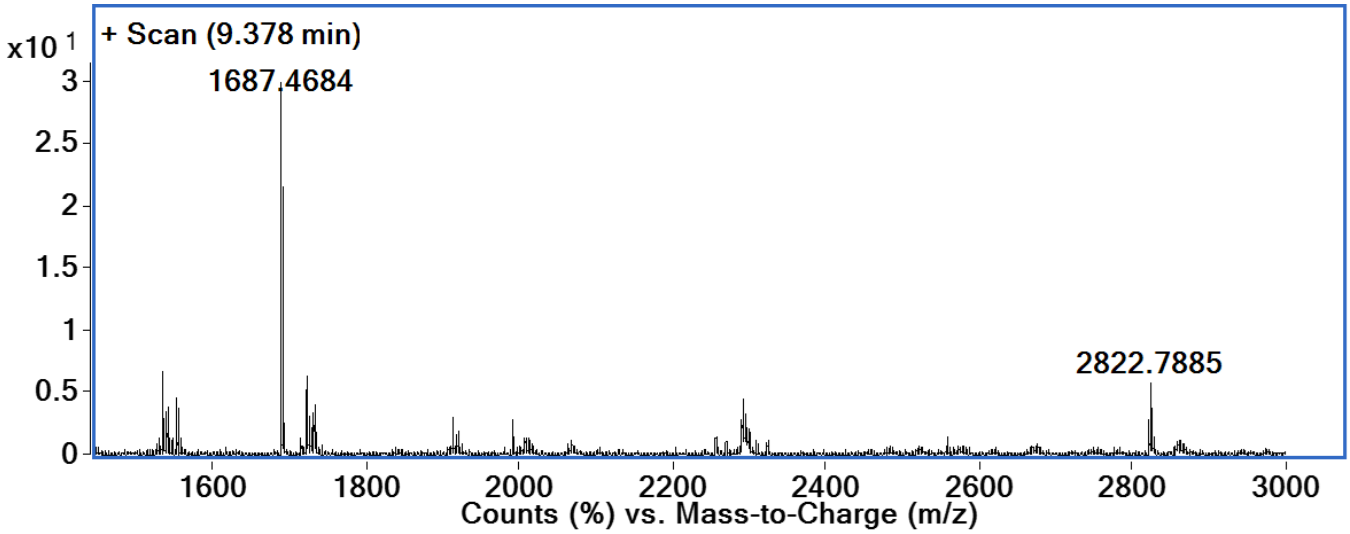
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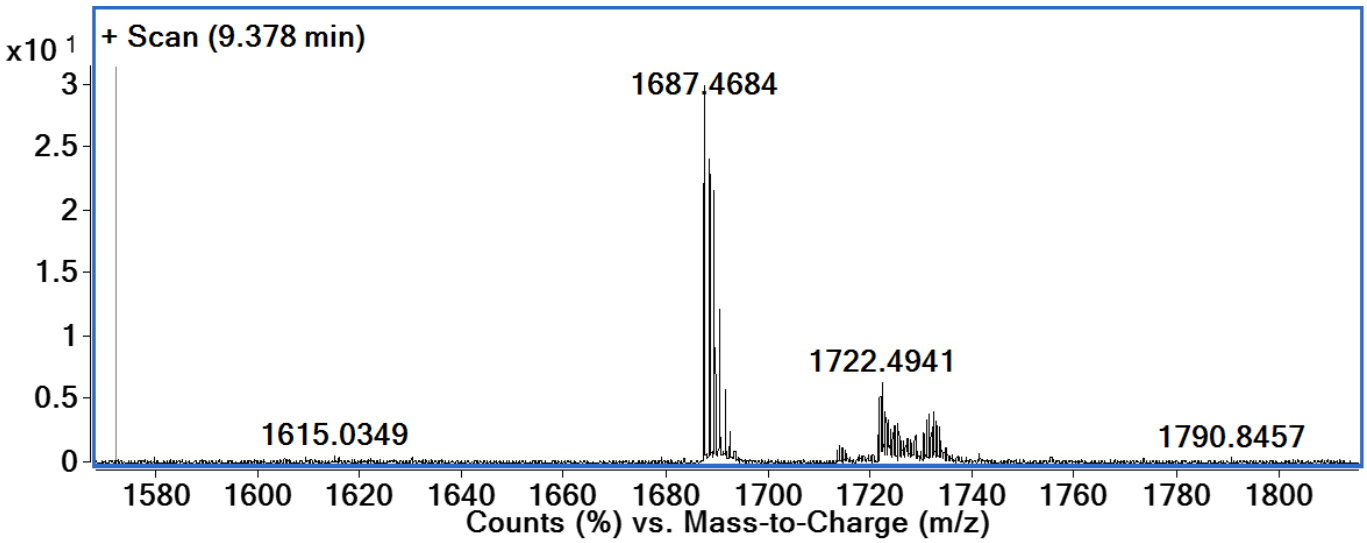
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Counts (%) vs. Mass-to-Charge (m/z)

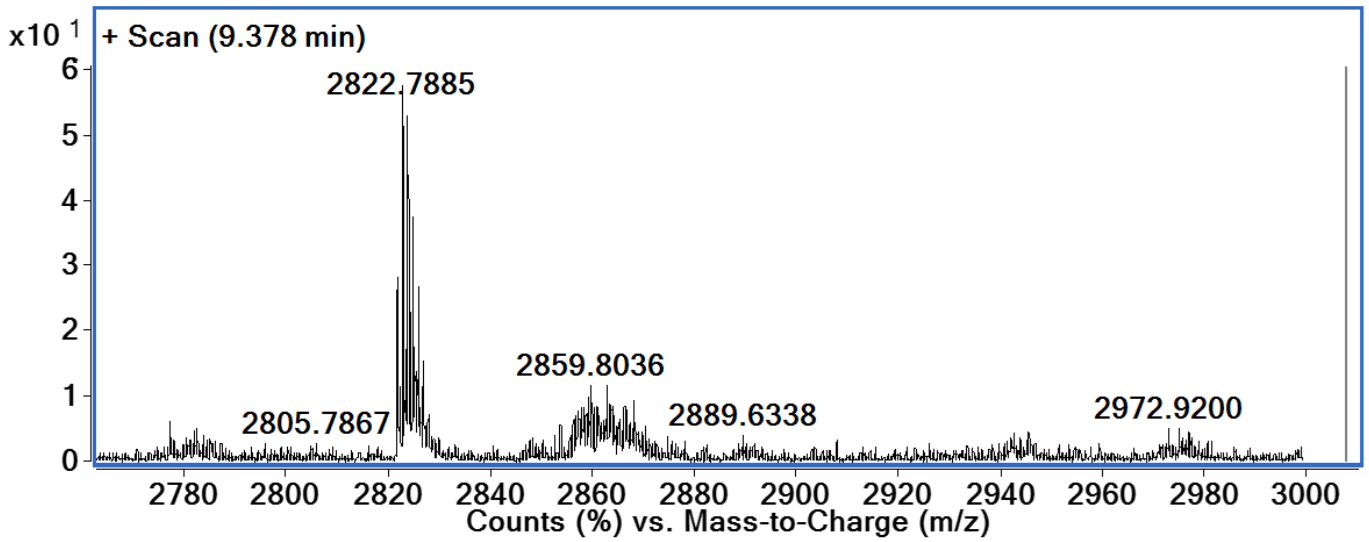
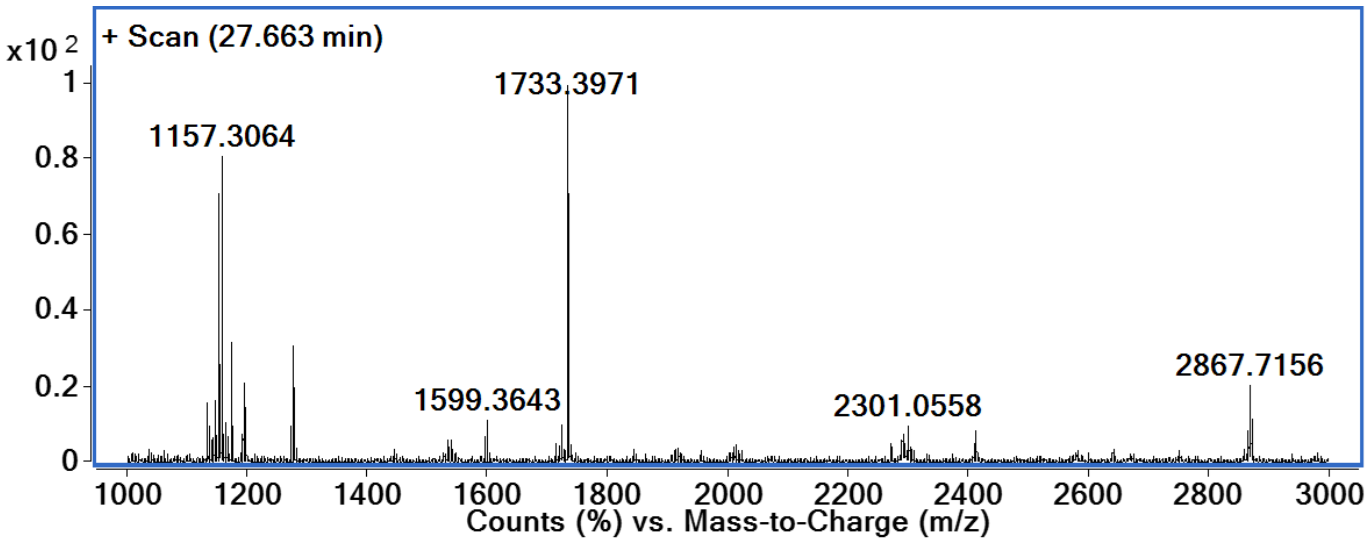


Figure S1. Examples of ESI-MS spectra of the **1a_CD** at 1:5 molar ratio between indolizine **1a** and CD. Peaks corresponding to: β-CD (MNa^+ ion at *m/z* 1157), the formation of 1:1 inclusion complex (M^+-Br + CD ion at *m/z* 1687) and 1:2 (M^+-Br + 2CD ion at *m/z* 2822) have been identified.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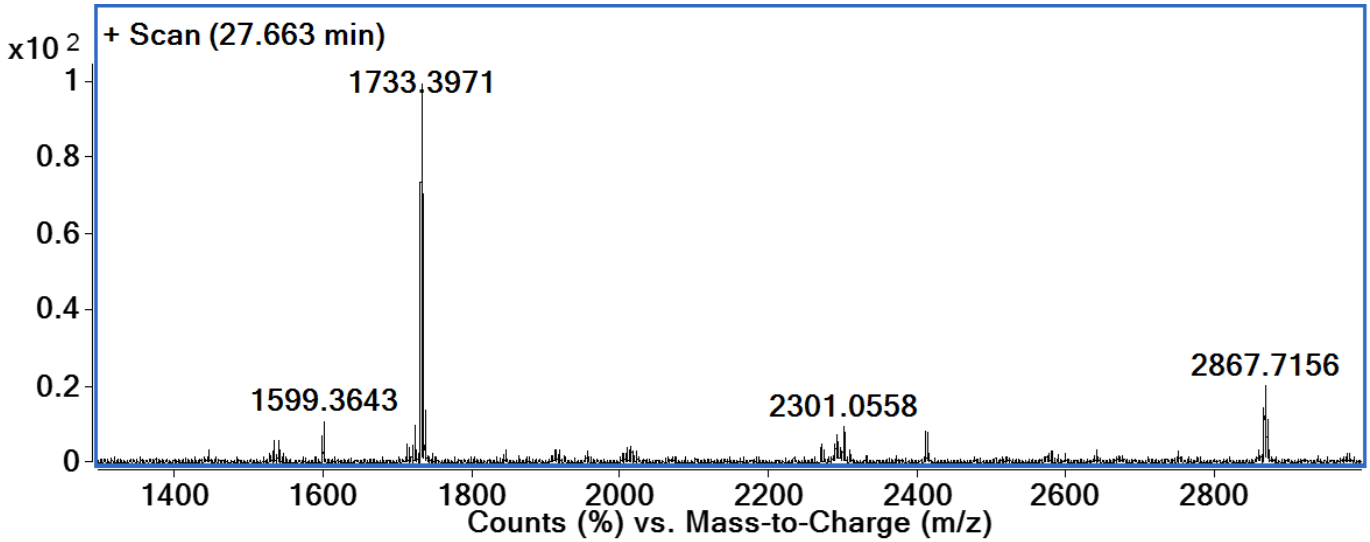
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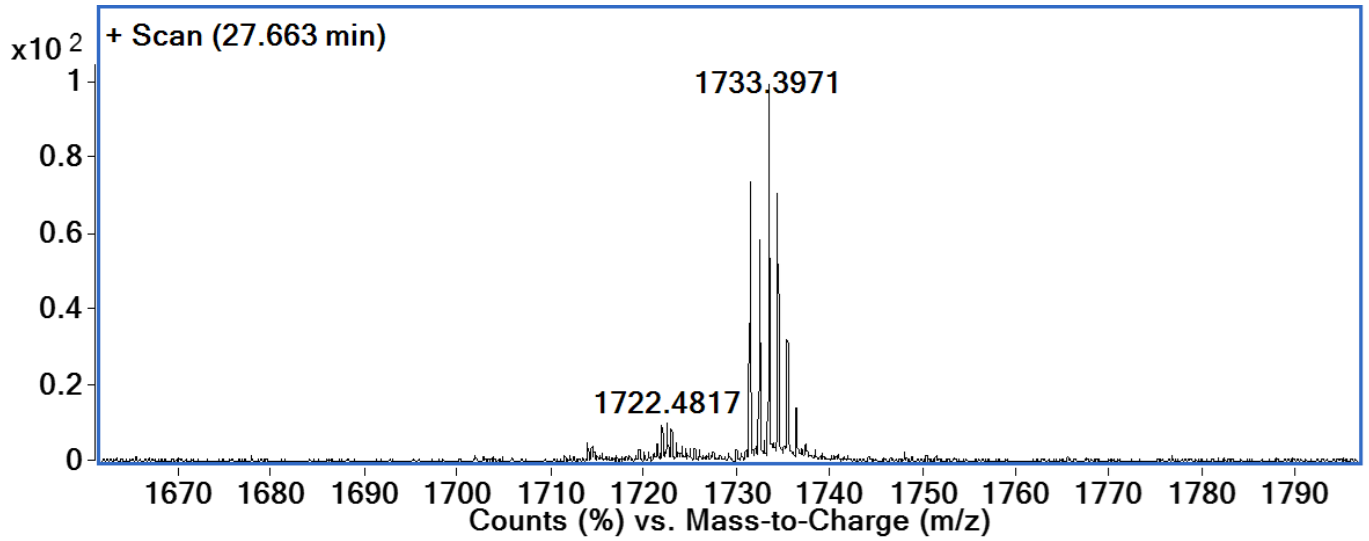
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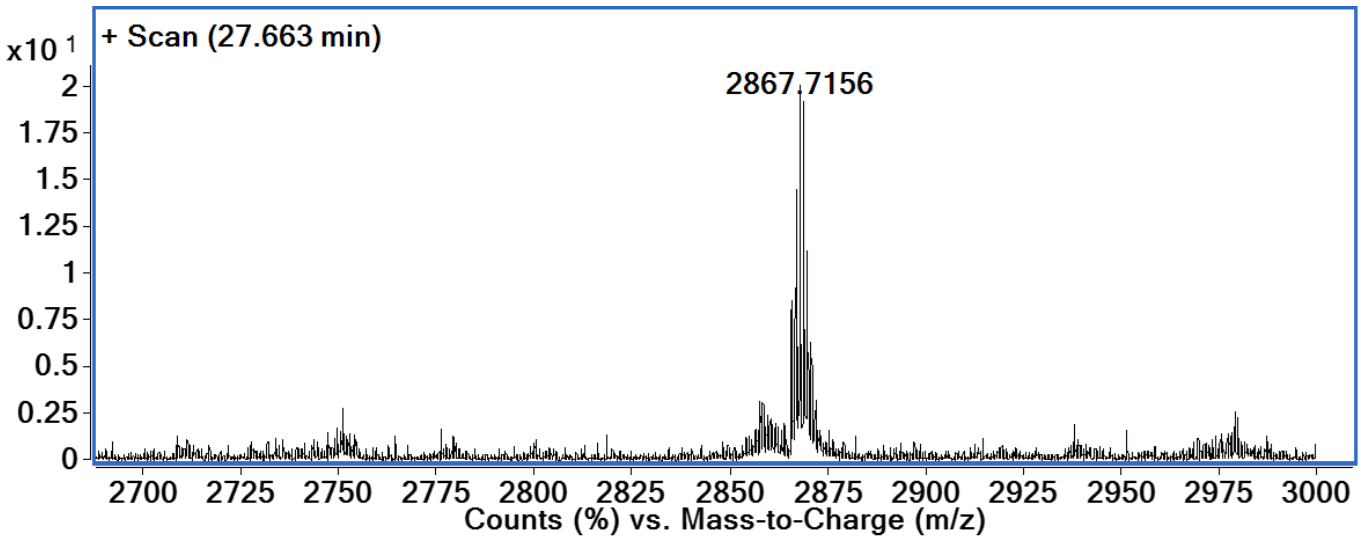
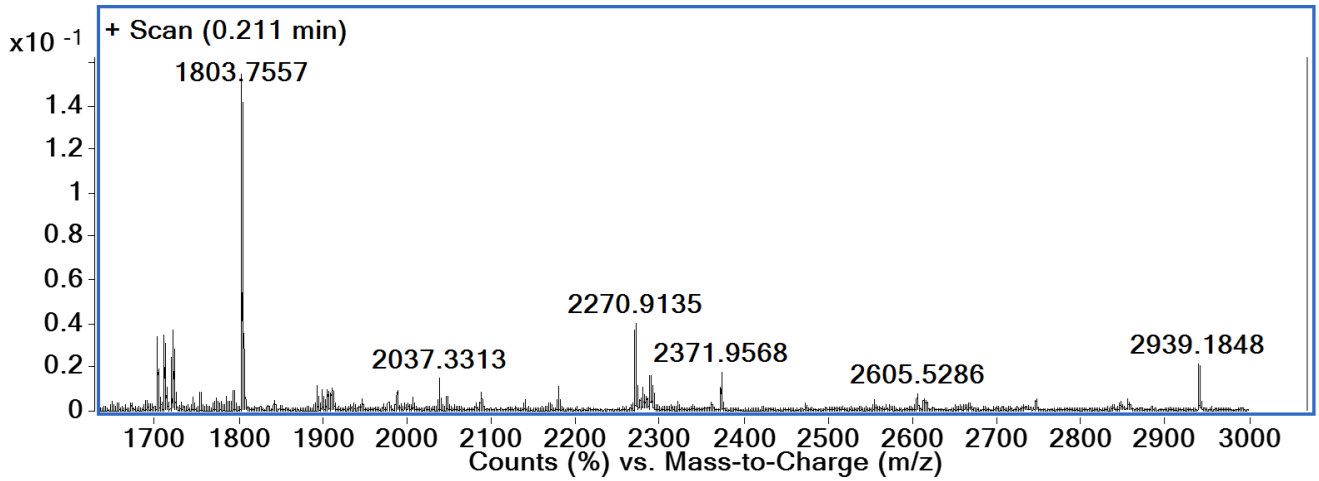


Figure S2. Examples of ESI-MS spectra of the **1b_CD** at 1:5 molar ratio between indolizine **1b** and CD. Peaks corresponding to: β-CD (MNa^+ ion at *m/z* 1157), the formation of 1:1 inclusion complex (M^+-Br + CD ion at *m/z* 1733) and 1:2 (M^+-Br + 2CD ion at *m/z* 2867) have been identified.



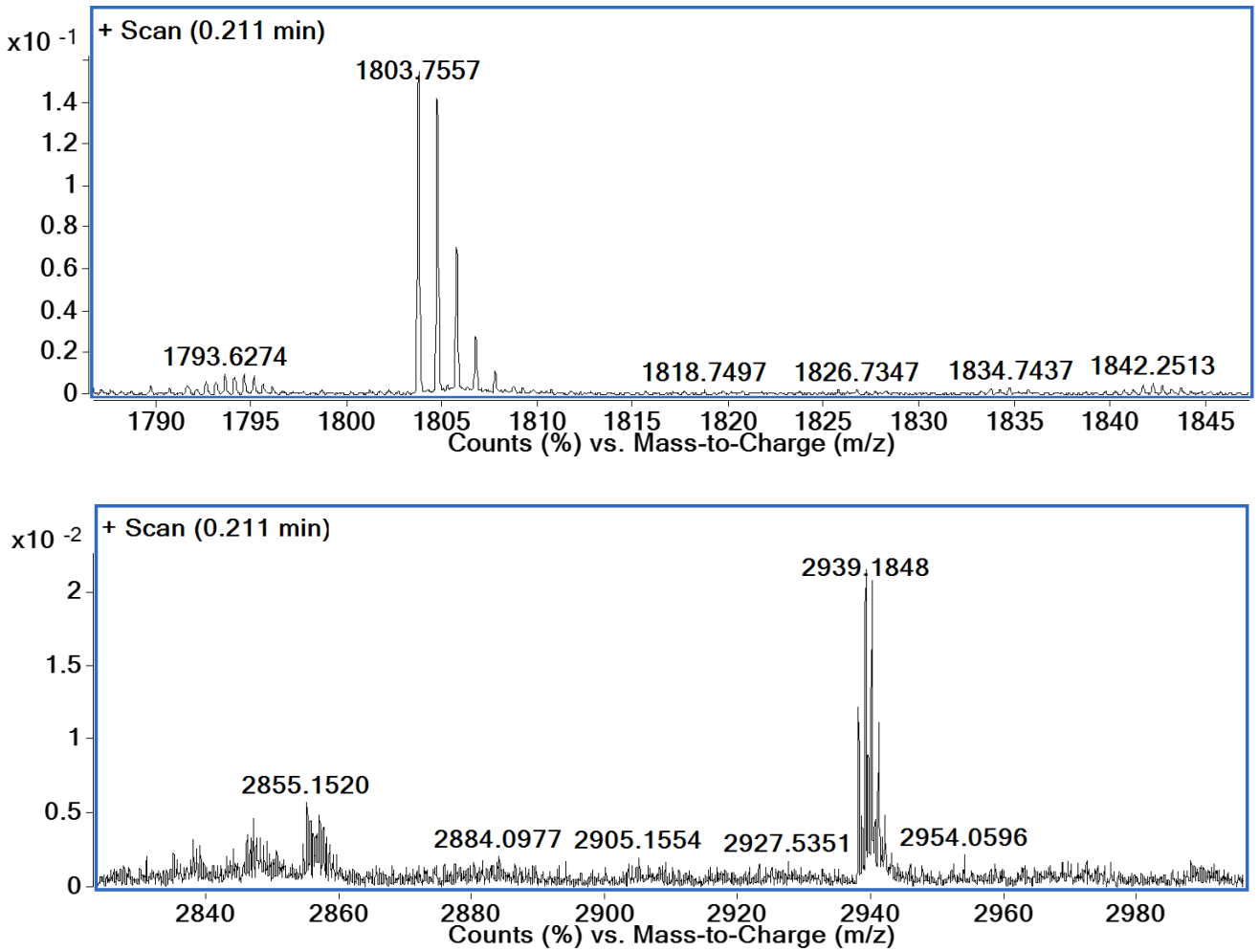
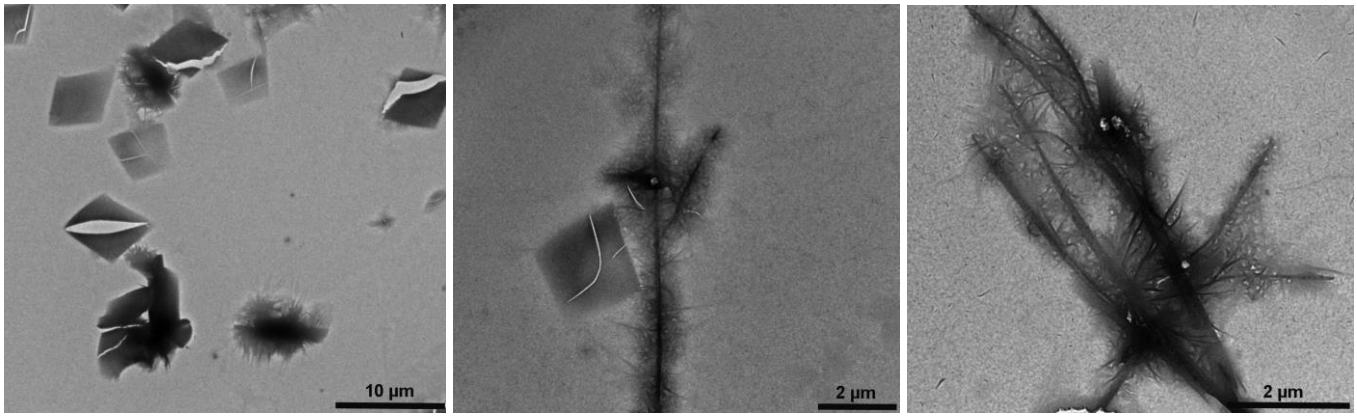
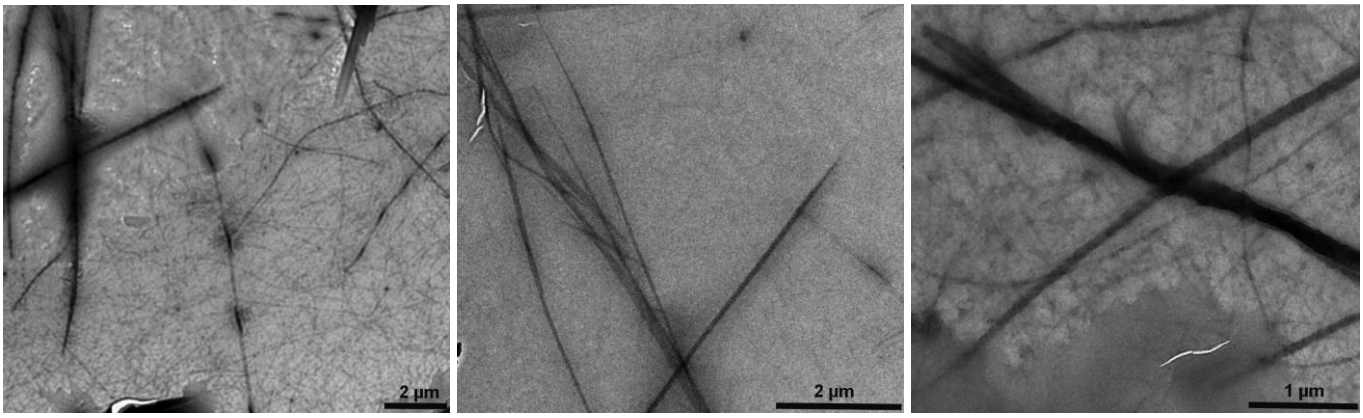


Figure S3. Examples of ESI-MS spectra of the **1c_CD** at 1:5 molar ratio between indolizine **1c** and CD. Peaks corresponding to: the formation of 1:1 inclusion complex (M^+-Br + CD ion at *m/z* 1803) and 1:2 (M^+-Br + 2CD ion at *m/z* 2939) have been identified.

(A)



(B)



(C)

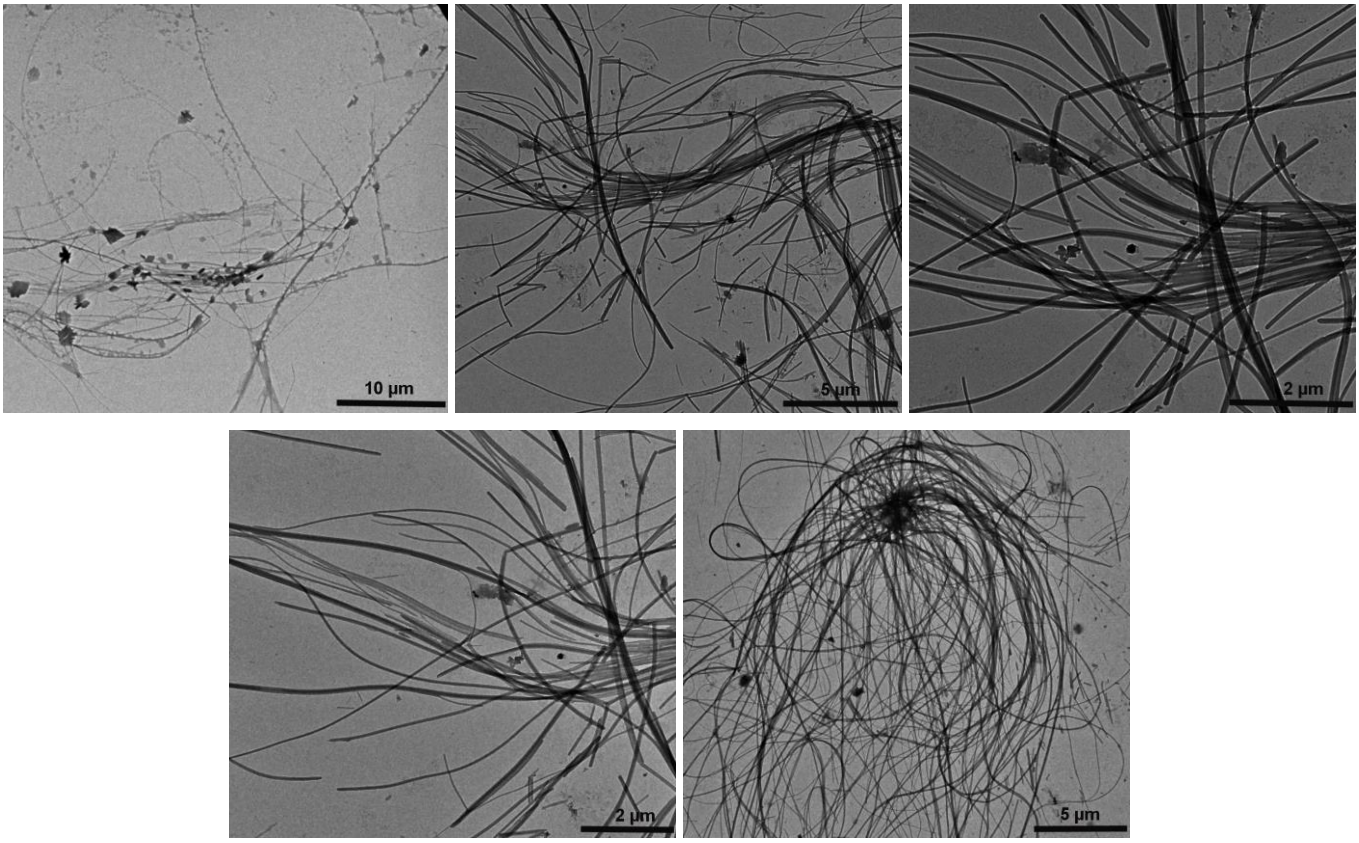


Figure S4: Examples of TEM images for compounds **1a_CD** (**A**); **1b_CD** (**B**); **1c_CD** (**C**).

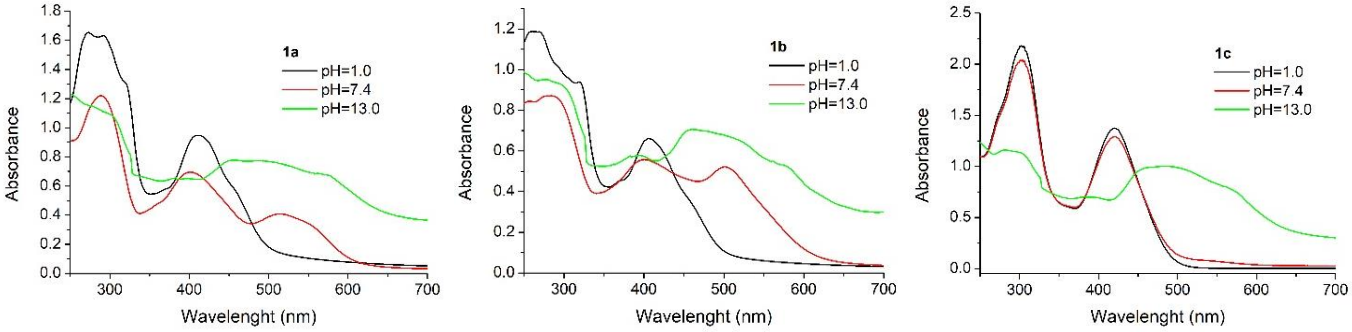


Figure S5: UV-Vis spectra of compounds **1(a-c)** at pH value of 1.0 (0.1 M HCl), 7.4 (1xTAE) and 13.0 (0.1 M NaOH).

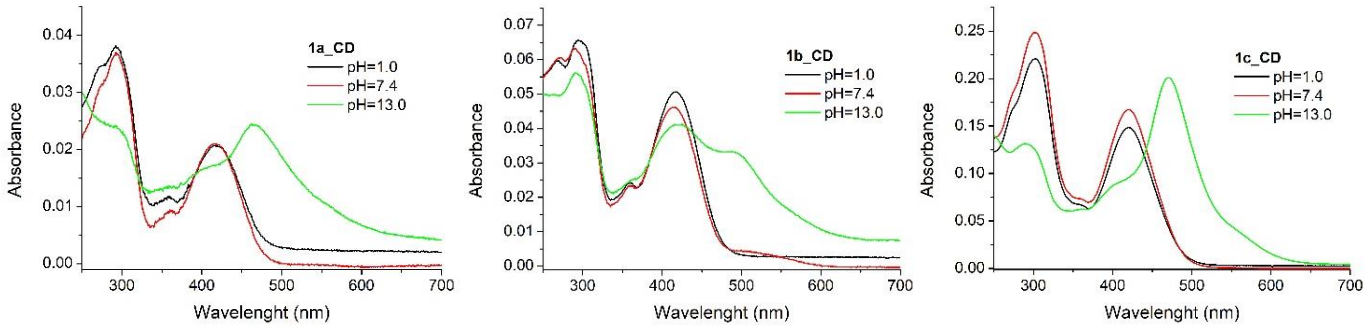
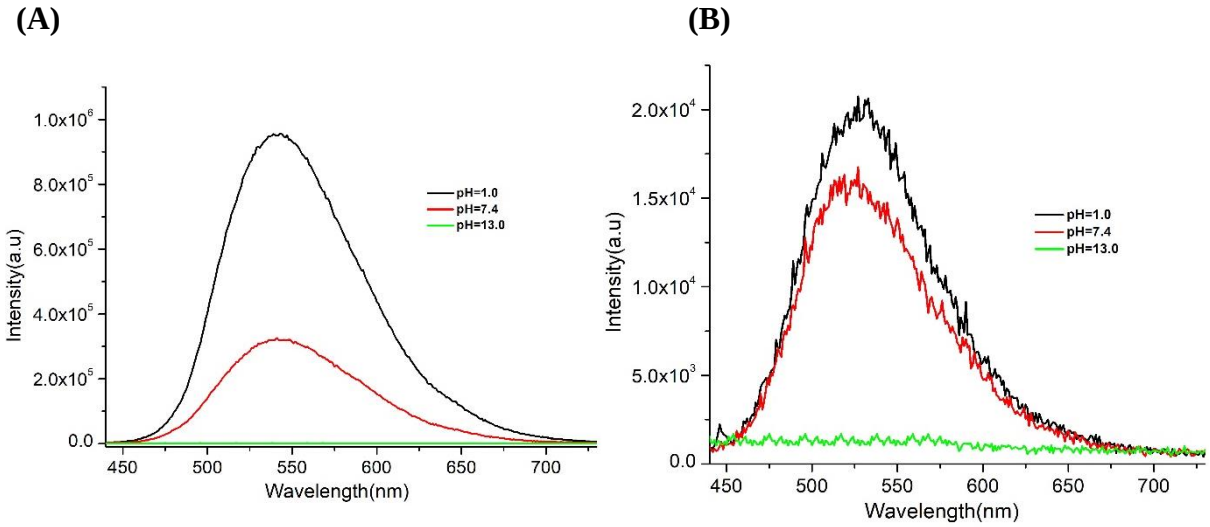


Figure S6: UV-Vis spectra of compounds **1(a-c)_CD** at pH value of 1.0 (0.1 M HCl), 7.4 (1xTAE) and 13.0 (0.1 M NaOH).



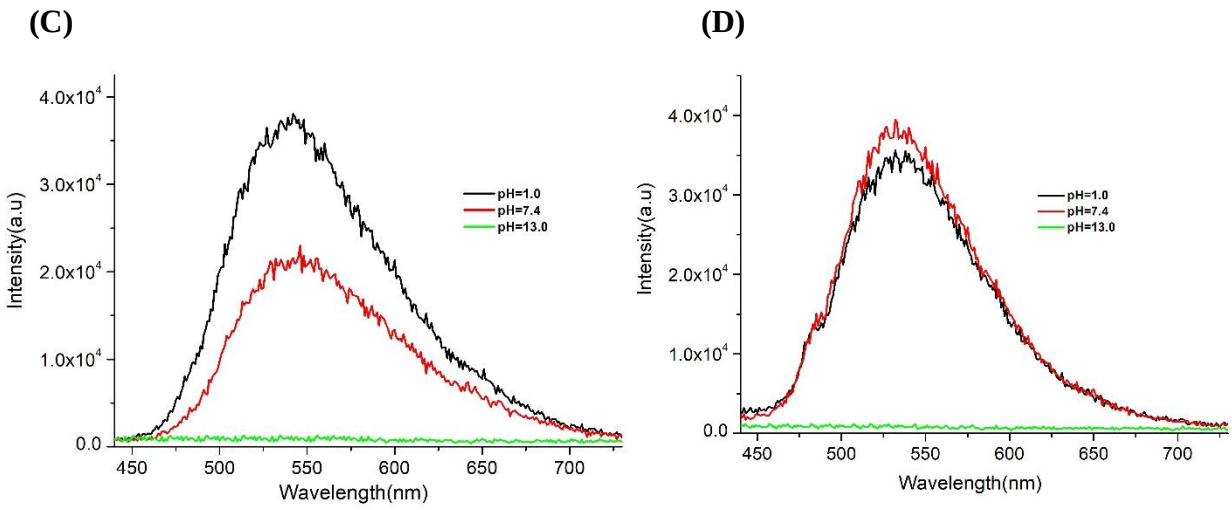


Figure S7: Fluorescence spectra at pH = 1.0 (0.1 M HCl), 7.4 (1xTAE) and 13.0 (0.1 M NaOH)for compounds: **(A)** compound **1b**, **(B)**compound **1b_CD**, **(C)** compound **1c** and **(D)** compound **1c_CD**.

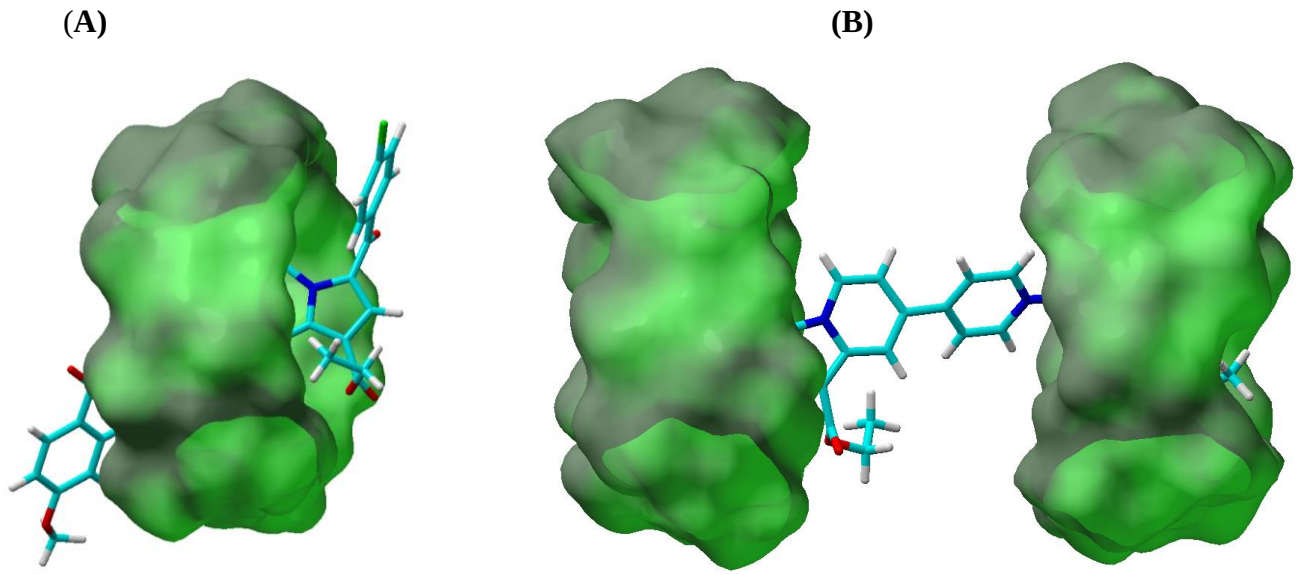


Figure S8: Examples of molecular docking models of compound **1b** in complex with β-CD showing the possibility of the 1:1 (**A**) and 1:2 (**B**) inclusion complexes formation**.**

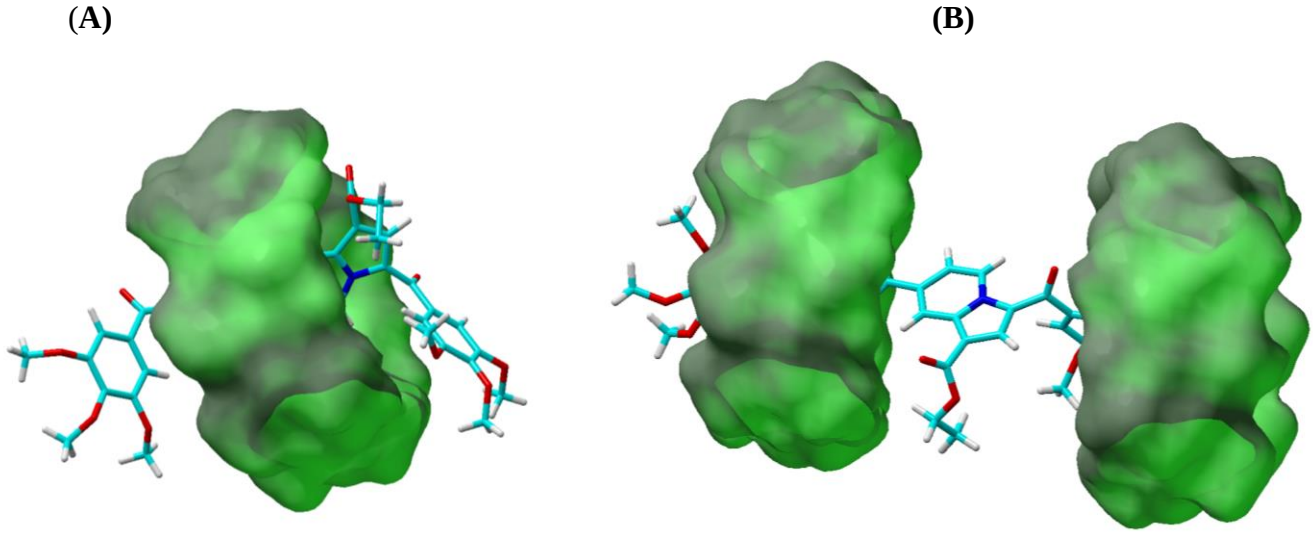


Figure S9: Examples of molecular docking models of compound **1c** in complex with β-CD showing the possibility of the 1:1 (**A**) and 1:2 (**B**) inclusion complexes formation**.**

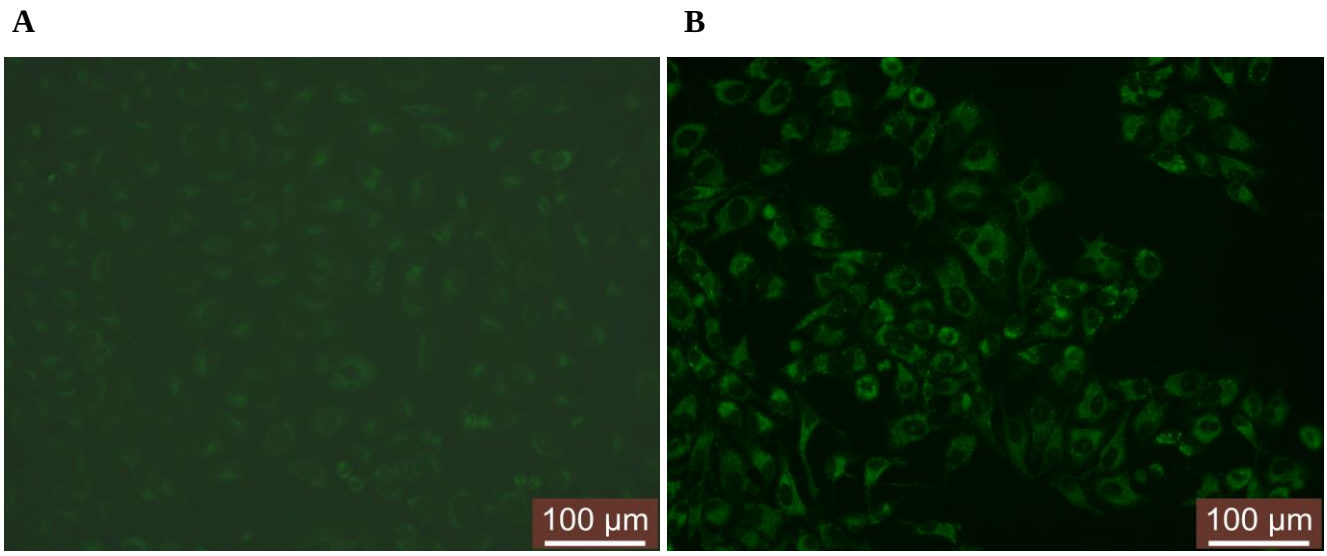


Figure S10. Compound **1b_CD** uptake into HeLa cells after 15 min (left) and 24 hours (right) incubation.

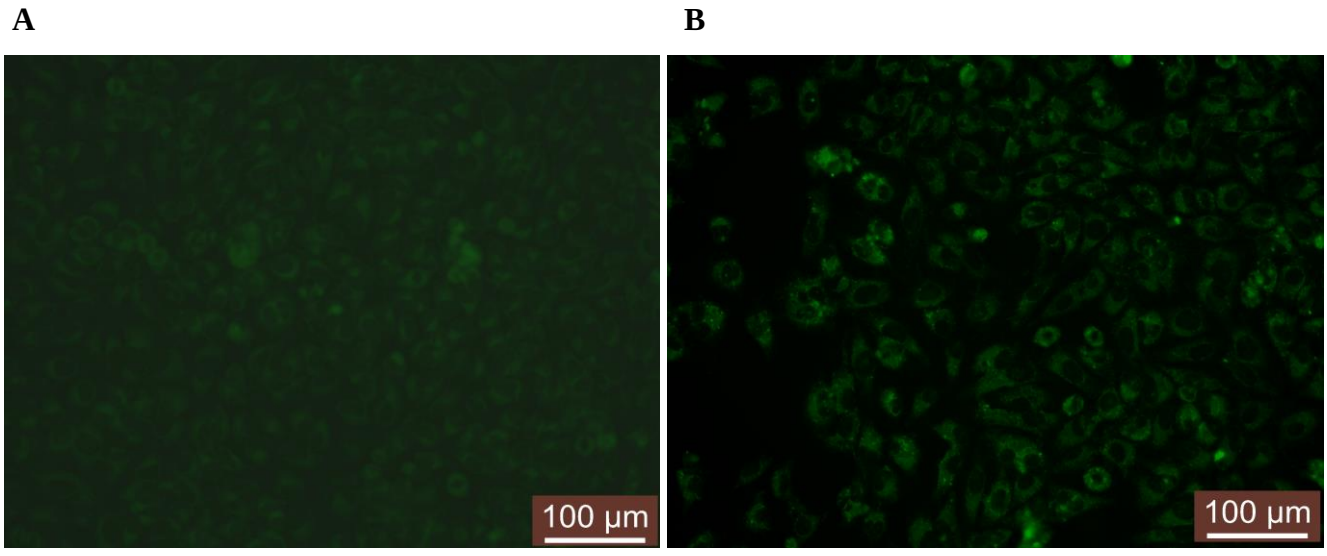


Figure S11. Compound **1c_CD** uptake into HeLa cells after 15 min (left) and 24 hours (right) incubation.

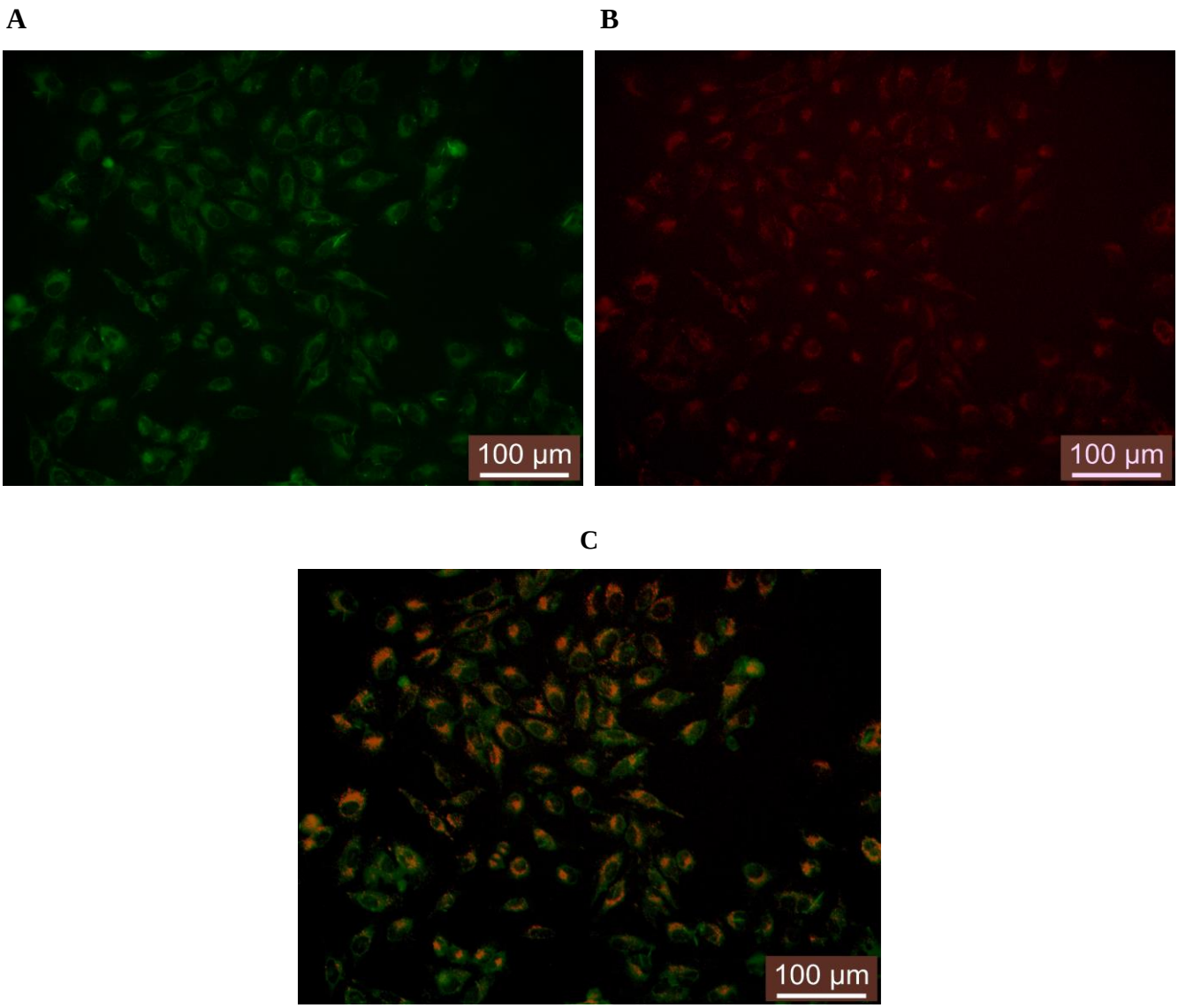


Figure S12. Examples of images for intracellular distribution of compound **1b_CD** after 24 hours (A) compared to LysoTracker Red (B) and corresponding overlay (C).

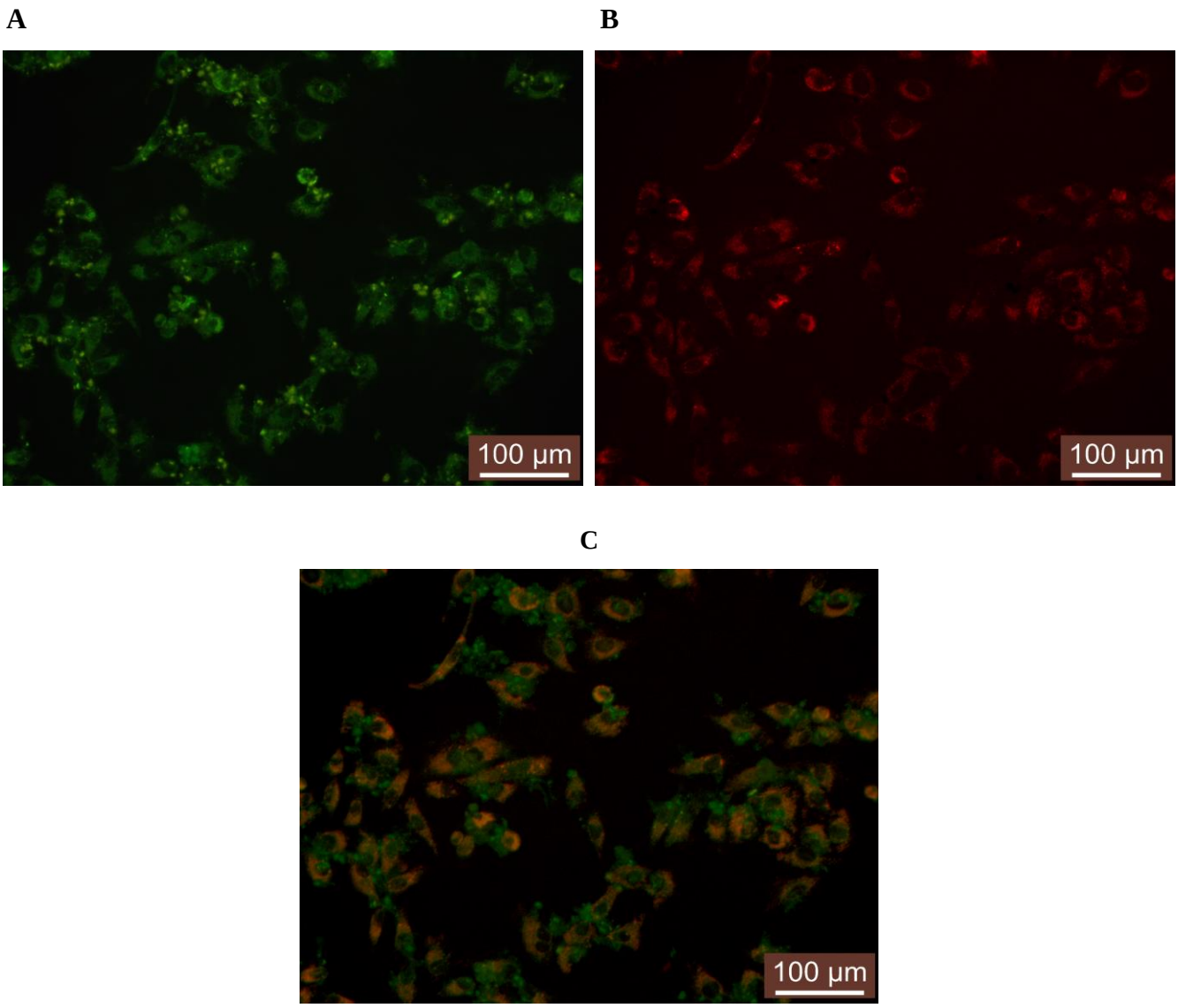


Figure S13. Examples of images for intracellular distribution of compound **1c_CD** after 24 hours (A) compared to LysoTracker Red (B) and corresponding overlay (C).

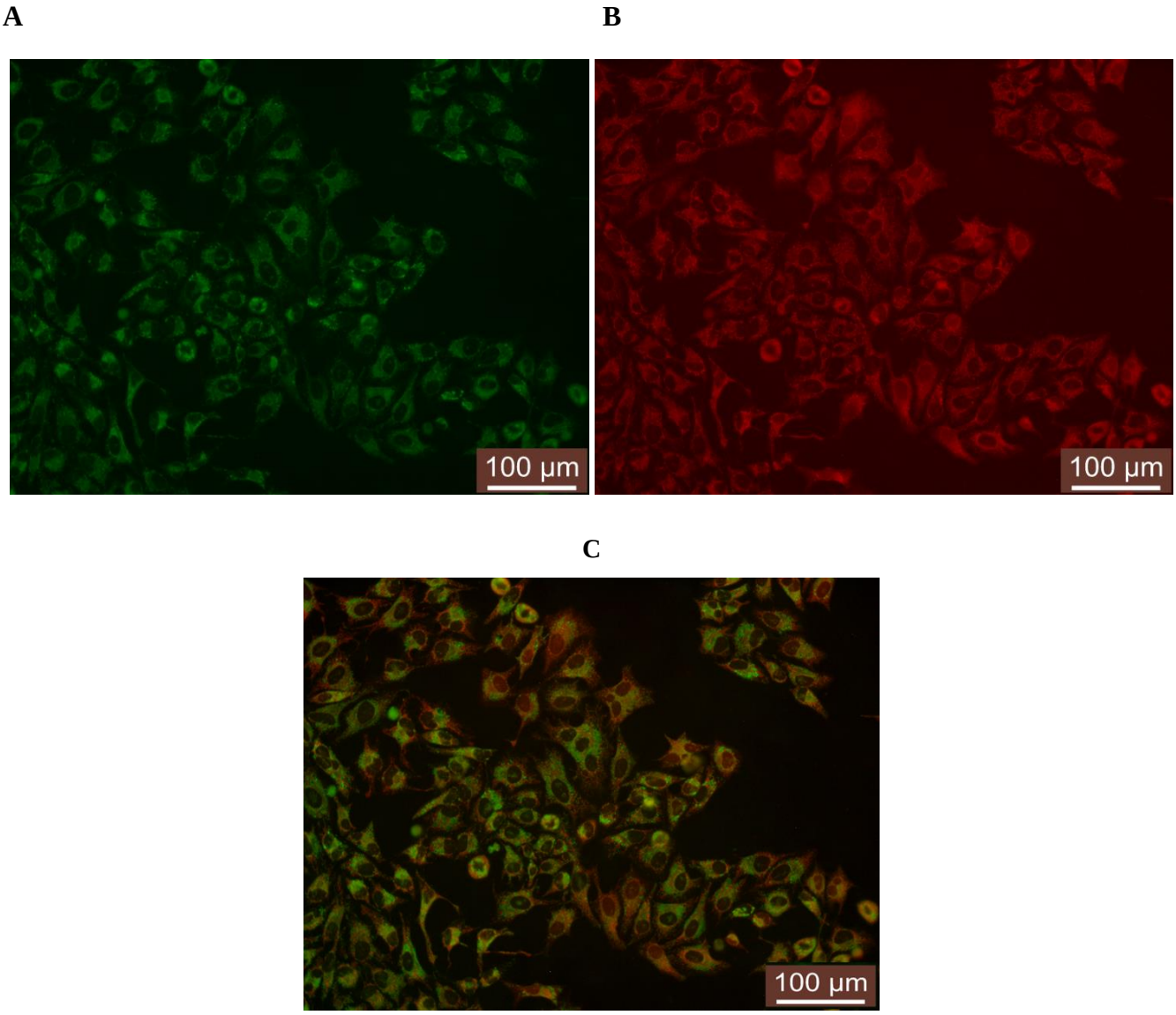


Figure S14. Examples of images for intracellular distribution of compound **1b_CD** after 24 hours (A) compared to MitoTracker Red (B) and corresponding overlay (C).

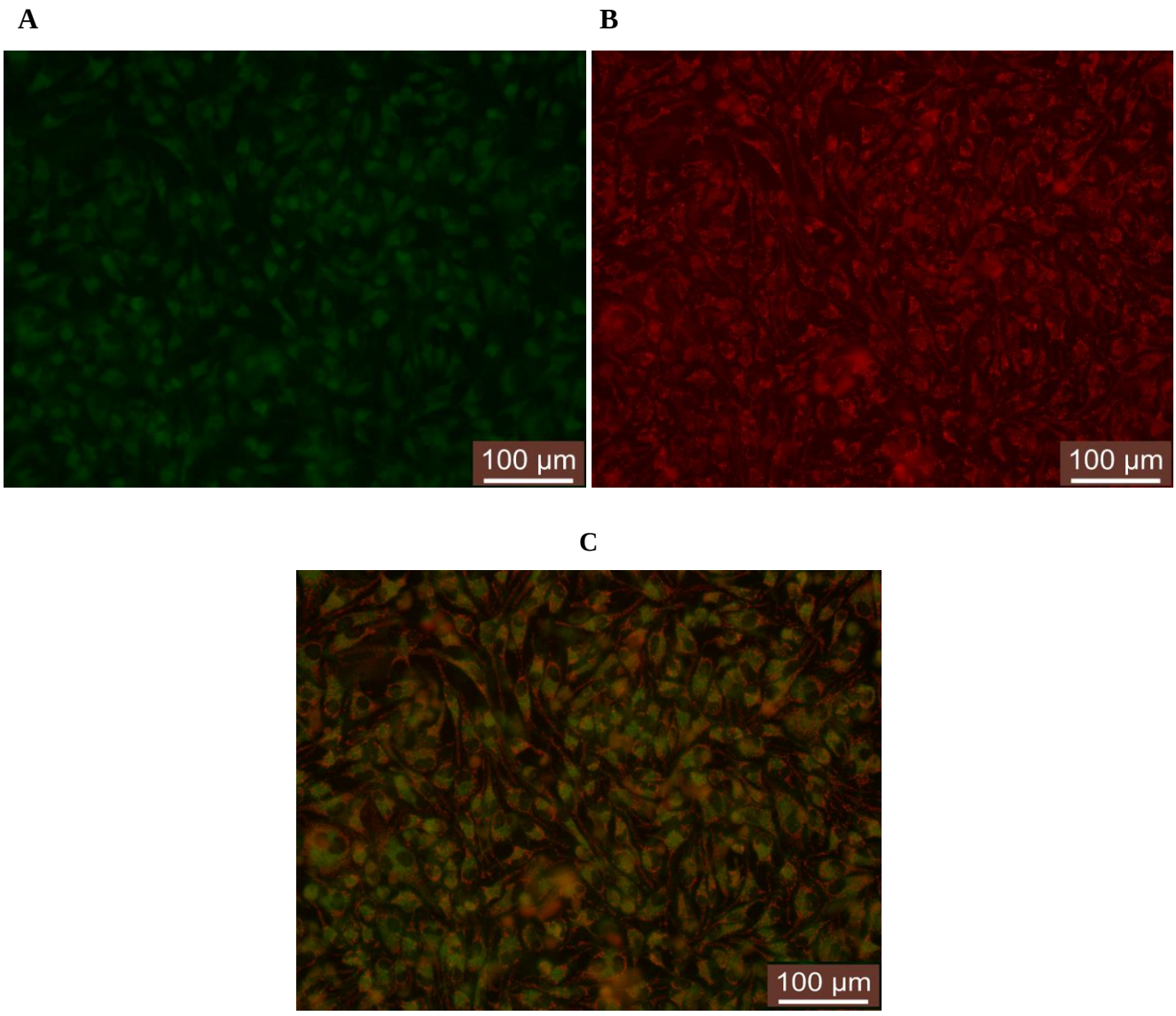


Figure S15. Examples of images for intracellular distribution of compound **1c_CD** after 24 hours (A) compared to MitoTracker Red (B) and corresponding overlay (C).