Near-Infrared-Emitting Meso-Substituted Heptamethine Cyanine Dyes: From the Synthesis to Photophysics

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ABSTRACT: Cyanine dyes are a class of functional organic dyes characterized by a π-conjugated poly-methinic chain linking two heterocyclic ring systems. These dyes are widely recognized for their versatile applications across industrial and technological fields, including photosensitization and optical materials and biological labeling.

Heptamethine cyanine dyes were synthesized in good yields by the reaction between quaternary indoles and a pentamethinic salt, under mild reaction conditions. These compounds were used as precursors to prepare meso-substituted derivatives. The cyanine dye precursors presented UV-Vis absorption, related to fully allowed electronic transitions and fluorescence emission in the NIR region, without any evidence of aggregation in both ground and excited states. The substitution at the meso position showed a fundamental role in their photophysics.

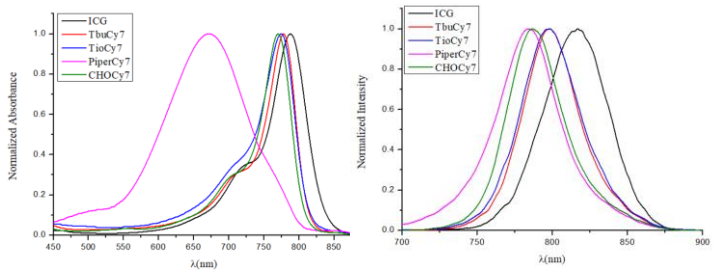
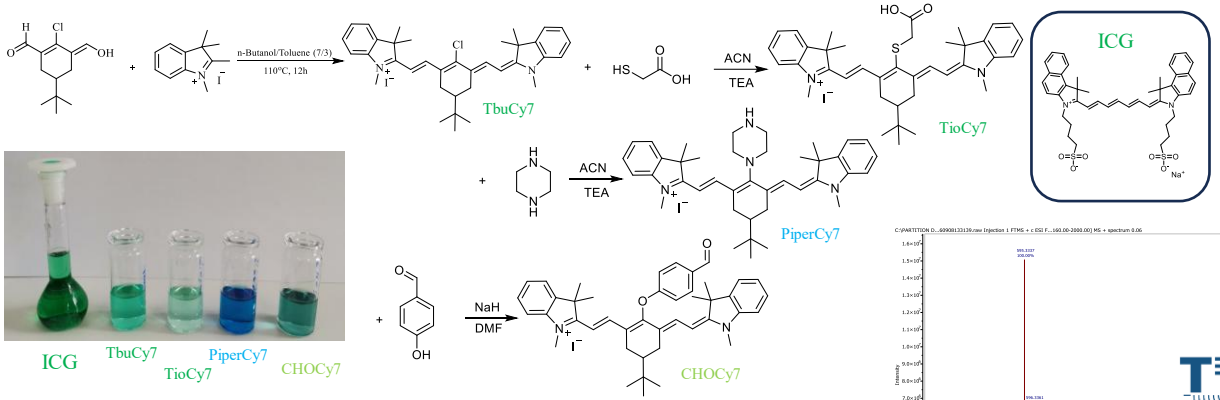


Figure 1. *Normalized absorbance and emission spectra of Heptacyanine dyes in EtOH*

Table 1. *Photophysical properties of Cy7 series*

Comp.	MW.	λ_{ex} (nm)	λ_{em} (nm)	ε (l/mol ·cm)	Stokes (nm, cm^{-1})
ICG	**774.98**	722, **788**	**816**	**910602**	28 (**435**)
TbuCy7	**539.31**	706, **778**	**797**	**107862**	19 (**306**)
TioCy7	**595.33**	706, **770**	**798**	**178599**	28 (**456**)
PirazCy7	**589.42**	**672**	**785**	**9440**	113 (**2142**)
CHOCy7	**625.37**	706, **770**	**787**	**172628**	17 (**281**)



Scheme 1. *The synthesis of Heptamethine cyanine dyes, and the colour of their ethanolic solution in UV-Vis concentration*

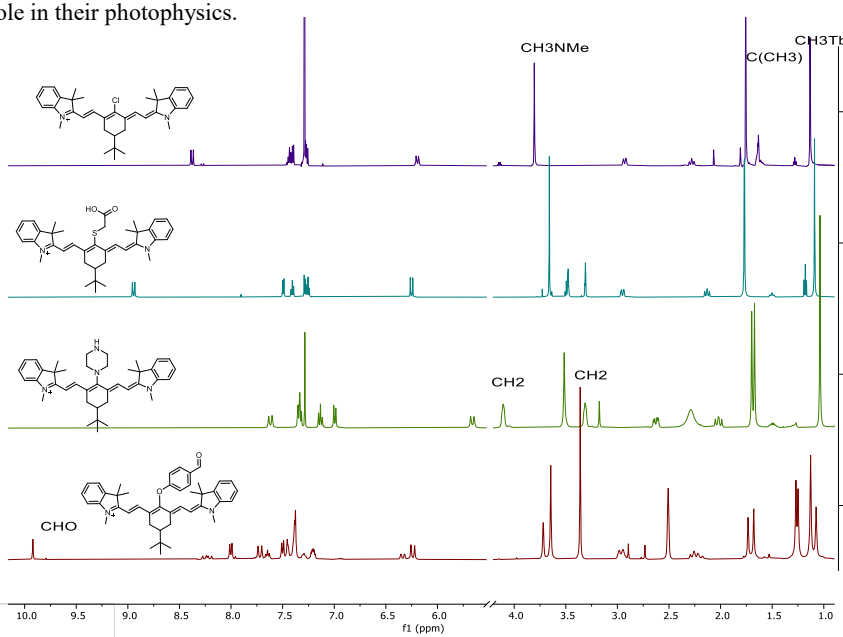


Figure 2. *^{1}H-NMR spectra of Heptacyanine dyes ($CDCl_3$, 400MHz)*

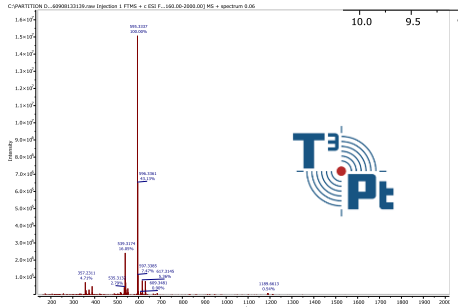


Figure 3. *HRMS (ESI+) spectra of TioCy7*

Equipments:
Bruker ASCEND 600/400 MHz NMR spectrometer;
Bruker FT-IR Vector 22 spectrophotometer;
Shimadzu QP-2010 PLUS mass spectrometer;
HRMS Thermo Scientific LTQ Orbitrap XL

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https://chem.ubbcluj.ro/~hetorgmet/research/grants/t3-pt/

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