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# Fluorosolvatochromism and hyperpolarizability of one-arm and two-arms nitro-compounds bearing heterocyclic rings

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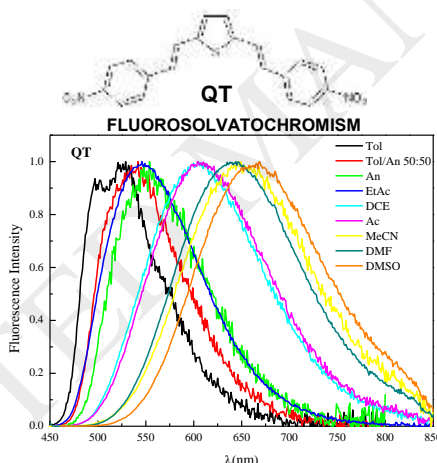
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## Graphical abstract

Strong fluorsolvatochromism exhibited by compounds with Acceptor- $\pi$ -Het and Acceptor- $\pi$ -Het- $\pi$ -Acceptor structures in agreement with the substantial photoinduced intramolecular charge transfer (from the heteroaromatics to the nitro groups) allowed hyperpolarizability coefficients of significant value to be estimated through the solvatochromic method ( $\beta_{CT}$  up to  $1030 \times 10^{-30}$  esu<sup>-1</sup> cm<sup>5</sup>, larger for the thiophen-derivatives and for the two-arms compounds).



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## Highlights

- Synthesis and spectral behaviour in many solvents of different polarity of six mono- and two-branched nitro-derivatives bearing pyridine, furan or thiophene rings.
- Strong fluorsolvatochromism in agreement with substantial photoinduced intramolecular charge transfer, from the heteroaromatics to the nitro groups, undisclosed by quantum mechanical DFT calculations.
- High hyperpolarizability coefficient  $\beta_{CT}$  estimated through a solvatochromic method.
- The new Acceptor- $\pi$ -Core  $\pi$ -Acceptor structural motif of interest for new efficient NLO materials.

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