The synthesis and light absorbing properties of heptamethine cyanine chromophores based on benzoxazole derivatives.

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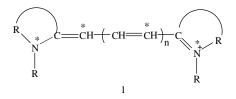
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Abstract

A novel near infrared (NIR) absorbing dyes were synthesized by using bis-aldehyde formyl aromatic compounds and heteroaryl derivatives with the reactive methylene group. These dyes provided a range of the NIR wavelength region about 720 nm value. Also, the light absorbing properties of these dyes were investigated in our experiment results. In generally, these NIR colorants may be potential used for optical recording media, DNA sequencing probe and laser beam printings.

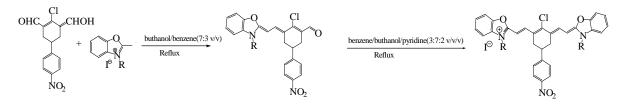
1. Introduction

Polymethine cyanine dyes have the general structure 1 and absorb in a wide range of wavelengths, from 340 to 1400nm. In structure 1, R denotes the heteroaromatic residue, and λ_{max} is affected strongly by the electronic characteristics of R. the length of an ethylene unit in the conjugating bridge also strongly affects λ_{max} , and near-infrared absorption generally can be attained for n>3.



2. Experiment and Discussion

General procedure for the synthesis of heptamethinecyanines : benzoxazole



The reaction of 1-chloro-2-hydromethylene-4-(4-mitro)phenyl-5-formyl cyclohexene and 1,1,2-benzoxazole iodine salts in a mixture of 1-butanol and benzene (7:3) was heated under reflux. During the reaction water was removed azotropically using a Dean-Stark condenser. The reaction was reflux $3 \sim 4$ hrs and completed with an intense green color material. The solvent was removed at reduced pressure, the resulting residue redissolved in methanol and precipitated with ether. The product was separated by filtration, washed with water and diethyl ether. Finally the cyanine dye was dried in an air and obtained green color material.

R	λ_{max}/nm (in CH ₂ Cl ₂)	λ _{max} /nm (in CHCl ₃)	λ _{max} /nm (in HCON(CH ₃) ₂)	λ _{max} /nm (in CH ₃ OH)
CH ₃	726	722	723	712
C ₂ H ₅	724	720	723	712
C ₃ H ₇	723	722	727	715
C ₄ H ₉	722	722	727	716
C ₆ H ₁₃	727	721	728	714
C ₈ H ₁₇	725	720	728	716

3. Conclusion

Our experiments were investigated NIR absorbing dyes with a absorption $maxima(\lambda_{max})$ about 712~728nm. The cyanine chromophores were shown some change in the spectrum with a various organic solvents. As mentioned before the cyanine dyes have found uses as functional dyes, e.q. near-infrared absorbs, lager light filter and bio-probe labels.

4. Reference

- 1. Fabian J., Nakazumi H and Matsuoka M., Chem Rev 92, pp 1197~1226(1992).
- 2. Mitsuitotsu Chemicals Co. Ltd, Japan Kokai 57-11090.
- 3. Williams, R. J., Lipowska, M., Patonay, G.; Strekowski, L. Anal, Chem. 65, 601(1993).
- 4. Ernst, L. A.; Gupta, R. K.; Mujumdar, S. R.; Waggoner, A. S. Cytometry 10: 3(1989).
- 5. Matsuoka M, editor. Infrared absorption dyes. New York Plenum Press 1990.

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