TITLE: The Optimization of Pentamethine Carbocyanine Dyes By Means of Microwave Assisted Organic Synthesis

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Introduction: Various pentamethine carbocyanine dyes were synthesized using microwave methodology. The synthesis outlined herein drastically reduced the reaction times of pentamethine carbocyanine dye syntheses from hours to minutes, as well as producing increased or comparable yields (33-98 %) to the conventional heating method. Each cyanine dye was optimized by varying temperature and keeping reaction time constant at 20 minutes. The desired products were verified by ¹H NMR (Bruker Avance, 400 MHz) and melting point, and show comparable purity to the conventional method.

Method: The synthesis of pentamethine cyanine dyes was carried out by reacting corresponding indolenine salt with chosen alkyl halide under neat conditions in a closed vessel microwave (CEM Discover LabMate).

Two equivalents of various indolinium salts were reacted with β-substituted malonaldehydebis(phenylimine)monohydrochloride, in the presence of sodium acetate and acetic anhydride as a catalyst, reactions went to completion after 15-20 minutes.

Results: Microwave assisted organic synthesis (MAOS) of the chosen pentamethine cyanine dyes has shown to drastically reduce reaction times compared to the conventional oil bath method.

Conclusion: The synthesis of various substituted pentamethine carbocyanine dyes was completed using microwave irradiation. Optimal reaction conditions were found at a constant reaction time of 20 minutes for all dyes. Both reaction times and yields were improved significantly using MAOS, which was paired with reasonable purity shown by ¹H NMR (Bruker Avance, 400 MHz) spectra.