

Title.

"Accelerated photobleaching of a cyanine dye in the presence of a ternary target DNA, PNA probe, dye catalytic complex; a novel molecular diagnostic"

Authors.

M. Wang¹, R. Holmes-Davis¹, Z. Rafinski², B. Jedrzejewska², K. Y. Choi⁴, M. Zwick⁴, C. Bupp⁴, A. Izmailov³, J. Paczkowski², B. Warner¹, H. Koshinsky^{1*}

Affiliations

1. Investigen Inc., Hercules, CA
2. Faculty of Chemical Technology & Engineering, University of Technology and Life Sciences, Bydgoszcz, Poland
3. Advanced Scientific Consulting, Etobicoke, Ontario, Canada
4. Previously at Investigen

Corresponding Author*

510-964-9700, ceo@investigen.com

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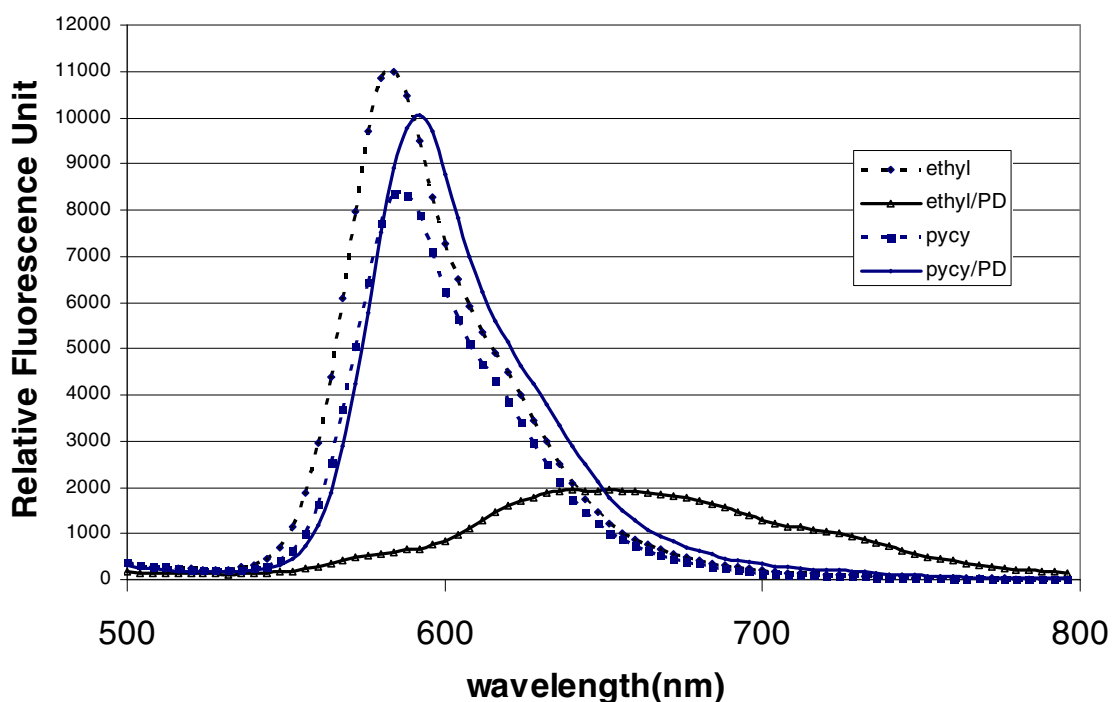
S4. ¹H NMR spectra of photodecomposition product # **I**.

S5. Effects of oxygen presence on the absorbance maxima of DiSC₂(3)

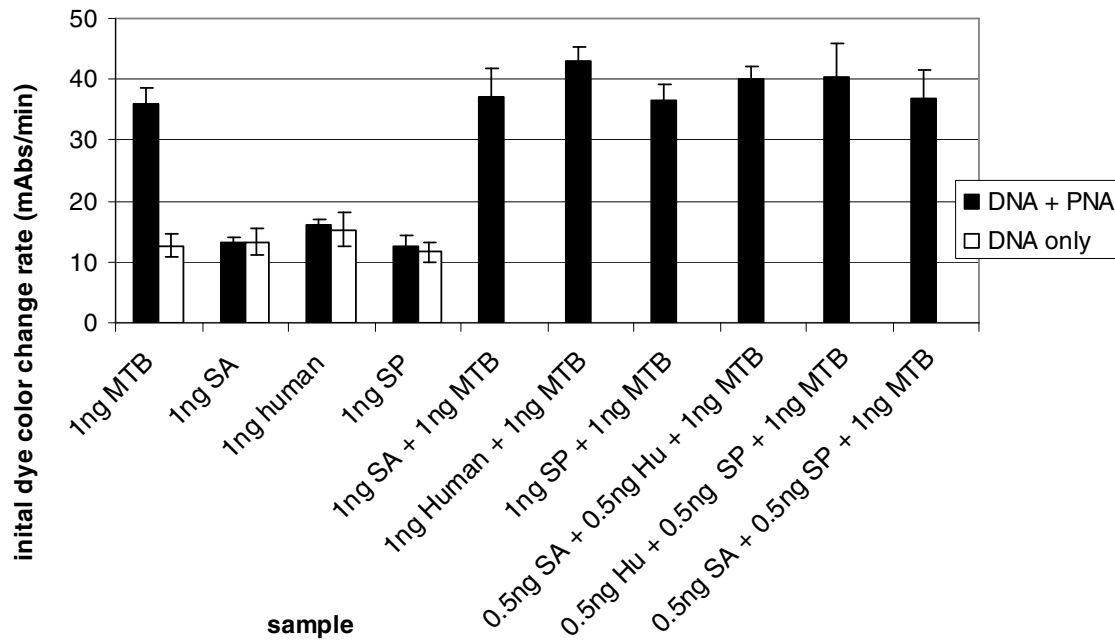
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		PNA sequence	DNA sequence
1	TB14(gel lane 1)	GTCGTCAGACCCAAAAC	GTTTTGGGTCTGACGAC
2	TB19(gel lane 2)	TGAACCGCCCCGGCATG	CATGCCGGGGCGGTTCA
3	TB15(gel lane 3)	ACCAAGTAGACGGGCGA	TCGCCCGTCTACTTGGT
4	TB20(gel lane 4)	CATCCAACCGTCGGTCCG	CGACCGACGGTTGGATG
5	TB23	GTTTTGGGTCTGACGAC	GTCGTCAGACCCAAAAC

S1. PNA names and sequences. All PNAs have a C-terminal carboxamide. The modification on the N-terminal is Lysine.

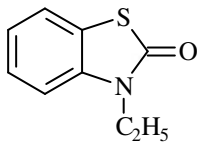


S2. Fluorescence emission spectra of 2.25 μM DiSC₂(3) or DiSC_{py}(3), alone or with 0.25 μM PNA-DNA duplex. PNA TB23 was used, the reactions were in 10mM Homopipes buffer, pH 5 and 470nm was the excitation wavelength.



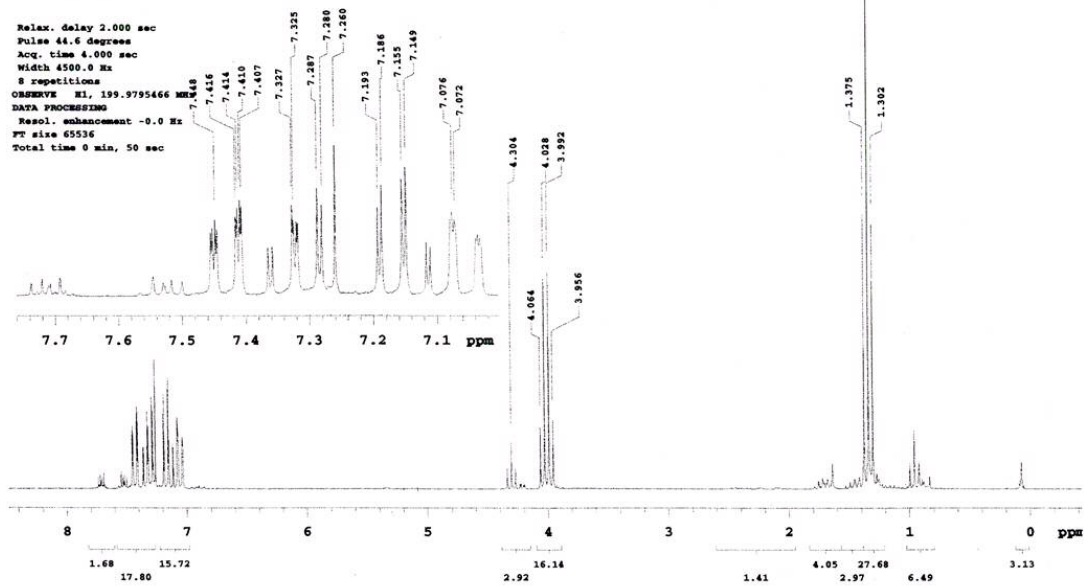
S3 Detection of MTB DNA in the presence of non-specific DNA. The initial (first 4 minutes) photobleaching rate of smartDNA reactions with *M. tuberculosis* (MTB) DNA alone, non-*M. tuberculosis* species DNA alone, and mixtures of DNA in the presence and absence of *M. tuberculosis* specific PNA probe, TB19. Reaction conditions are 10mM Homopipes buffer, pH5.0, with 0.05% Tween-80, the final concentration of PNA in the 50 μ l reaction is 160nM. SP is *Streptococcus pneumoniae* DNA. SA is *Staphylococcus aureus* DNA. Hu is Human DNA.

h5322
I
Z. Rafinski
2H

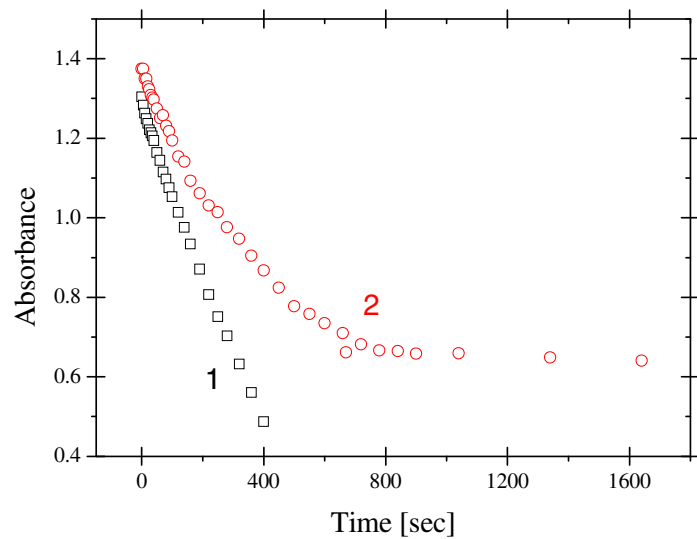


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Ambient temperature
File: h5322
GEMINI-200MHz "nmr"

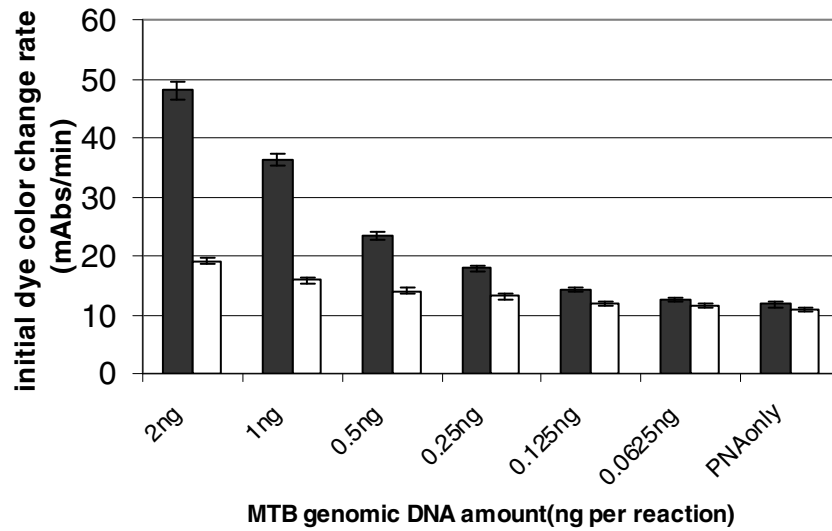
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S repetitions
OBSERVE M1 199.9795466 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
PT size 65536
Total time 0 min, 50 sec



S4. ¹H NMR spectra of photodecomposition product # I.



S5. Effects of oxygen presence on the absorbance maxima of $\text{DiSC}_2(3)$. The changes of the absorption intensity at λ_{max} during irradiation of $\text{DiSC}_2(3)$ in phosphate buffer solution in: **1** oxygen saturated solution and **2** in argon saturated solution. Time of argon bubbling was 100 minutes.



S6. Effects of sodium azide on a smartDNA assay. The final concentration of the PNA probe, TB01, is 80nM, and of DiSC₂(3) is 9μM, with 2 ng of *M. tuberculosis* (MTB) genomic DNA. The black bars are initial photobleaching rates in Homopipes buffer, pH 5.0, 10mM, and the white bars are the initial photobleaching rate in the presence of 0.1% sodium azide