Supporting information for:

Fluorescent hybridization probes for sensitive and selective DNA and RNA detection

Angel A. Martí, Steffen Jockusch, Nathan Stevens, Jingyue Ju, Nicholas J. Turro

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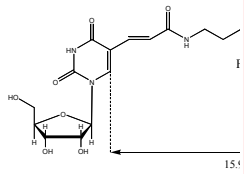

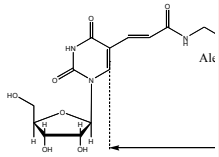

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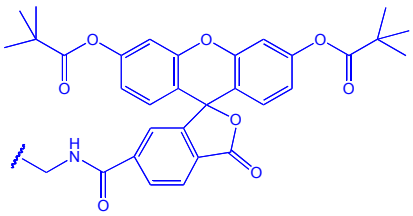
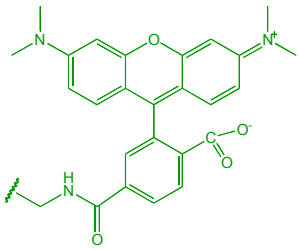
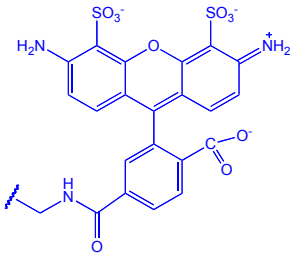


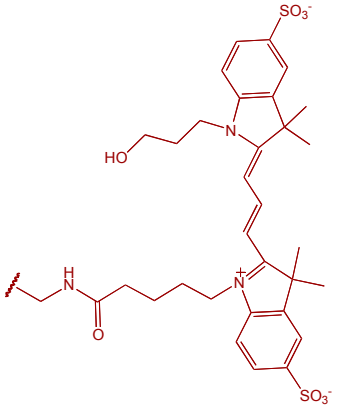
Fam



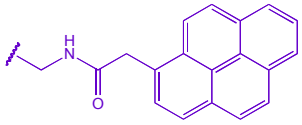
Tamra



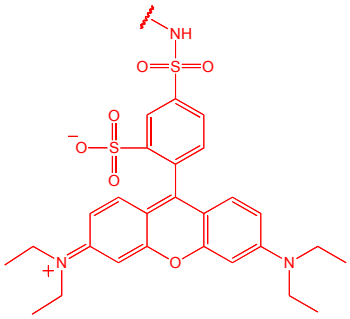
Alexa 488



Cy5



Pyrene



Red-X

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The distances between the dyes were estimated using the following assumptions:¶
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The RNA helix can be described as a cylinder with a radius of 13 Å, a height that increases 2.6 Å per base pair and a

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The distance from the base to the fluorophore is that of the fluorophore linker.¶
The distance from the edge of the cylinder to the fluorophore is the fluorophore linker minus the distance from linking position on the base to the edge of the cylinder (ca. 6.7 Å), which leaves an effective radius of 13 – 6.7 = 6.3 Å. This is because the cylinder is

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The linker length for Alexa488, Fam and Tam is taken as 15.9 Å while the linker length for Cy5 is 20.85 Å.¶
¶
Example: Calculation of the distance

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¶
The position of the fluorophore in the cylinder can be described by the angle between the dyes (33˚/base × 7 bases = 231˚), the vertical displacement which depends on the number of bases between the dyes (2.6 Å/base × 5 bases = 18.2 Å), and a representative radius equal to the effective RNA radius (6.3 Å) plus the length of the fluorophore's linker; Alexa488: 6.3 + 15.9 = 22.2 Å, Cy5: 6.3 + 20.85 = 27.2 Å (see figure below). ¶
¶
... [1]

from Cy5 to Alexa488 in BP-2d

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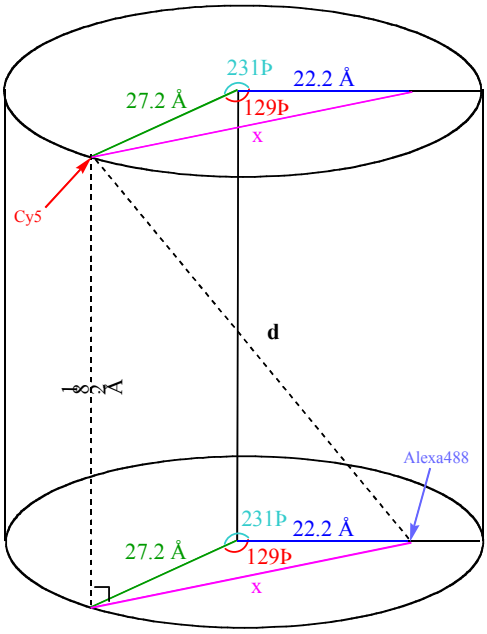

The cosine law can be used to determine the length of x.

$c^2 = a^2 + b^2 - 2ac \cos(c')$

where *c'* is the angle between a and b. Then:

$c^2 = 27.2^2 + 22.2^2 - (27.2)(22.2) \cos 129 = 44.6$ Å

Then, if x is 44.7 Å, using Pythagoras' theorem the value of d results:

$d^2 = 44.7^2 + 18.2^2 = 2323.2$; d = 48.2 Å