

Addition/Correction pubs.acs.org/JACS

Correction to "Synthetic, Functional Thymidine-Derived Polydeoxyribonucleotide Analogues from a Six-Membered Cyclic Phosphoester"

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J. Am. Chem. Soc. 2017, 139 (15), 5467-5473. DOI: 10.1021/jacs.7b01116

Supporting Information

There are mistakes in the stereochemical structures for (R)-5 and (S)-5 in the original manuscript in the Abstract graphic,

Chart 1. Original and Corrected Chemical Structures of (R)-5 and (S)-5



Scheme 1, Scheme 2, Figure 2, Figure 3, Table 2, and the Supporting Information (the chemical structures are shown here as original and corrected structures in Chart 1). These changes do not affect any of the conclusions. The corrected abstract graphic, figures, schemes, and tables are shown below. The corrected structures are provided in the revised Supporting Information. We apologize to the reader for any inconvenience.



Scheme 2. Polymerization of 5 with 4-Methoxybenzyl Alcohol as the Initiator and TBD as the Catalyst^a



^aAlthough the polymer is illustrated with only one regiochemistry and no stereochemistry, ³¹P NMR spectra suggested that the polymers contained regioisomeric and diastereoisomeric repeat units.





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Reaction coordinate

Figure 2. Reaction coordinate diagram of using DMAP as activator to promote cyclization of 6 at the B3LYP/6-31+G* level of theory.



Figure 3. Use of 1D-NOESY to identify the diastereomers (a) (S)-5 and (b) (R)-5, with atomic distances of 6.6 and 4.2 Å, respectively, calculated from DFT geometric optimization at the B3LYP/6-31+G* level of theory.

ASSOCIATED CONTENT

S Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/jacs.8b01661.

Experimental procedures, spectroscopic data for all new compounds including ¹H, ¹³C, and ³¹P NMR spectra, TGA, DSC, and details of computational chemistry (PDF)

ACKNOWLEDGMENTS

We thank Yelena Lipskerova of Chemical Abstracts Service for drawing our attention to the mistakes in the stereochemical assignments of the chemical structures.

Table 2. Condition Screening for Cyclization of 6 with 7 Using Various Solvents and Bases at -78 °C



^{*a*}The (R)/(S) ratio was determined by 31 P NMR of reaction crude.

