Supporting Information
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SUPPORTING INFORMATION

A Reliable Synthesis of 3-Amino-5-Alkyl and 5-Amino-3-Alkyl Isoxazoles

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Supporting information

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NMR study summary of phenyl (3-cyclobutylisoxazol-5-yl)carbamate (A) and phenyl (5-cyclobutylisoxazol-3-yl)carbamate (B).

| NMR Instrument: 600 MHz | Solvent: DMSO-d$_6$ |

Result Summary

A series of NMR experiments were run on both compounds in DMSO-d$_6$ solution on a 600 MHz Bruker Avance II instrument equipped with a TCI CryoProbe at 300 K. For phenyl (3-cyclobutylisoxazol-5-yl)carbamate (A), experiments including 1D $^1$H, $^{13}$C, $^{13}$C-DEPT, 2D $^1$H-$^1$H COSY, $^1$H-$^1$H ROESY, $^1$H-$^{13}$C HSQC & HMBC and $^1$H-$^{15}$N HMBC were collected; and phenyl (5-cyclobutylisoxazol-3-yl)carbamate (B), only 1D $^1$H, 2D $^1$H-$^1$H ROESY, $^1$H-$^{13}$C HMBC and $^1$H-$^{15}$N HMBC experiments were measured (see below).

Proton assignments were achieved for both compounds, as shown in the annotated spectra of both phenyl (3-cyclobutylisoxazol-5-yl)carbamate (A) and phenyl (5-cyclobutylisoxazol-3-yl)carbamate (B). Carbon assignments were achieved via 2D HSQC and HMBC experiments.

Due to the nature of the structures of the two compounds, 2D $^1$H-$^{13}$C HMBC or 2D $^1$H-$^1$H ROESY were not able to distinguish them. These data were found to be consistent with both structures shown above. However, 2D $^1$H-$^{15}$N HMBC was able to distinguish the two compounds. For phenyl (3-
cyclobutylisoxazol-5-yl)carbamate (A), a correlation between H-6 to a nitrogen atom at 353.7 ppm was clearly observed, indicating that the there is an nitrogen atom within 2 or 3 bonds away from H-6, but the corresponding correlation peak was not observed for phenyl (5-cyclobutylisoxazol-3-yl)carbamate (B).