Table 1. Bond lengths (Å) for the conformers of **I**

| Bond | Conformer | | | | | | Mean value |
|---|---|---|---|---|---|---|---|
| | 1R, 1S | 2R, 2S | 3R, 3S | 4R, 4S | 5R, 5S | 6R, 6S | |
| C2 - S | 1.67 | 1.67 | 1.67 | 1.67 | 1.67 | 1.67 | 1.67 |
| O1 - C5' | 1.22 | 1.21 | 1.21 | 1.22 | 1.22 | 1.21 | 1.21 |
| O2 - C5' | 1.36 | 1.36 | 1.36 | 1.36 | 1.36 | 1.36 | 1.36 |
| N1 - C2 | 1.38 | 1.38 | 1.38 | 1.38 | 1.38 | 1.38 | 1.38 |
| C2 - N3 | 1.34 | 1.34 | 1.34 | 1.34 | 1.34 | 1.34 | 1.34 |
| N3 - C4 | 1.47 | 1.47 | 1.47 | 1.47 | 1.47 | 1.47 | 1.47 |
| C4 - C5 | 1.52 | 1.52 | 1.52 | 1.52 | 1.52 | 1.52 | 1.52 |
| C5 - C6 | 1.36 | 1.36 | 1.36 | 1.36 | 1.36 | 1.36 | 1.36 |
| C6 - N1 | 1.39 | 1.39 | 1.39 | 1.39 | 1.39 | 1.39 | 1.39 |
| C4 - C4' | 1.54 | 1.54 | 1.54 | 1.54 | 1.54 | 1.54 | 1.54 |
| C5 - C5' | 1.47 | 1.47 | 1.47 | 1.47 | 1.47 | 1.47 | 1.47 |
| C6 - C6' | 1.50 | 1.50 | 1.50 | 1.50 | 1.50 | 1.50 | 1.50 |
| O2 - C7 | 1.45 | 1.45 | 1.45 | 1.45 | 1.45 | 1.45 | 1.45 |
| C7 - C8 | 1.52 | 1.52 | 1.52 | 1.52 | 1.52 | 1.52 | 1.52 |
| N1 - H1 | 1.01 | 1.01 | 1.01 | 1.01 | 1.01 | 1.01 | 1.01 |
| N3 - H3 | 1.01 | 1.01 | 1.01 | 1.01 | 1.01 | 1.01 | 1.01 |
| C4 - H4 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 |
| C4' - H41' | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 |
| C4' - H42' | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 |
| C4' - H43' | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 |
| C6' - H61' | 1.09 | 1.10 | 1.10 | 1.08 | 1.08 | 1.10 | 1.09 |
| C6' - H62' | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 |
| C6' - H63' | 1.08 | 1.08 | 1.08 | 1.09 | 1.09 | 1.08 | 1.09 |
| C7 - H71 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 |
| C7 - H72 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 |
| C8 - H81 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 |
| C8 - H82 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 |
| C8 - H83 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 |