Supplementary Material

A concise synthesis of isoguanine 2'-deoxyriboside and its adenine-like triplex formation when incorporated into DNA

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Table of Contents

Compound 2: $^1$H NMR (250.1 MHz, CDCl$_3$) S2
Compound 2: $^{13}$C NMR (62.9 MHz, CDCl$_3$) S2
Compounds 3 and 4: $^1$H NMR (250.1 MHz, CDCl$_3$) S3
Compound 5: $^1$H NMR (250.1 MHz, (CD$_3$)$_2$SO) S4
Compound 5: $^{13}$C NMR (62.9 MHz, (CD$_3$)$_2$SO) S4
Compound 6: $^1$H NMR (250.1 MHz, (CD$_3$)$_2$SO) S5
Compound 6: $^{13}$C NMR (62.9 MHz, (CD$_3$)$_2$SO) S5
Compound 7: $^1$H NMR (250.1 MHz, (CD$_3$)$_2$SO) S6
Compound 7: $^{13}$C NMR (62.9 MHz, (CD$_3$)$_2$SO) S6
Compound 8: $^1$H NMR (250.1 MHz, (CD$_3$)$_2$SO) S7
Compound 8: $^{13}$C NMR (62.9 MHz, (CD$_3$)$_2$SO) S7
Compound 9: $^1$H NMR (250.1 MHz, (CD$_3$)$_2$SO) S8
Compound 9: $^{13}$C NMR (62.9 MHz, (CD$_3$)$_2$SO) S8
Compound 11: $^1$H NMR (250.1 MHz, (CD$_3$)$_2$SO) S9
Compound 11: $^{13}$C NMR (62.9 MHz, (CD$_3$)$_2$SO) S9
Compound 13: $^1$H NMR (250.1 MHz, (CD$_3$)$_2$SO) S10
Compound 13: $^{13}$C NMR (62.9 MHz, (CD$_3$)$_2$SO) S10
Compound 14: $^1$H NMR (250.1 MHz, (CD$_3$)$_2$SO) S11
Compound 14: $^{13}$C NMR (62.9 MHz, (CD$_3$)$_2$SO) S11
Compound 14: $^{31}$P NMR (101.3 MHz, (CD$_3$)$_2$SO) S12
Compound 15: $^1$H NMR (250.1 MHz, (CD$_3$)$_2$SO) S13
Compound 15: $^{13}$C NMR (62.9 MHz, (CD$_3$)$_2$SO) S13
Compound 15: $^{31}$P NMR (101.3 MHz, (CD$_3$)$_2$SO) S14
Compound 2: $^1$H NMR (250.1 MHz, CDCl$_3$)

![NMR spectrum of Compound 2: $^1$H NMR (250.1 MHz, CDCl$_3$)](image)

Compound 2: $^{13}$C NMR (62.9 MHz, CDCl$_3$)

![NMR spectrum of Compound 2: $^{13}$C NMR (62.9 MHz, CDCl$_3$)](image)
Compounds 3 and 4: $^1\text{H}$ NMR (250.1 MHz, (CDCl$_3$))
Compound 5: $^1$H NMR (250.1 MHz, (CD$_3$)$_2$SO)

Compound 5: $^{13}$C NMR (62.9 MHz, (CD$_3$)$_2$SO)
Compound 6: $^1$H NMR (250.1 MHz, (CD$_3$)$_2$SO)

Compound 6: $^{13}$C NMR (62.9 MHz, (CD$_3$)$_2$SO)
Compound 7: $^1$H NMR (250.1 MHz, (CD$_3$)$_2$SO)

Compound 7: $^{13}$C NMR (62.9 MHz, (CD$_3$)$_2$SO)
Compound 8: $^1$H NMR (250.1 MHz, (CD$_3$)$_2$SO)

Compound 8: $^{13}$C NMR (62.9 MHz, (CD$_3$)$_2$SO)
Compound 9: $^1$H NMR (250.1 MHz, (CD$_3$)$_2$SO)

Compound 9: $^{13}$C NMR (62.9 MHz, (CD$_3$)$_2$SO)
Compound 11: $^1$H NMR (250.1 MHz, (CD$_3$)$_2$SO)

Compound 11: $^{13}$C NMR (62.9 MHz, (CD$_3$)$_2$SO)
Compound 13: $^1$H NMR (250.1 MHz, (CD$_3$)$_2$SO)

Compound 13: $^{13}$C NMR (62.9 MHz, (CD$_3$)$_2$SO)
Compound 14: $^1$H NMR (250.1 MHz, (CD$_3$)$_2$SO)

Compound 14: $^{13}$C NMR (62.9 MHz, (CD$_3$)$_2$SO)
Compound 14: $^{31}$P NMR (101.3 MHz, (CD$_3$)$_2$SO)
Compound 15: $^1$H NMR (250.1 MHz, (CD$_3$)$_2$SO)

Compound 15: $^{13}$C NMR (62.9 MHz, (CD$_3$)$_2$SO)
Compound 15: $^{31}$P NMR (101.3 MHz, (CD$_3$)$_2$SO)