Supplementary Information

8-Fluoro-*N*-2-isobutyryl-2'-deoxyguanosine: synthesis and stability

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electrospray detected for negative ions (2.6-2.8 min, background subtracted); d). high-resolution EI analysis on m/z 265.

Figure S30. ^{1}H NMR of products from the treatment of compound **4** with concentrated aqueous ammonium hydroxide at 55°C overnight. After the reaction mixture was cooled, it was lyophilized and purified by preparative C18-reverse phase column chromatography. The spectrum was recorded in DMSO-d_6 at 400.2 MHz.

Figure S31. COSY NMR of products from the treatment of compound **4** with concentrated aqueous ammonium hydroxide at 55°C overnight. After the reaction mixture was cooled, it was lyophilized and purified by preparative C18-reverse phase column chromatography. The spectrum was recorded in DMSO-d_6 at 400.2 MHz.

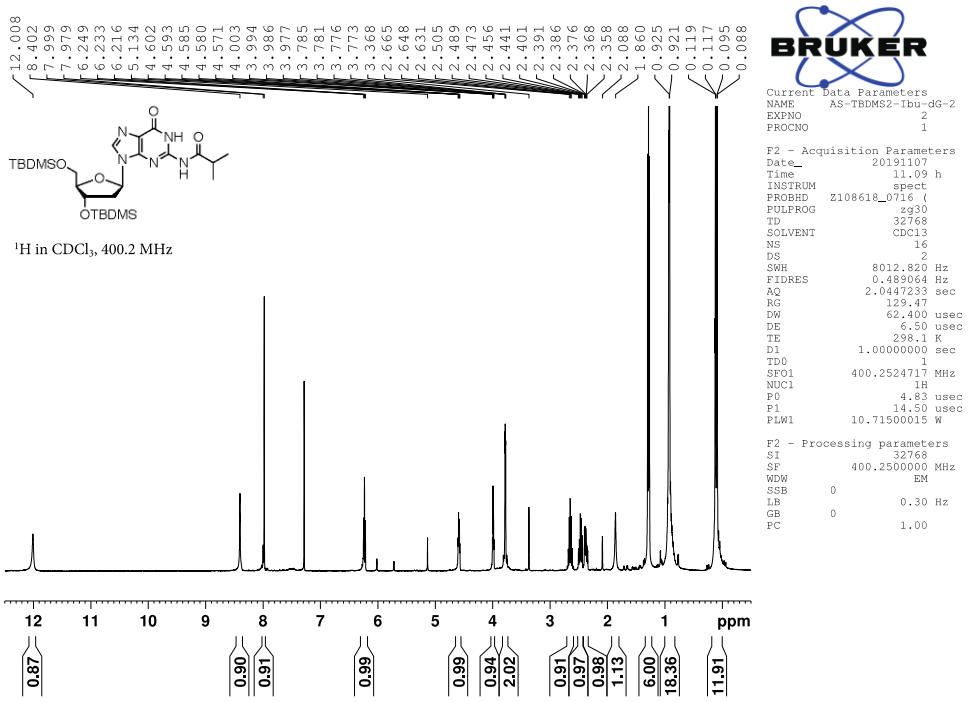


Figure S1. ^{1}H NMR of **6** in $CDCl_3$.

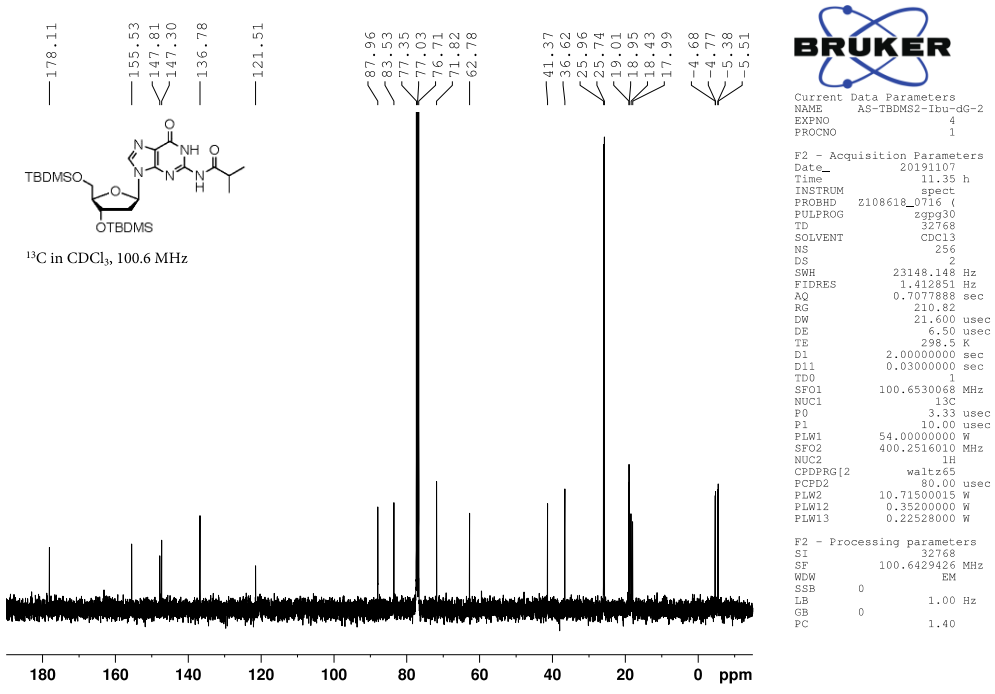


Figure S2. ^{13}C NMR of **6** in $CDCl_3$.

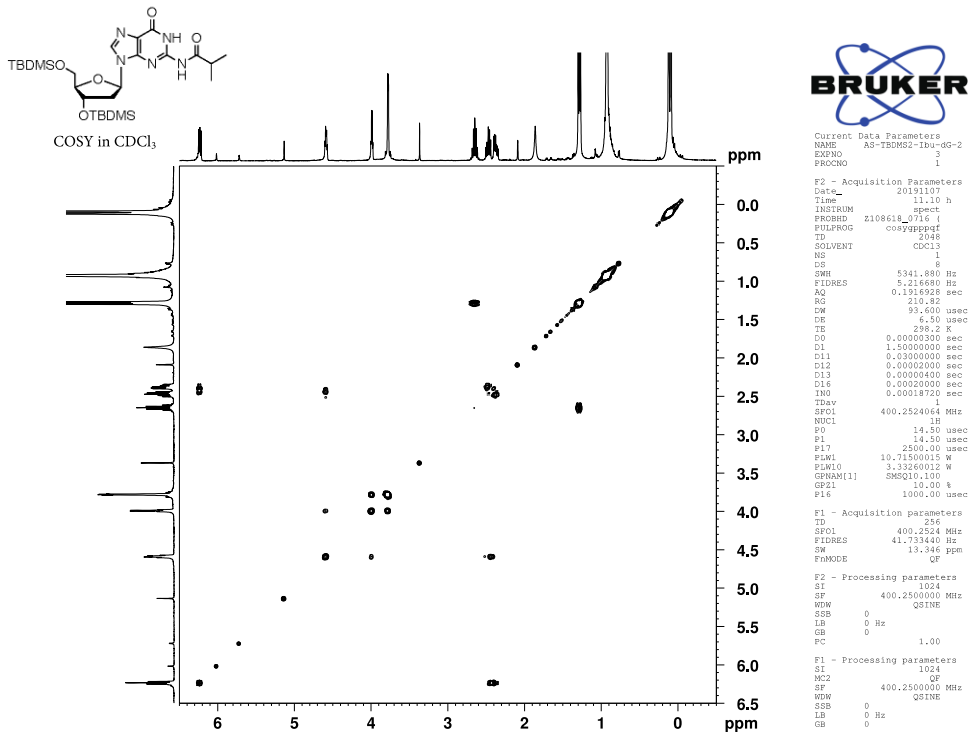


Figure S3. COSY NMR of **6** in $CDCl_3$.

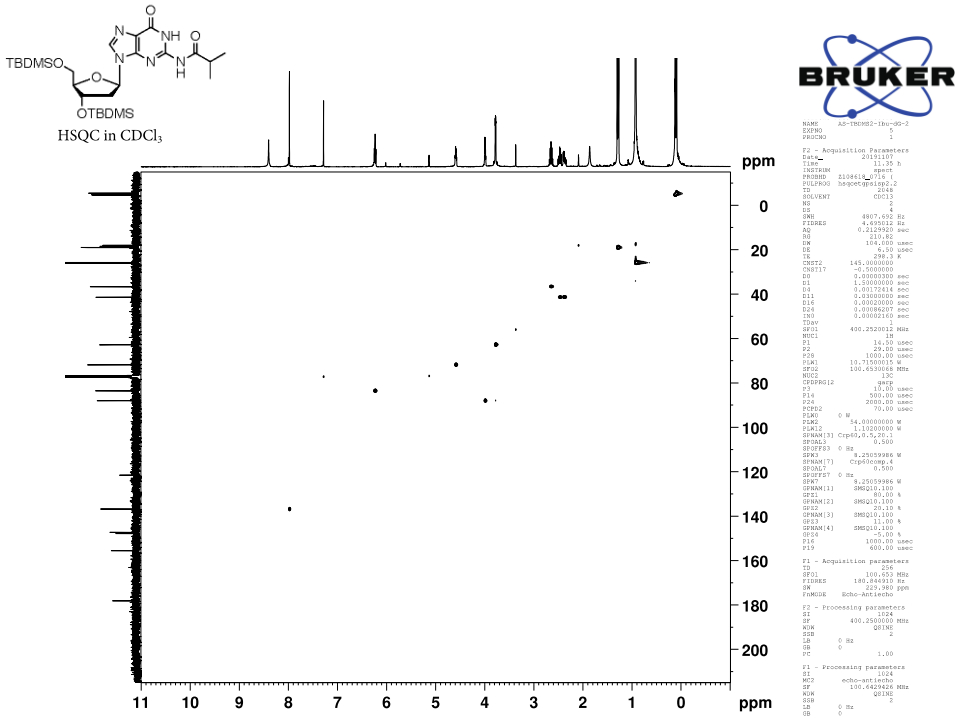


Figure S4. HSQC NMR of **6** in $CDCl_3$.

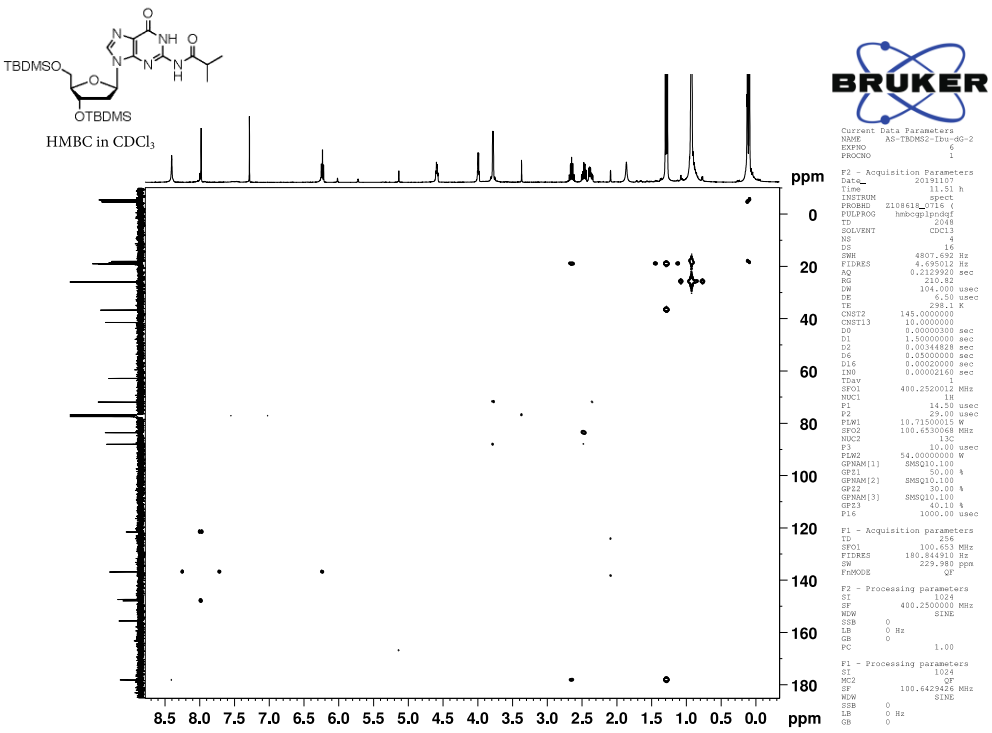


Figure S5. HMBC NMR of **6** in $CDCl_3$.

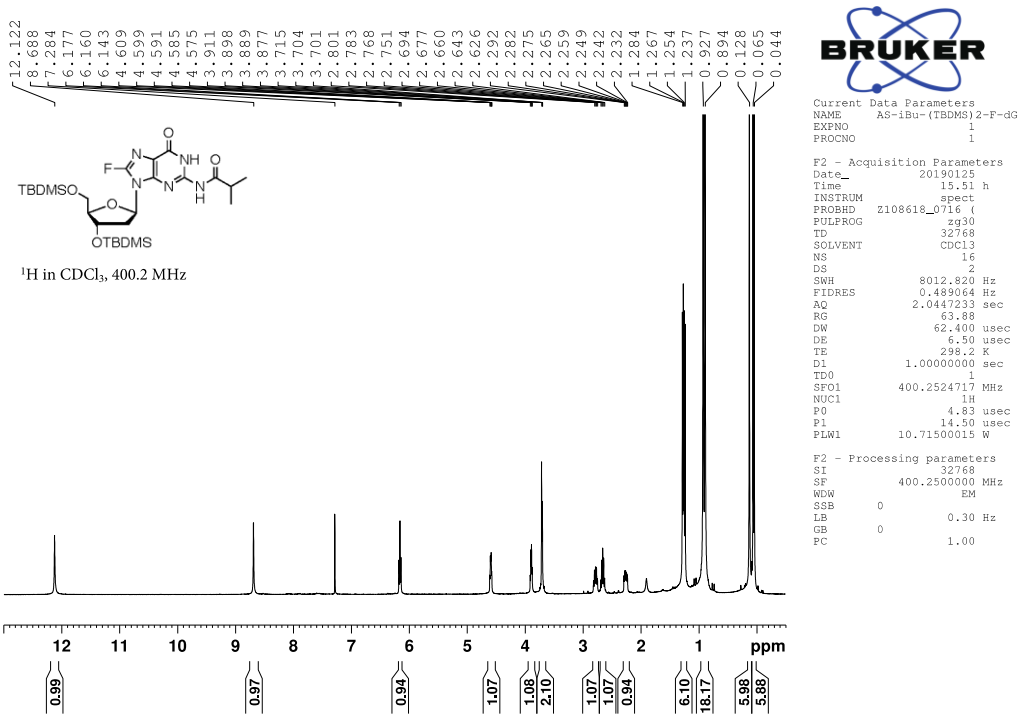
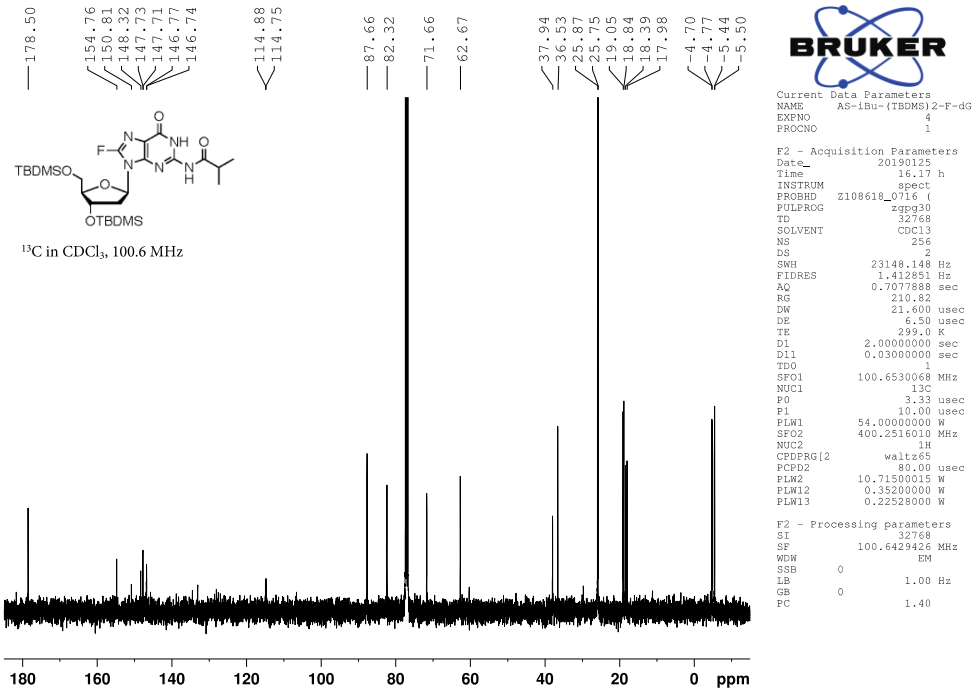


Figure S6. ^1H NMR of **7** in $CDCl_3$.



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PROCNO 1

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TE 299.0 K
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D11 0.03000000 sec
TD0 1
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NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 54.00000000 W
SFO2 400.2516010 MHz
NUC2 1H
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PCPD2 80.00 usec
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F2 - Processing parameters
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Figure S7. ^{13}C NMR of **7** in $CDCl_3$.

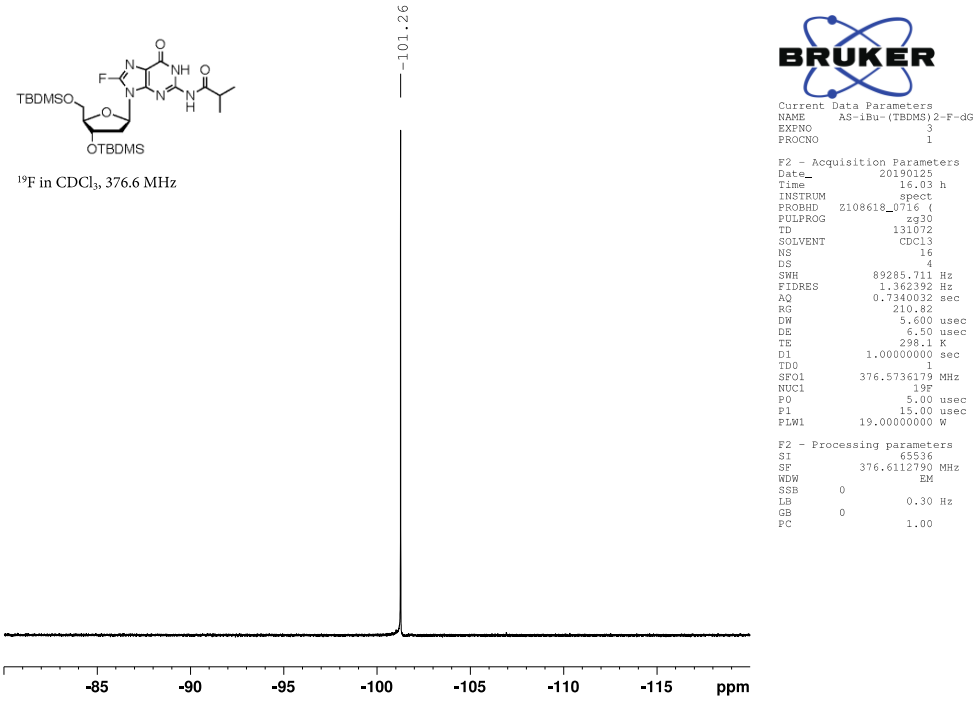

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Figure S8. ^{19}F NMR of **7** in $CDCl_3$.

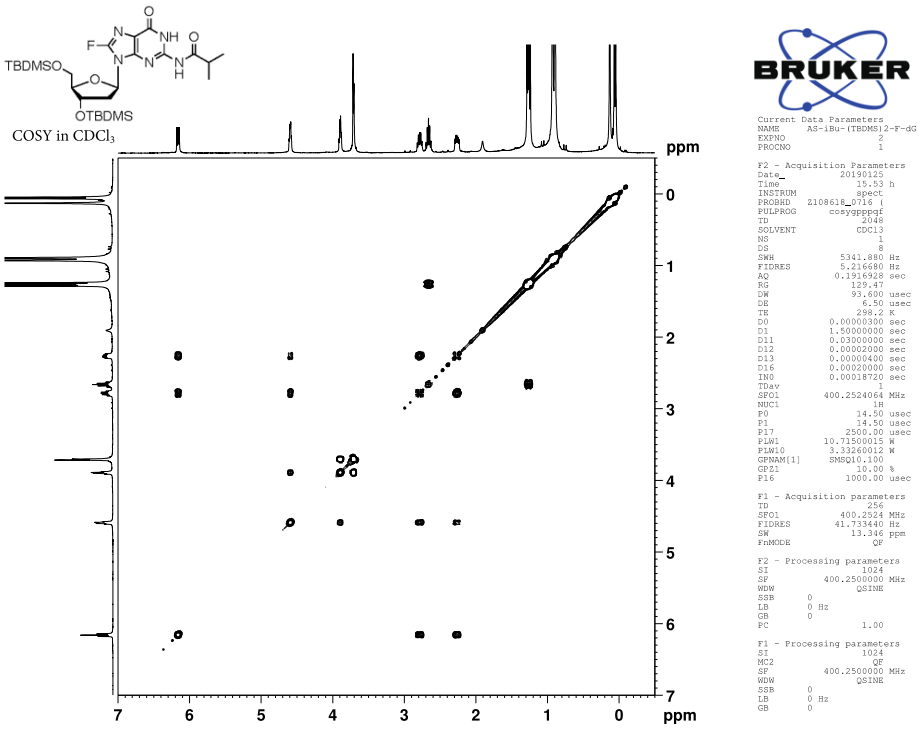


Figure S9. COSY NMR of **7** in $CDCl_3$.

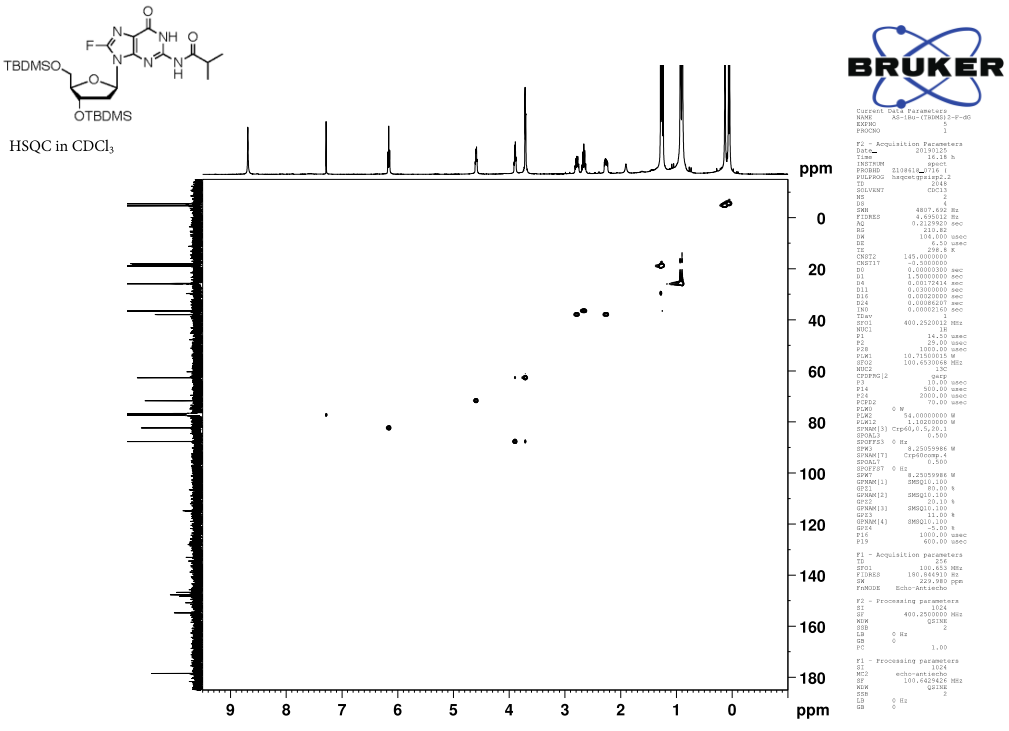


Figure S10. HSQC NMR of **7** in $CDCl_3$.

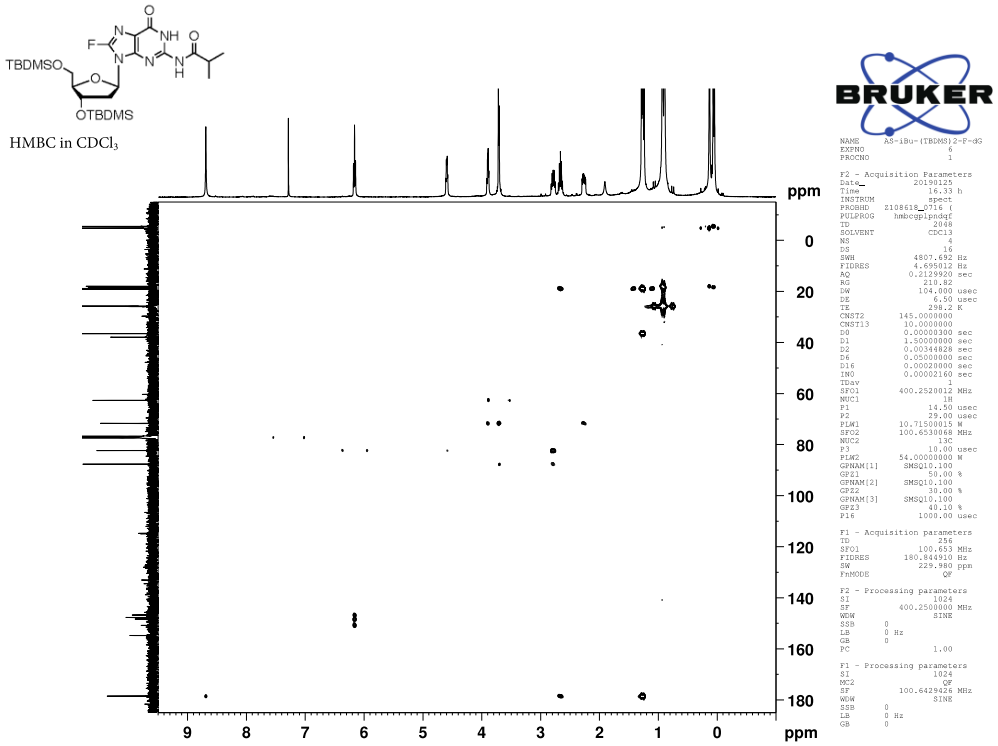


Figure S11. HMBC NMR of **7** in $CDCl_3$.

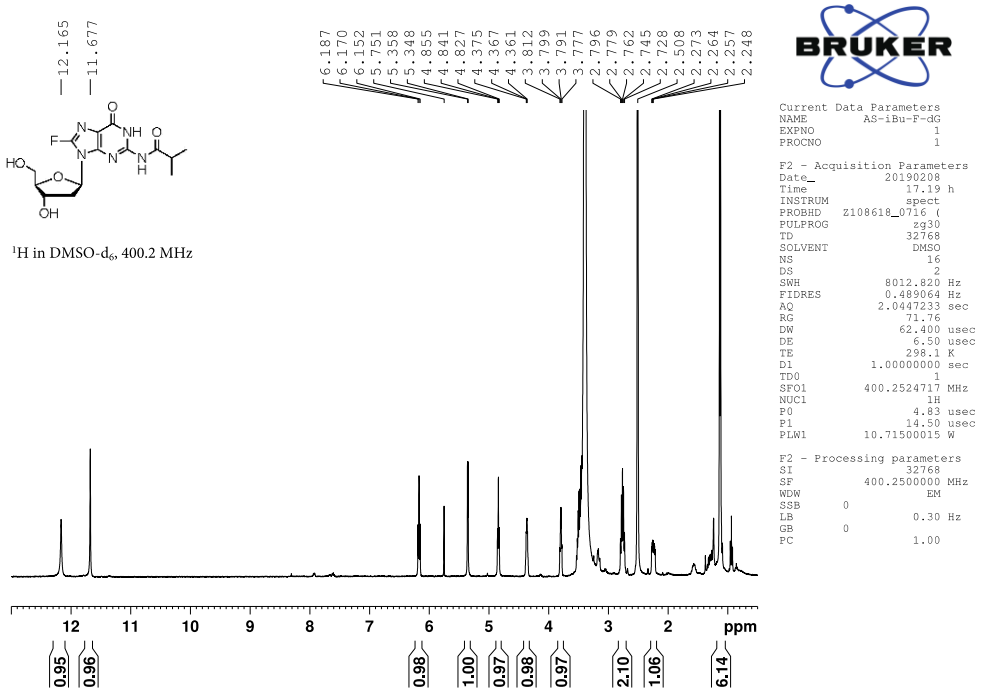


Figure S12. ^1H NMR of **4** in DMSO-d_6.

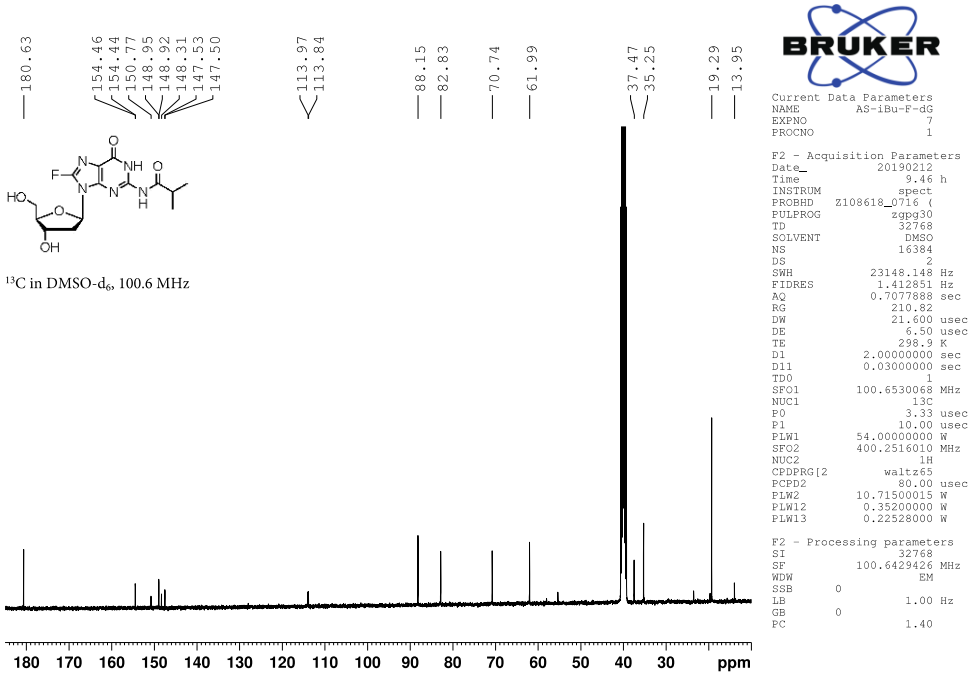


Figure S13. ^{13}C NMR of **4** in DMSO-d$_6$.

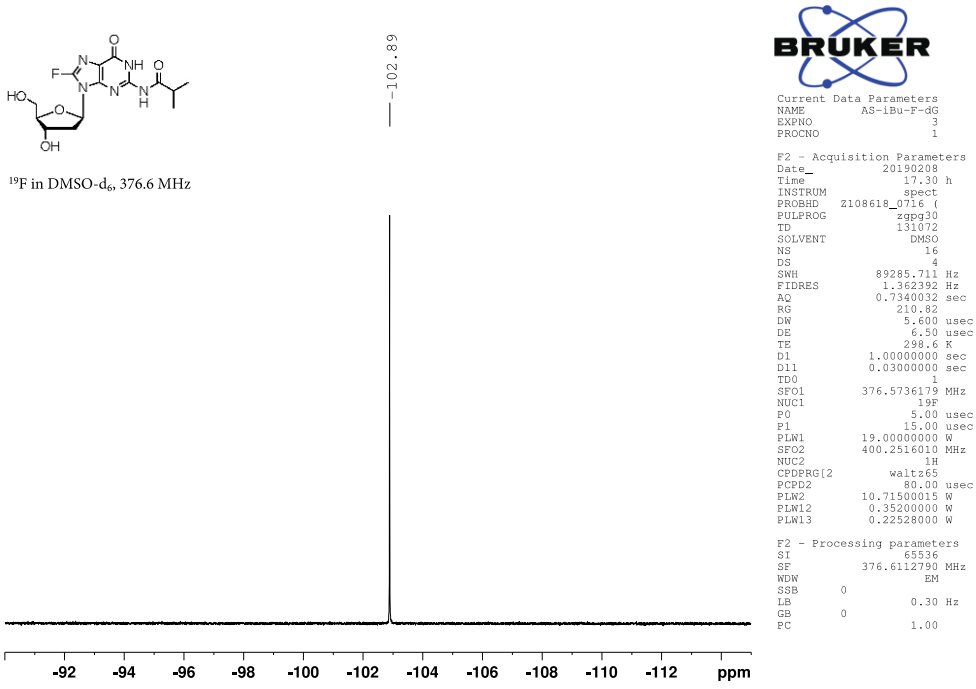


Figure S14. ^{19}F NMR of **4** in DMSO-d$_6$.

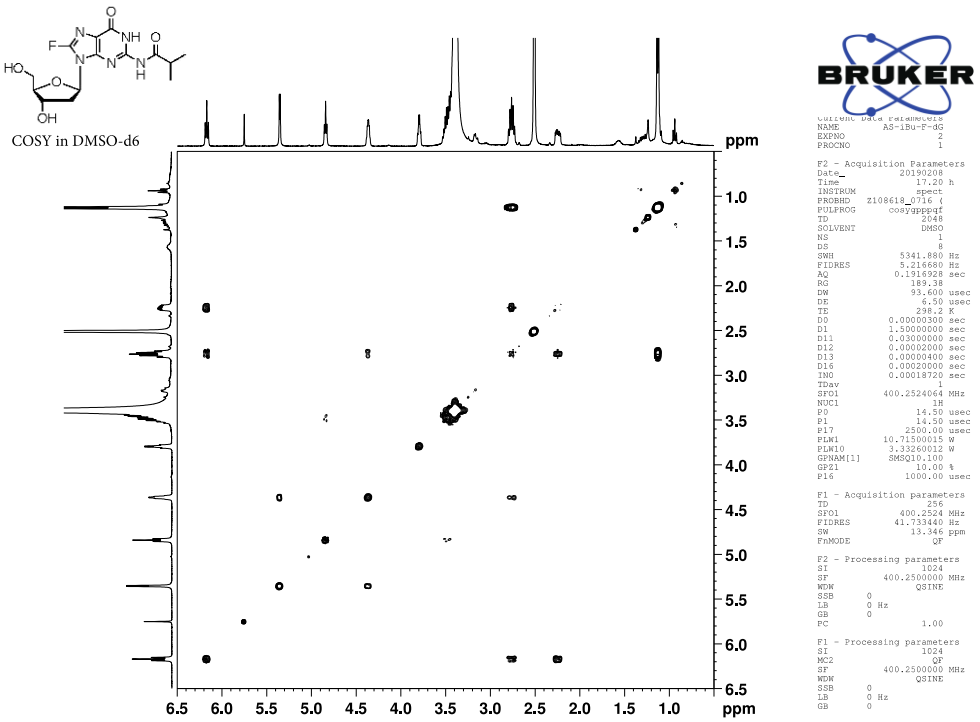


Figure S15. COSY NMR of **4** in DMSO-d$_6$.

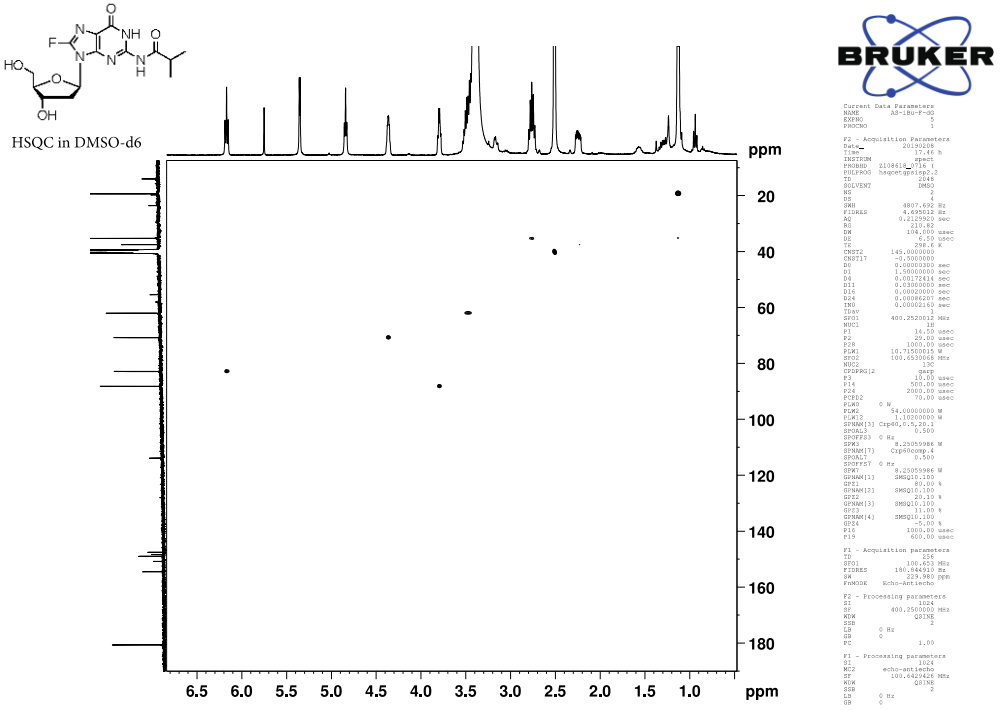


Figure S16. HSQC NMR of **4** in DMSO-d$_6$.

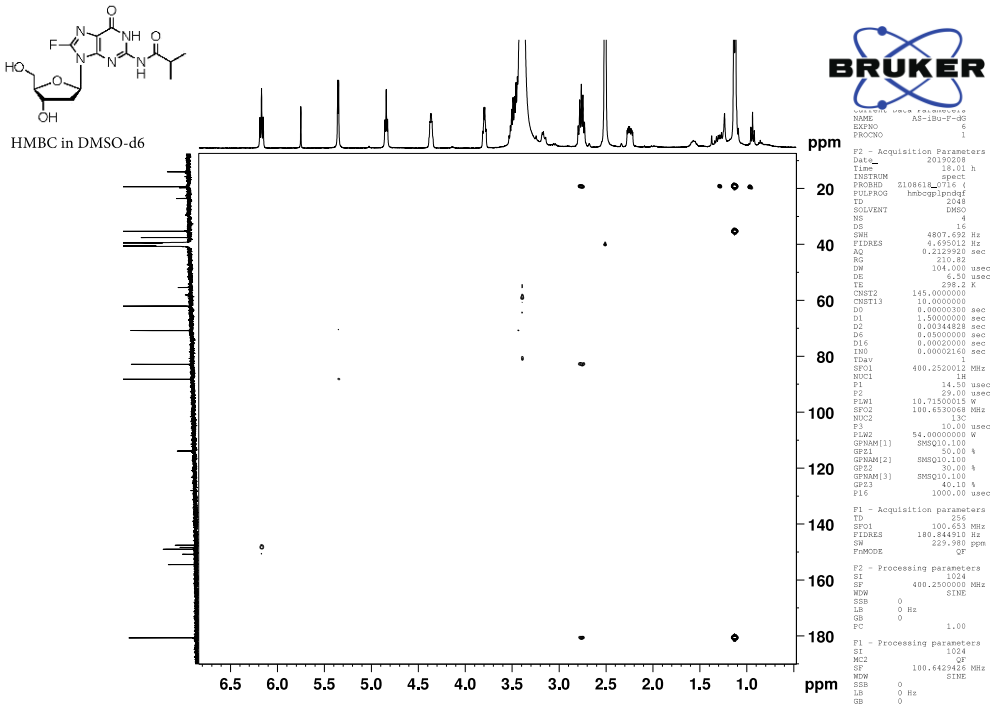


Figure S17. HMBC NMR of **4** in DMSO-d$_6$.

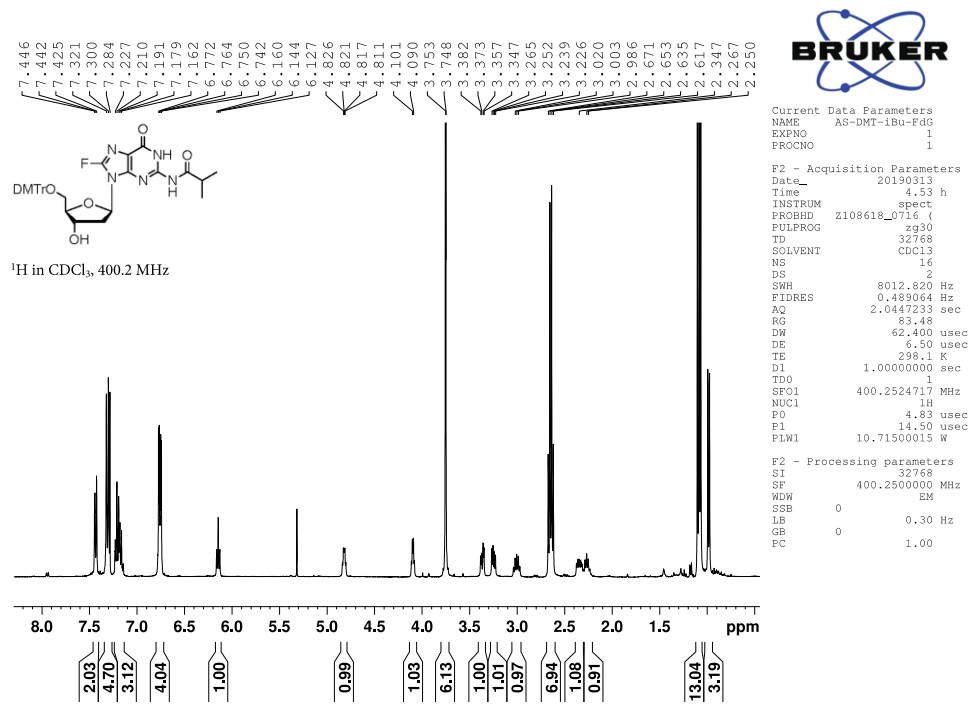


Figure S18. ^{1}H NMR of **10** in CDCl$_3$.

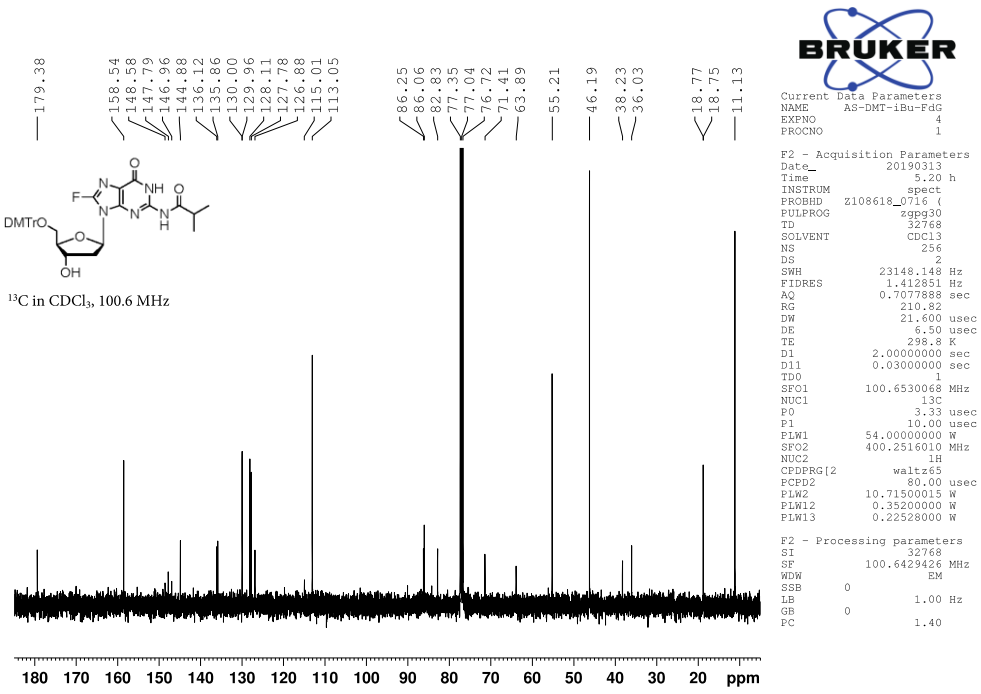


Figure S19. ^{13}C NMR of **10** in $CDCl_3$.

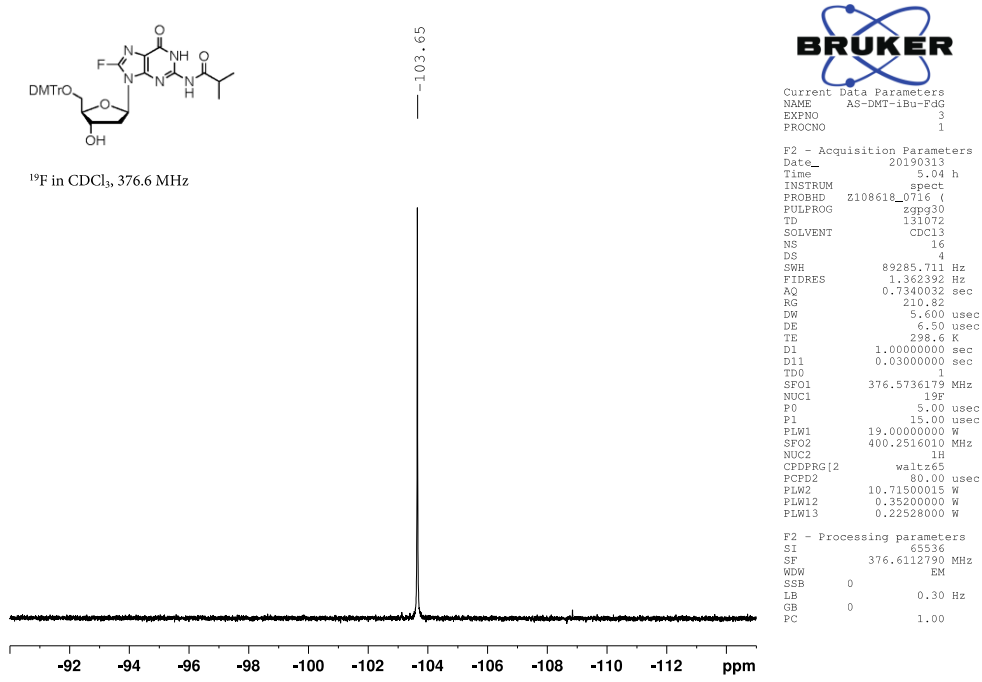


Figure S20. ^{19}F NMR of **10** in $CDCl_3$.

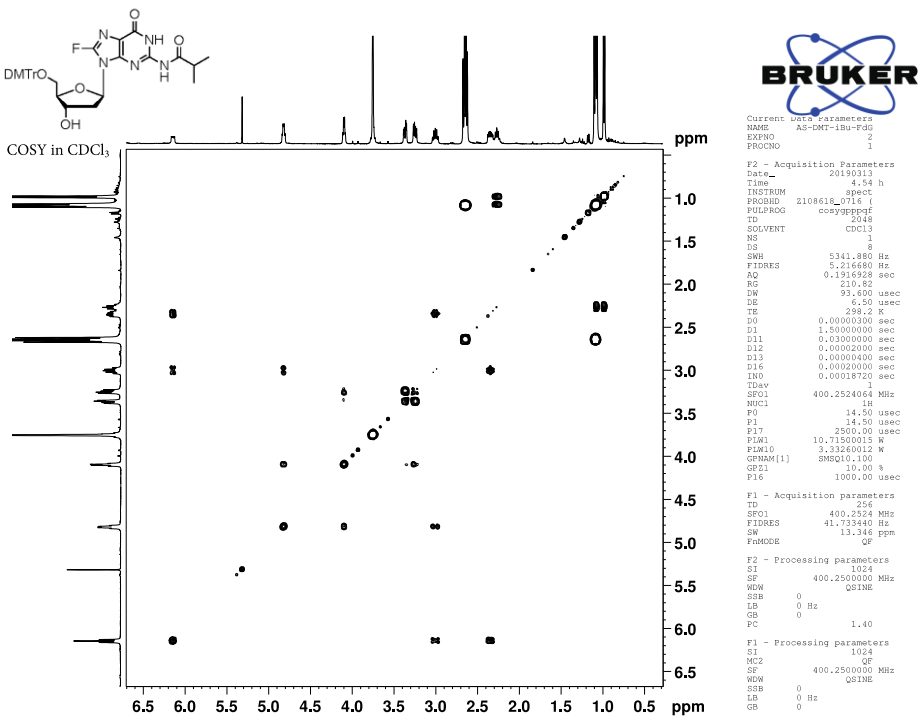


Figure S21. COSY NMR of **10** in $CDCl_3$.

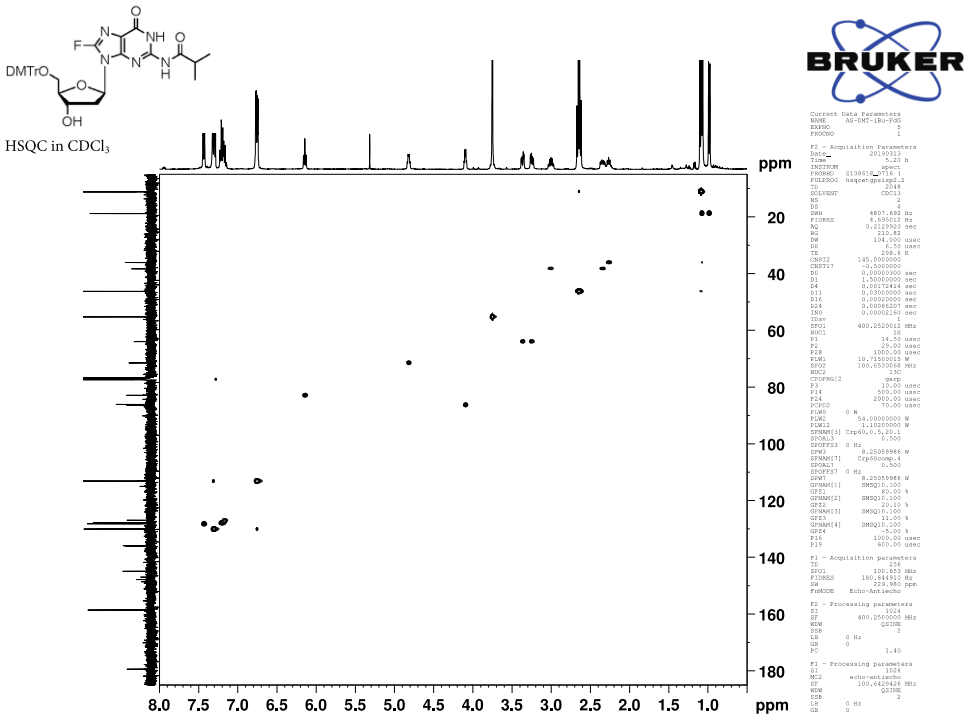


Figure S22. HSQC NMR of **10** in $CDCl_3$.

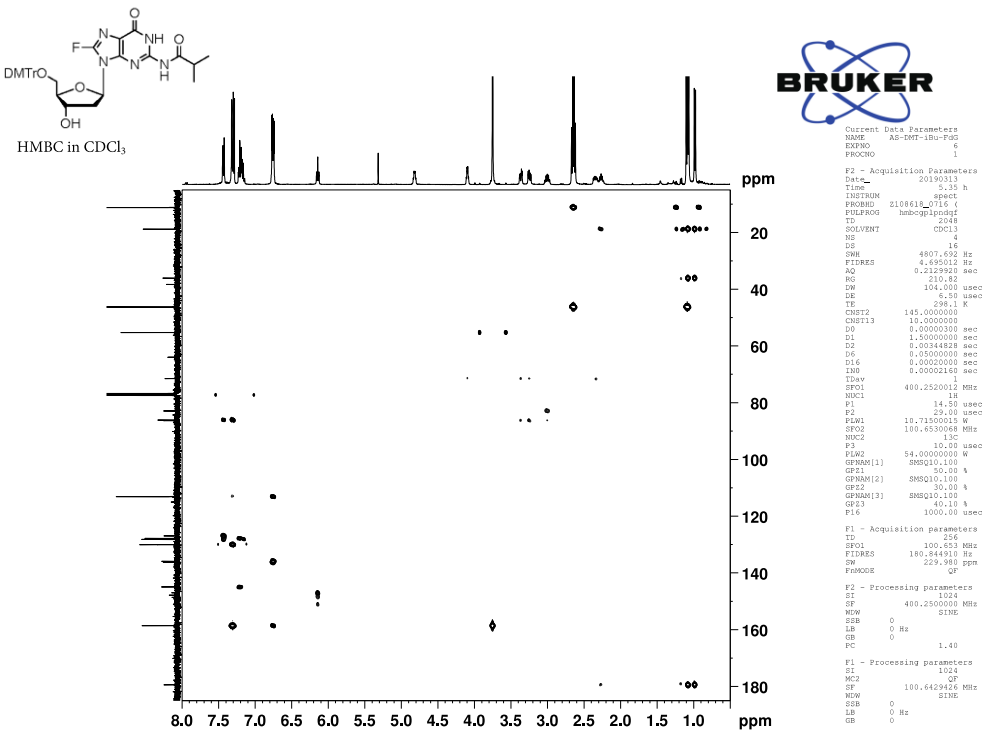


Figure 23. HSQC NMR of **10** in $CDCl_3$.

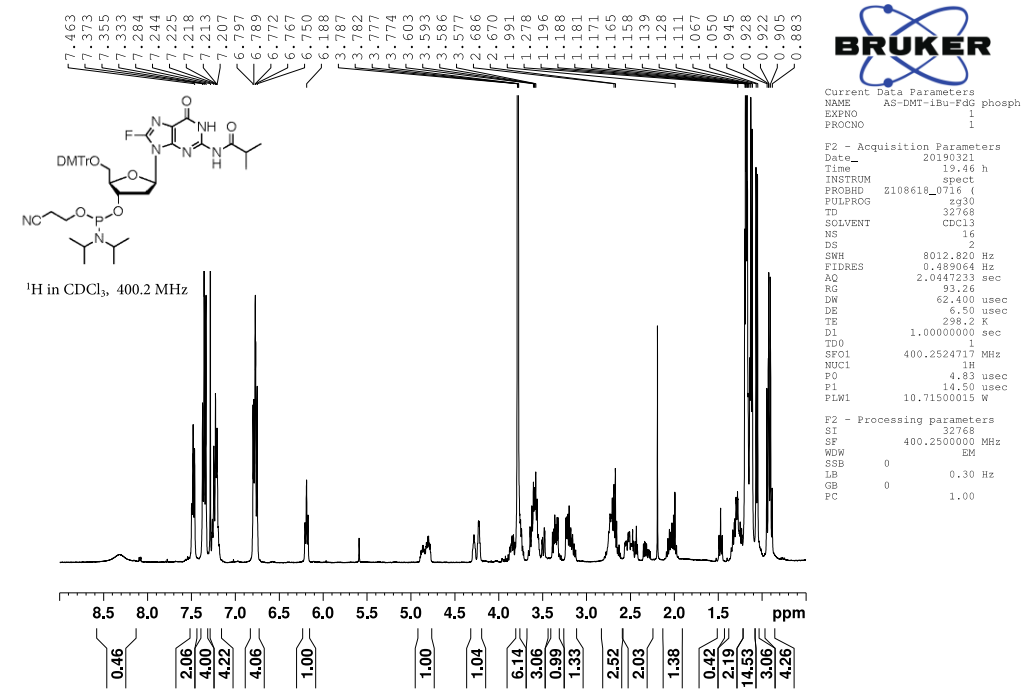
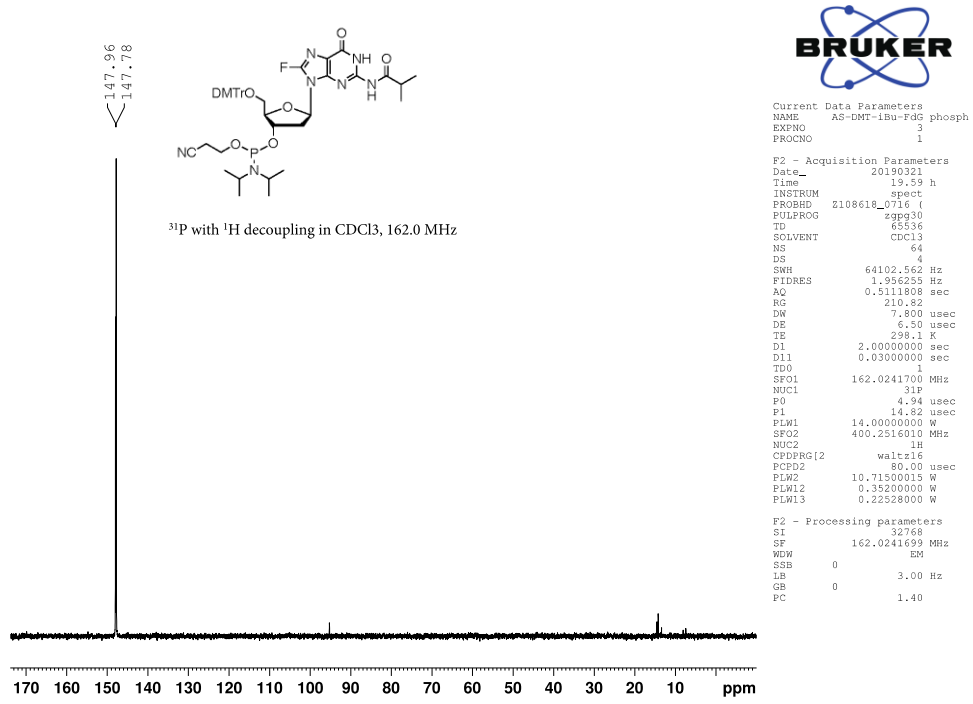


Figure S24. ^1H NMR of **11** in $CDCl_3$.



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D11 0.03000000 sec
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SFO1 162.0241700 MHz
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P0 4.94 usec
P1 14.82 usec
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SFO2 400.2516010 MHz
NUC2 1H
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F2 - Processing parameters
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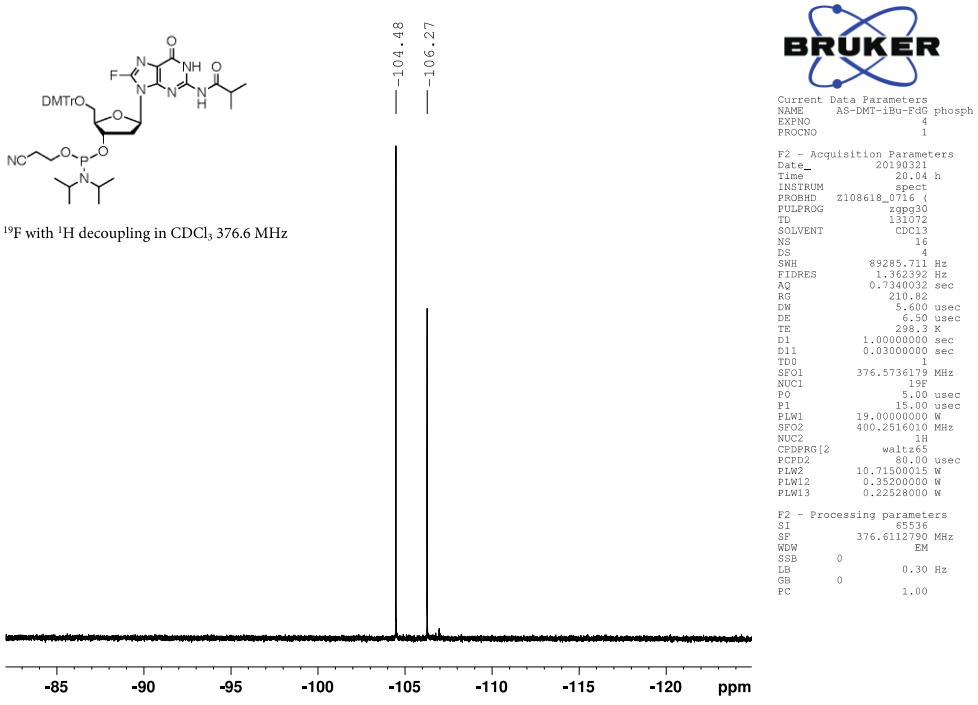
Figure S25. ^{31}P NMR of **10** in $CDCl_3$.



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FIDRES 1.362392 Hz
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DE 6.50 usec
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D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 376.5736179 MHz
NUC1 19F
P0 5.00 usec
P1 15.00 usec
PLW1 19.00000000 W
SFO2 400.2516010 MHz
NUC2 1H
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Figure S26. ^{19}F NMR of **10** in $CDCl_3$.

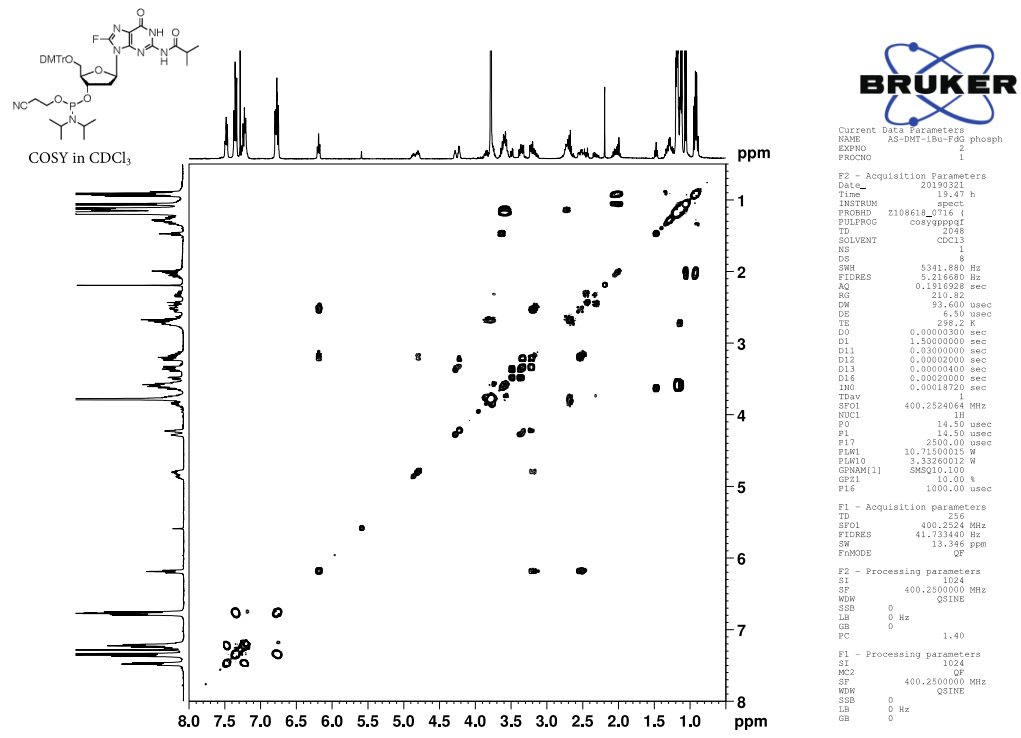

Figure S27. COSY NMR of **10** in $CDCl_3$.

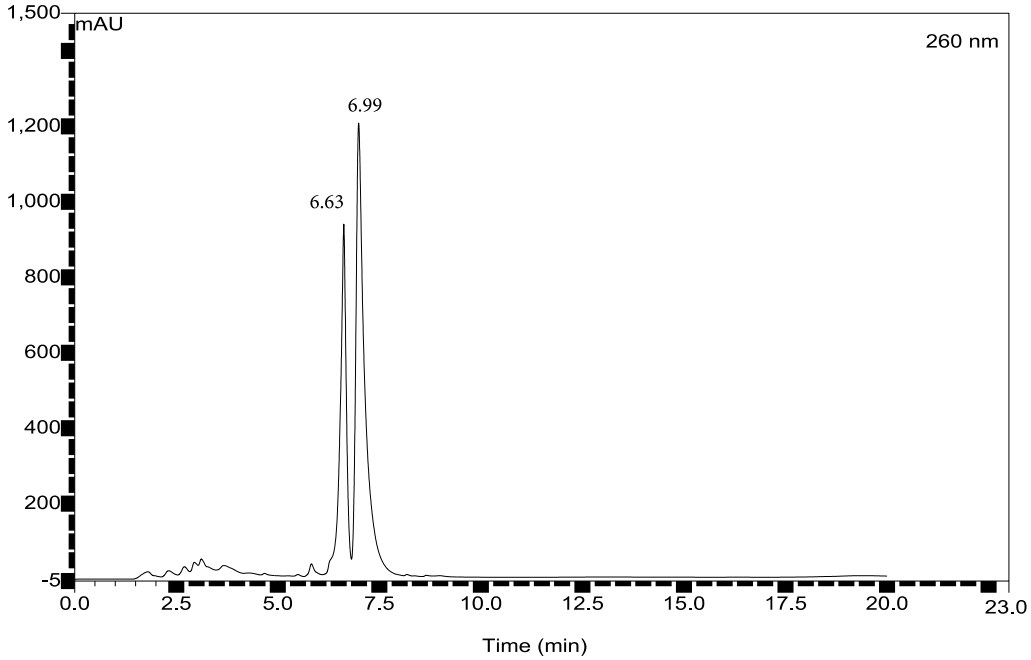

Figure S28. HPLC profile of the product where compound **4** was treated with concentrated aqueous ammonium hydroxide at 55°C overnight (as described in Scheme 3). The mixture was eluted off a Dionex Polar Advantage-2 C18 reverse phase column (4.6×150 mm) with a linear gradient of water–acetonitrile (100:0 to 60:40, v/v over 10 min) at 0.7 ml/min.

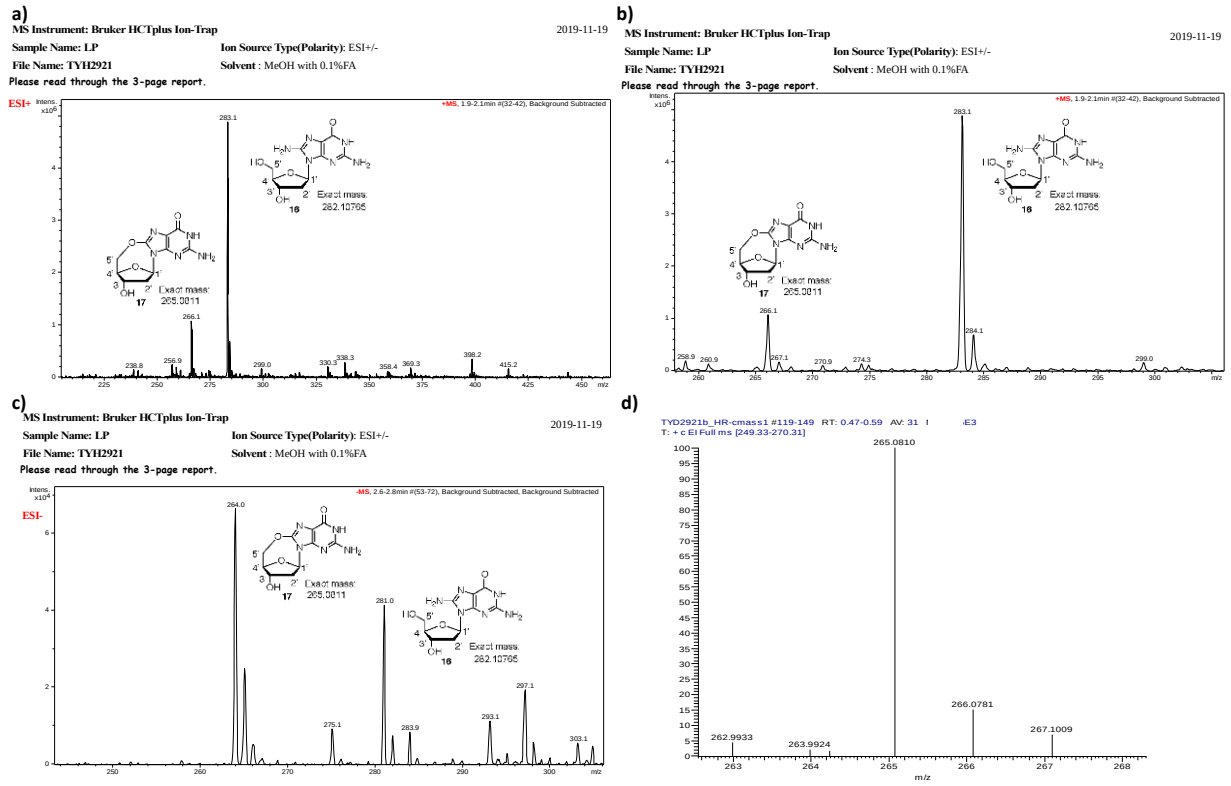

Figure S29. Mass spectra of products from the treatment of compound **4** with concentrated aqueous ammonium hydroxide at 55°C overnight. After the reaction mixture was cooled, it was lyophilized and purified by preparative C18-reverse phase column chromatography. a). Electrospray detected for positive ions (1.9-2.1min, background Subtracted); b). zoomed-in portion, electrospray detected for positive ions. (1.9-2.1min, background Subtracted); c). electrospray detected for negative ions (2.6-2.8 min, background Subtracted); d). high-res analysis on m/z 265.

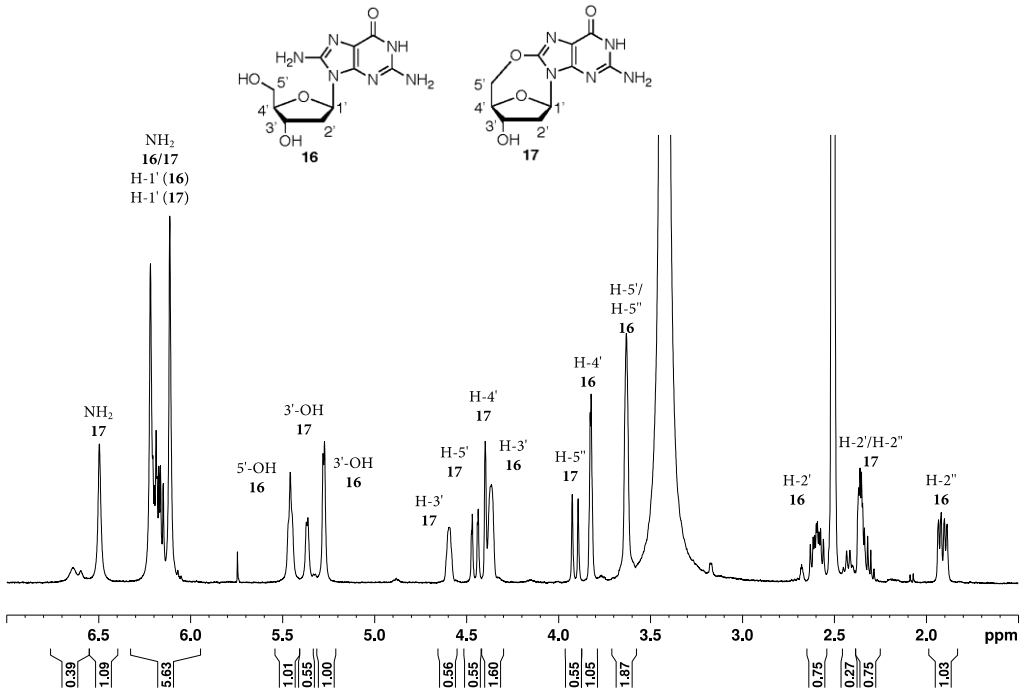

Figure S30. ^{1}H NMR of products from the treatment of compound **4** with concentrated aqueous ammonium hydroxide at 55°C overnight. After the reaction mixture was cooled, it was lyophilized and purified by preparative C18-reverse phase column chromatography. The spectrum was recorded in DMSO-d_6 at 400.2 MHz.

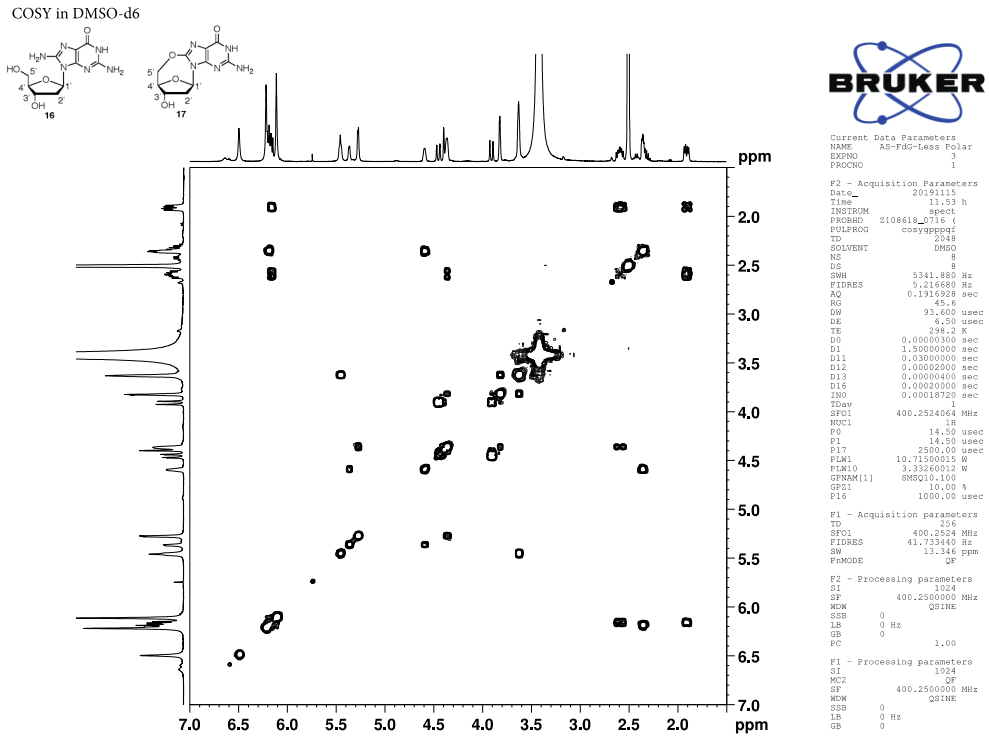

Figure S31. COSY NMR of products from the treatment of compound **4** with concentrated aqueous ammonium hydroxide at 55°C overnight. After the reaction mixture was cooled, it was lyophilized and purified by preparative C18-reverse phase column chromatography. The spectrum was recorded in DMSO-d_6 at 400.2 MHz.