

First characterisation of two important postulated intermediates in the formation of the HydT DNA lesion, a thymidine oxidation product.

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ELECTRONIC SUPPLAMENTARY INFORMATION

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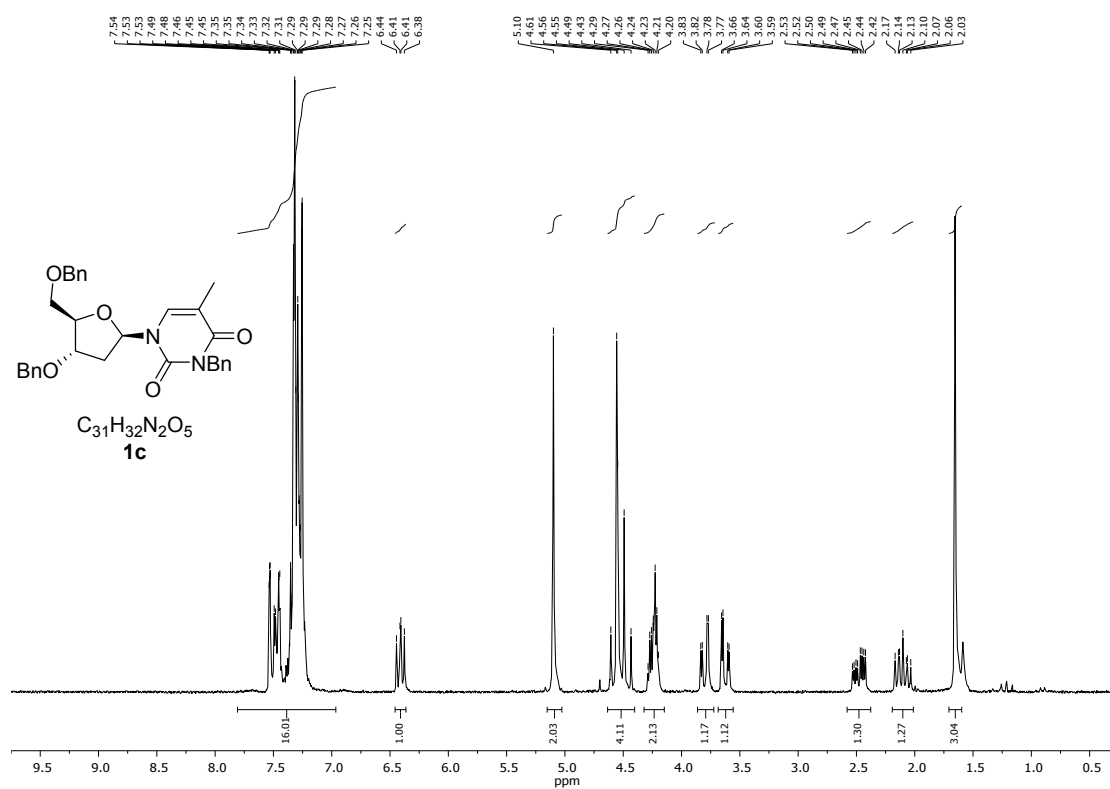


Figure S1: 1H NMR spectrum of **1c** (200 MHz, $CDCl_3$).

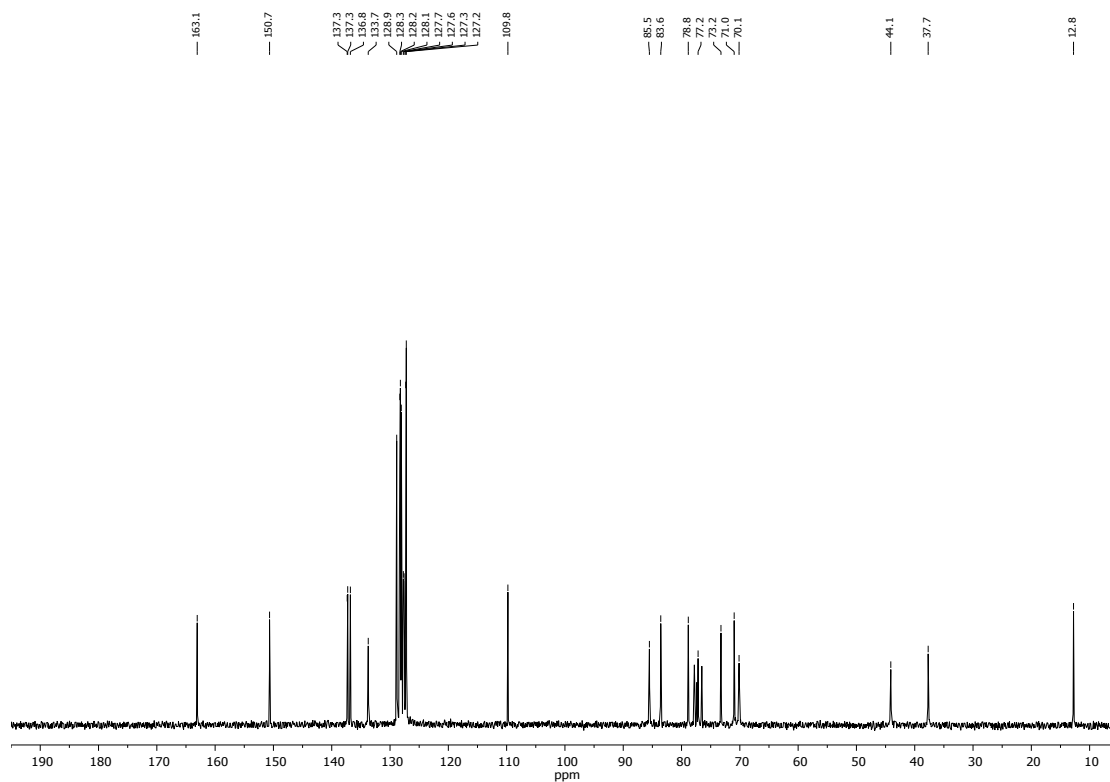


Figure S2: ^{13}C NMR spectrum of **1c** (50 MHz, $CDCl_3$).

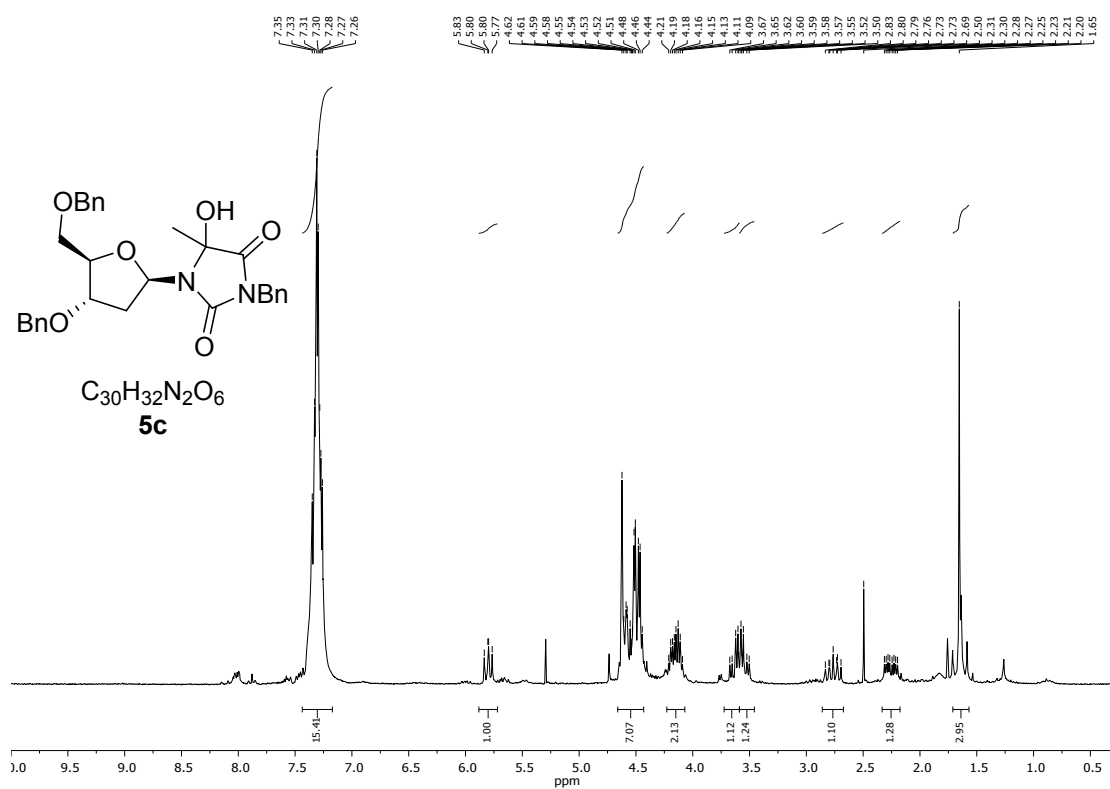


Figure S3: ^1H NMR spectrum of **5c** (200 MHz, CDCl_3).

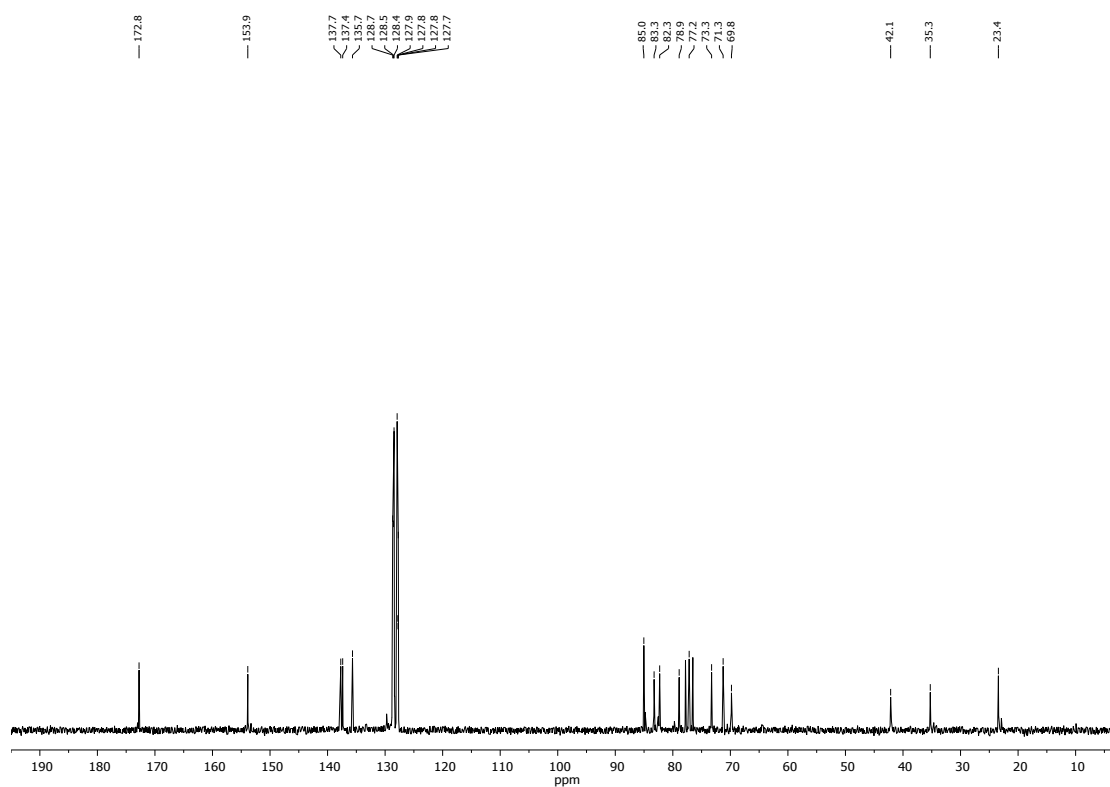


Figure S4: ^{13}C NMR spectrum of **5c** (50 MHz, CDCl_3).

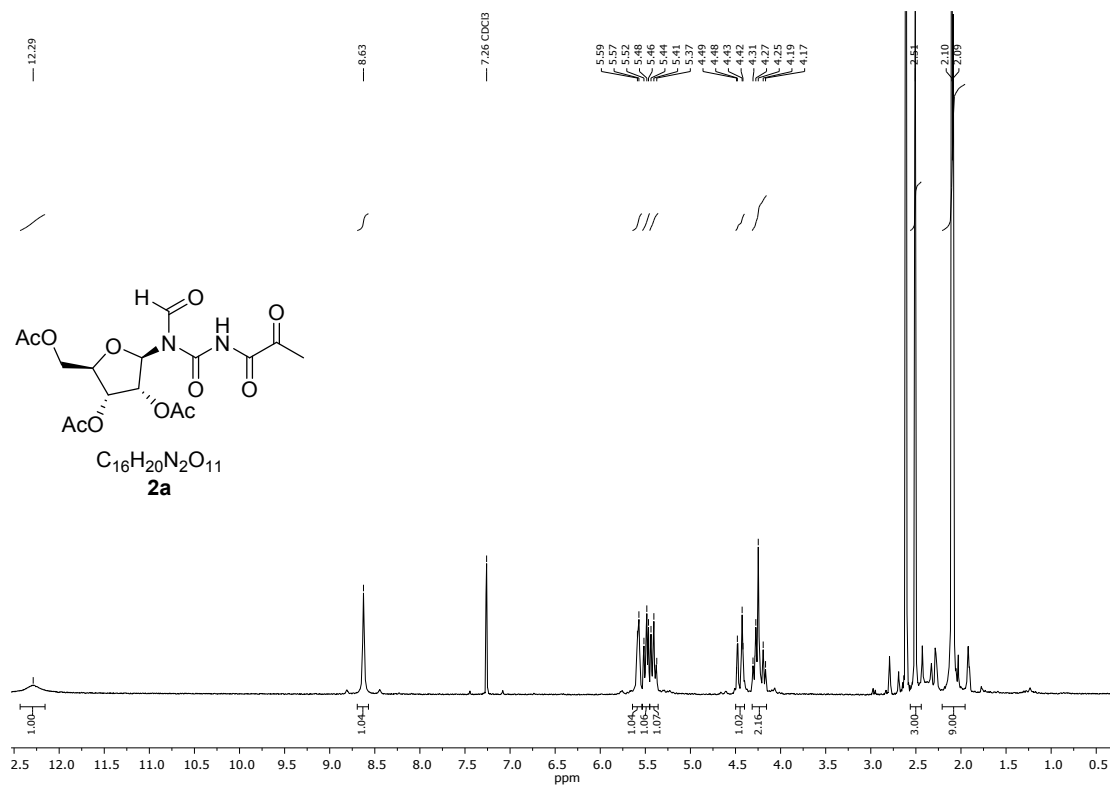


Figure S5: 1H NMR spectrum of crude ozonolysis product **2a** (200 MHz, $CDCl_3$).

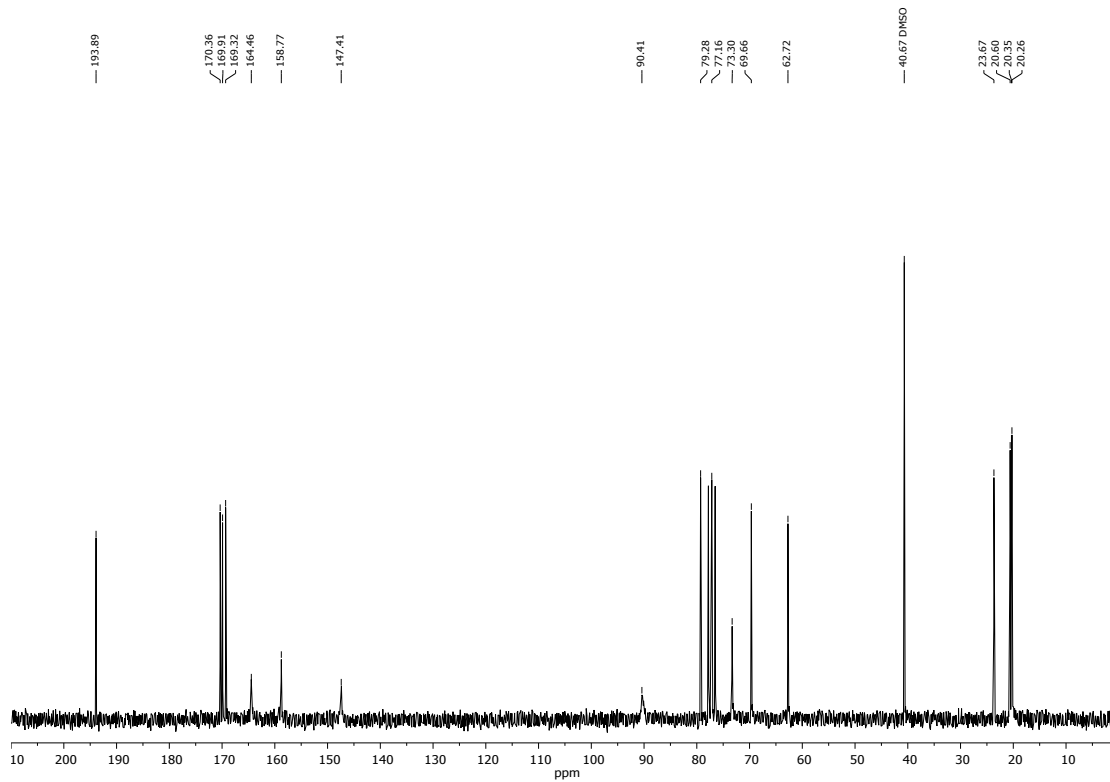


Figure S6: ^{13}C NMR spectrum of crude ozonolysis product **2a** (50 MHz, $CDCl_3$).

MPS017ESI+1#8 RT: 0.12 AV: 1 NL: 1.41E7
 T: {0,0} + p ESI corona sid=25.00 det=1106.00 Full ms [150.00-950.00]

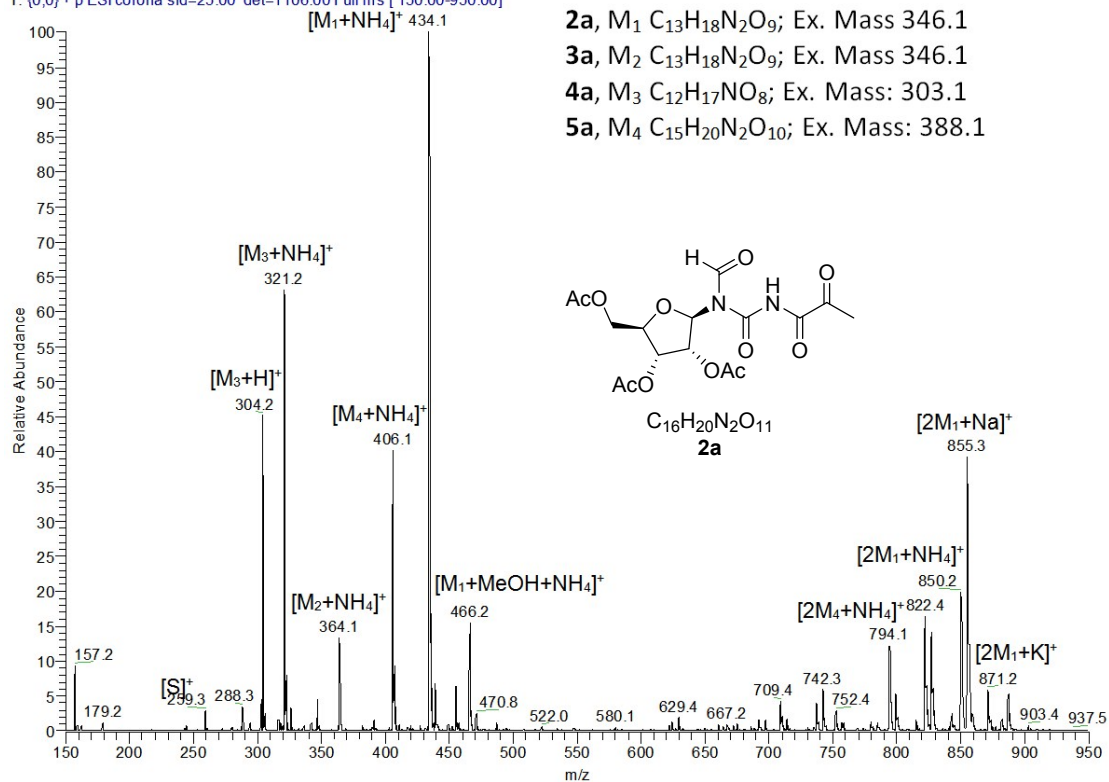


Figure S7: MS (ESI⁺) spectrum of crude ozonolysis product **2a**.

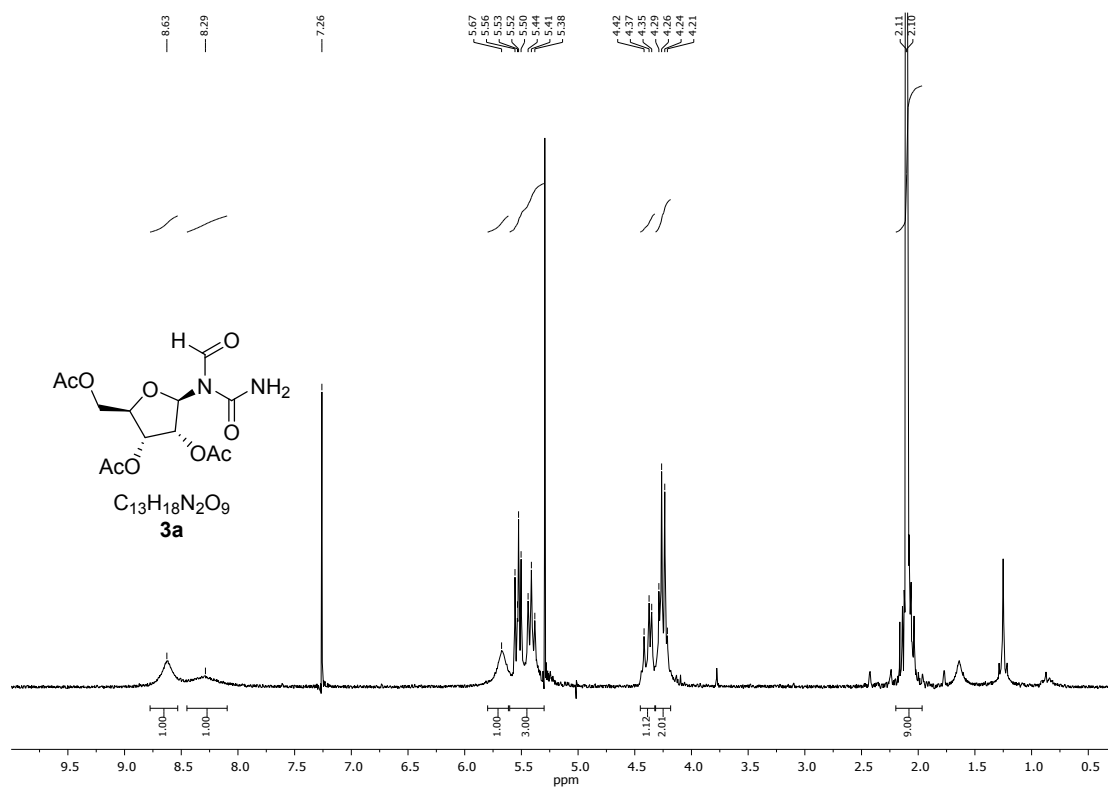


Figure S8: ¹H NMR spectrum of compound **3a** (200 MHz, CDCl₃).

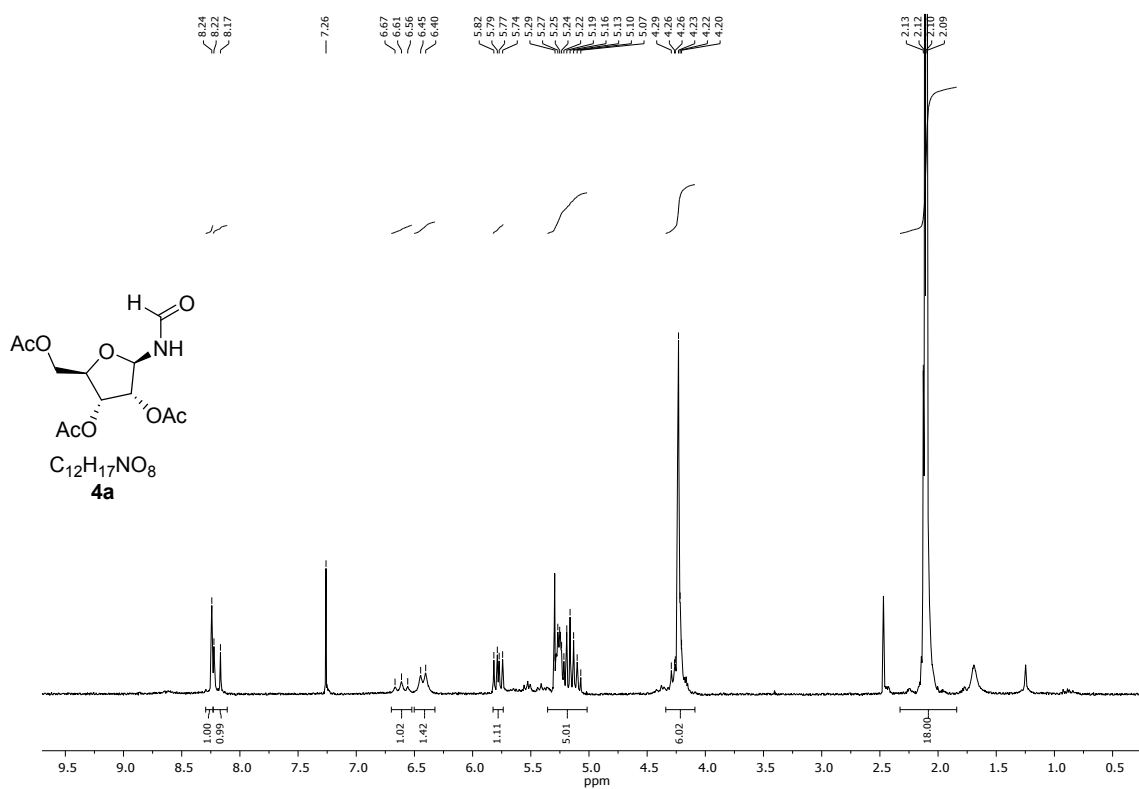


Figure S9: 1H NMR spectrum of compound **4a** (200 MHz, $CDCl_3$).

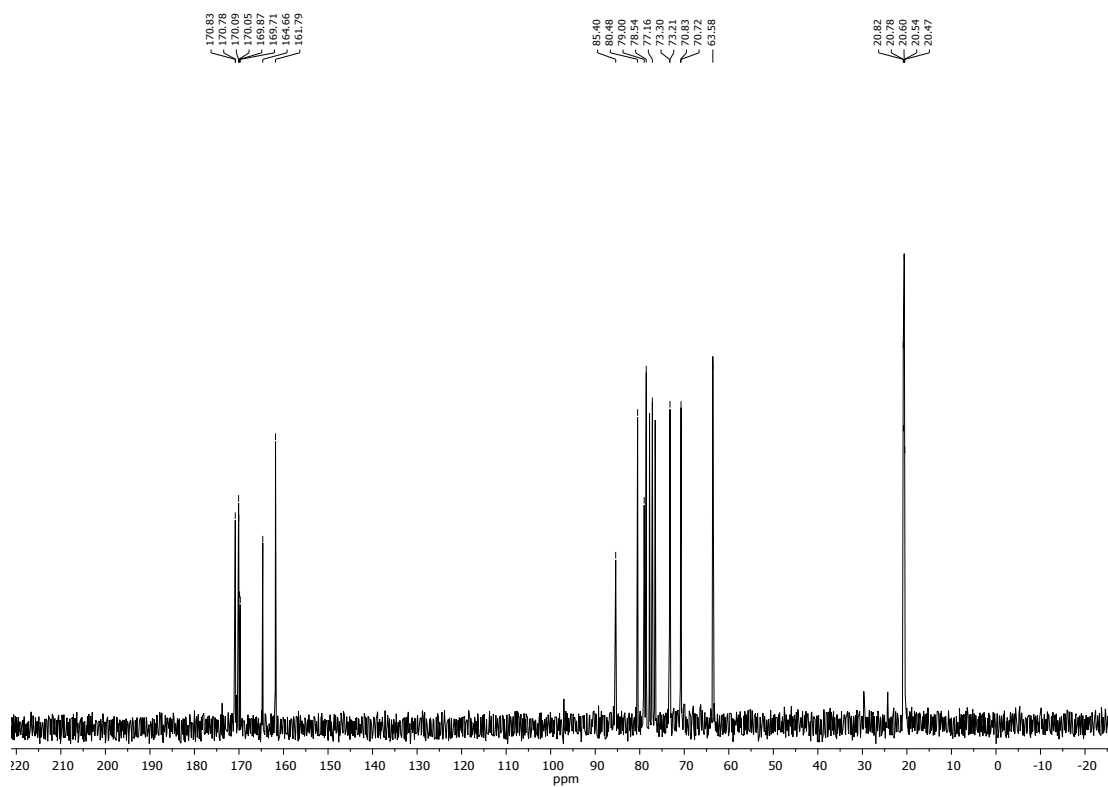


Figure S10: ^{13}C NMR spectrum of compound **4a** (50 MHz, $CDCl_3$).

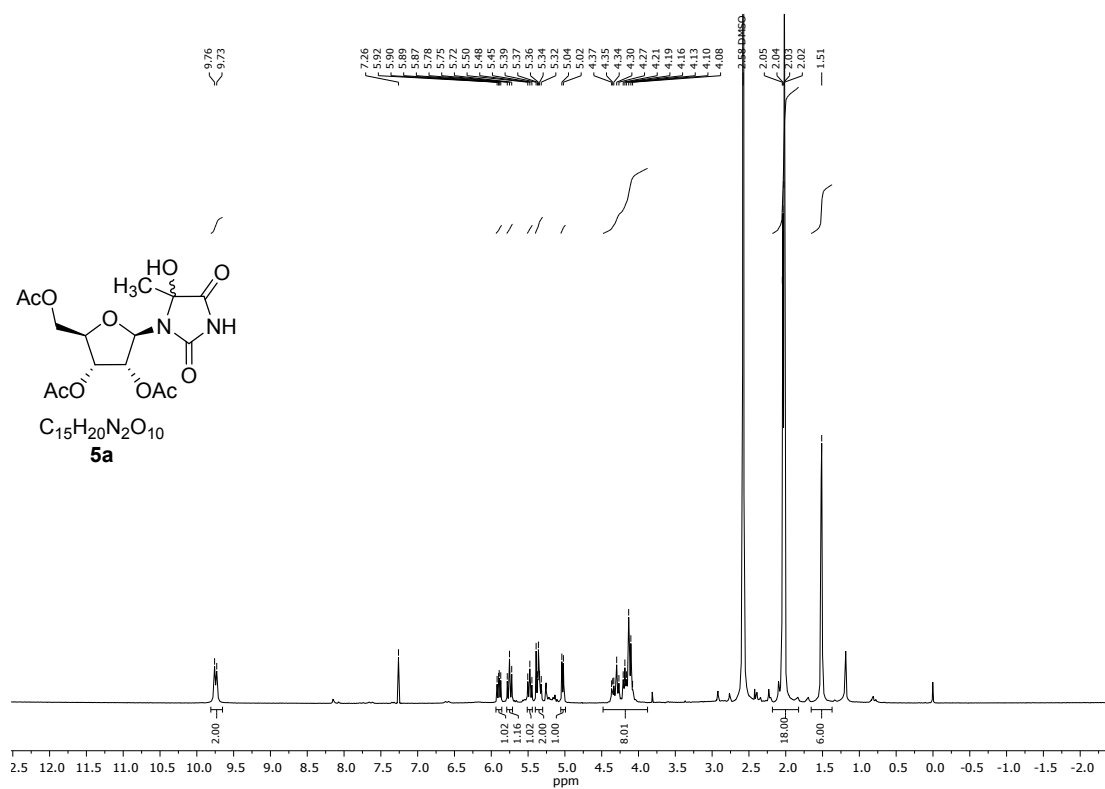


Figure S11: 1H NMR spectrum of compound **5a** (200 MHz, $CDCl_3$).

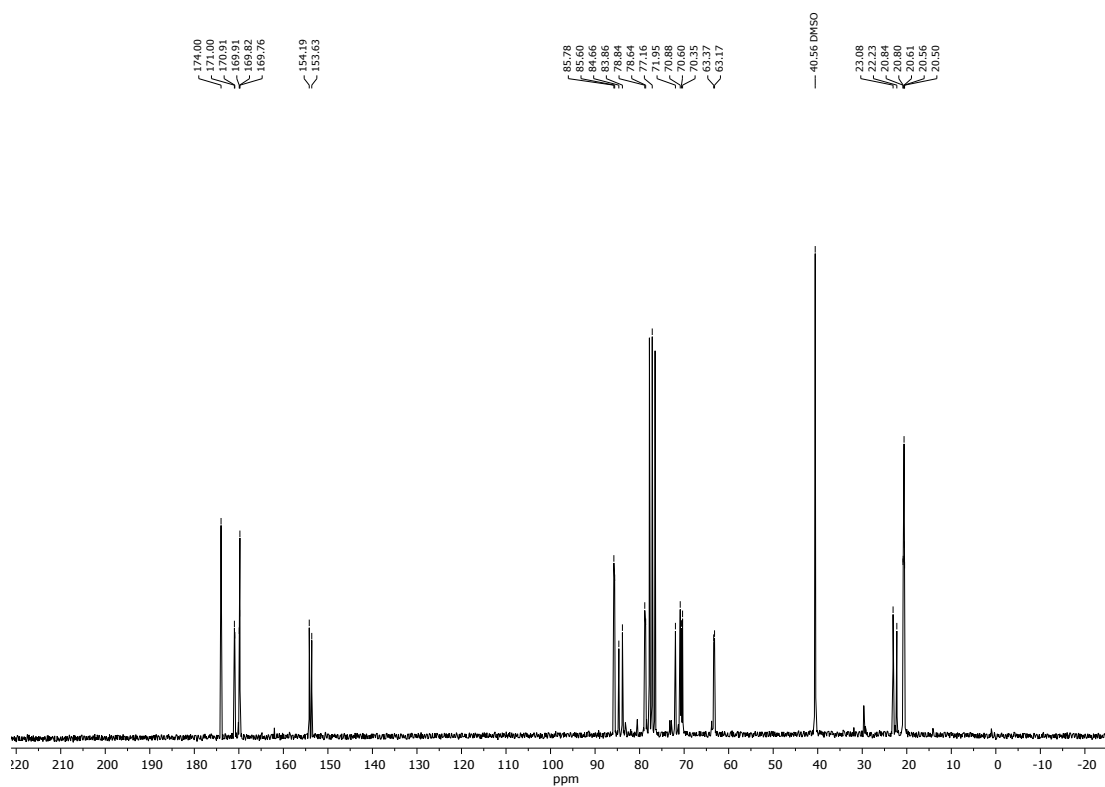


Figure S12: ^{13}C NMR spectrum of compound **5a** (50 MHz, $CDCl_3$).

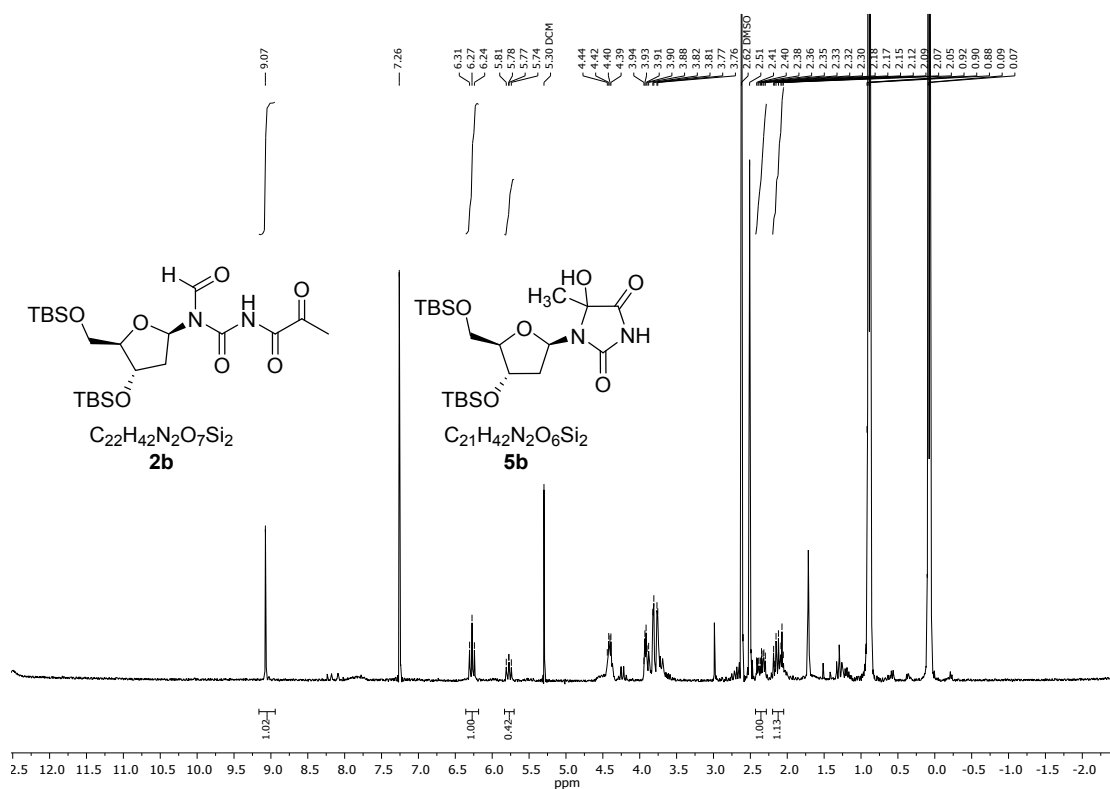


Figure S13: ¹H NMR spectrum of crude ozonolysis product (**2b** & **5b**) (200 MHz, CDCl₃).

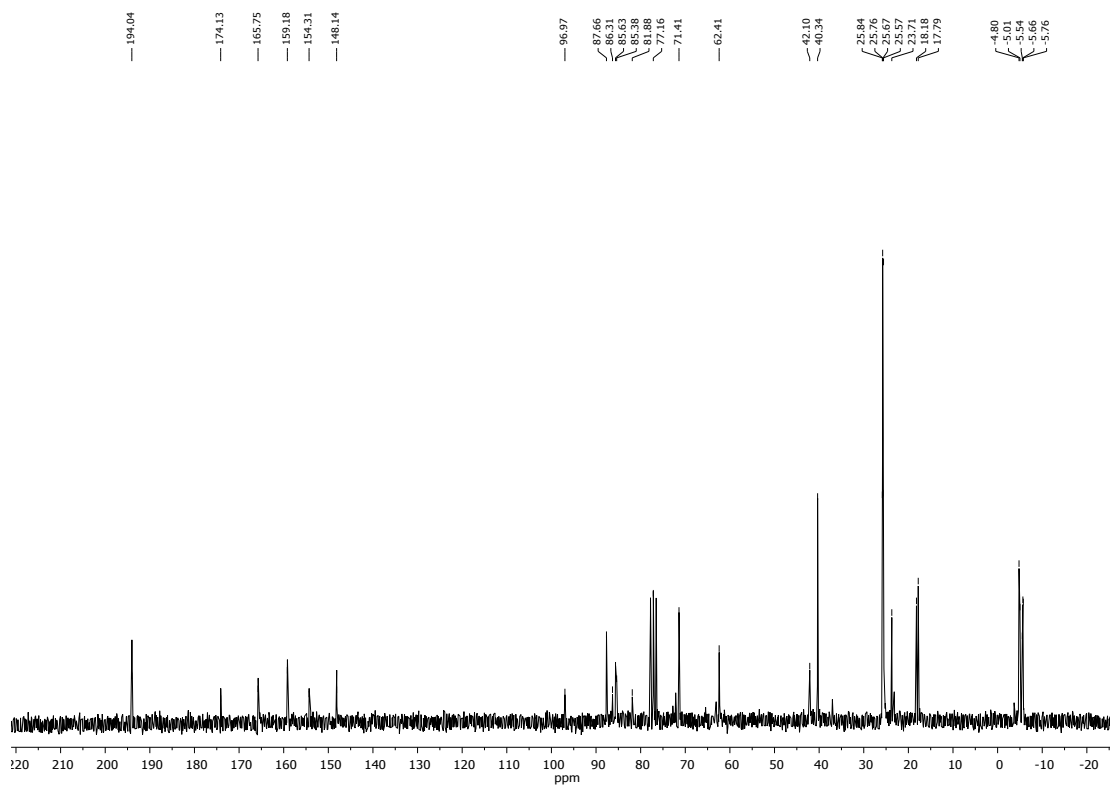
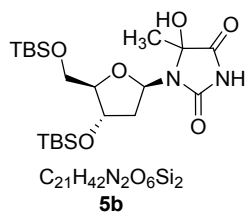
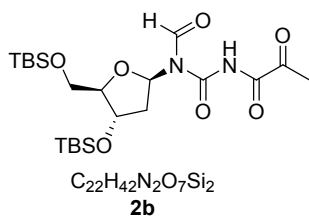


Figure S14: ¹³C NMR spectrum of crude ozonolysis product (**2b** & **5b**) (50 MHz, CDCl₃).



EX12_cr_ESI+4 #4-12 RT: 0.05-0.19 AV: 9 NL: 5.58E6

T: {0,0} +p ESI corona sid=25.00 det=1106.00 Full ms [100.00-1100.00]

2b, M_1 : $C_{22}H_{42}N_2O_7Si_2$; Ex. Mass: 502.2

3b, M_2 : $C_{19}H_{40}N_2O_5Si_2$; Ex. Mass: 432.2

4b, M_3 : $C_{18}H_{39}NO_4Si_2$; Ex. Mass: 389.2

5b, M_4 : $C_{21}H_{42}N_2O_6Si_2$; Ex. Mass: 474.3

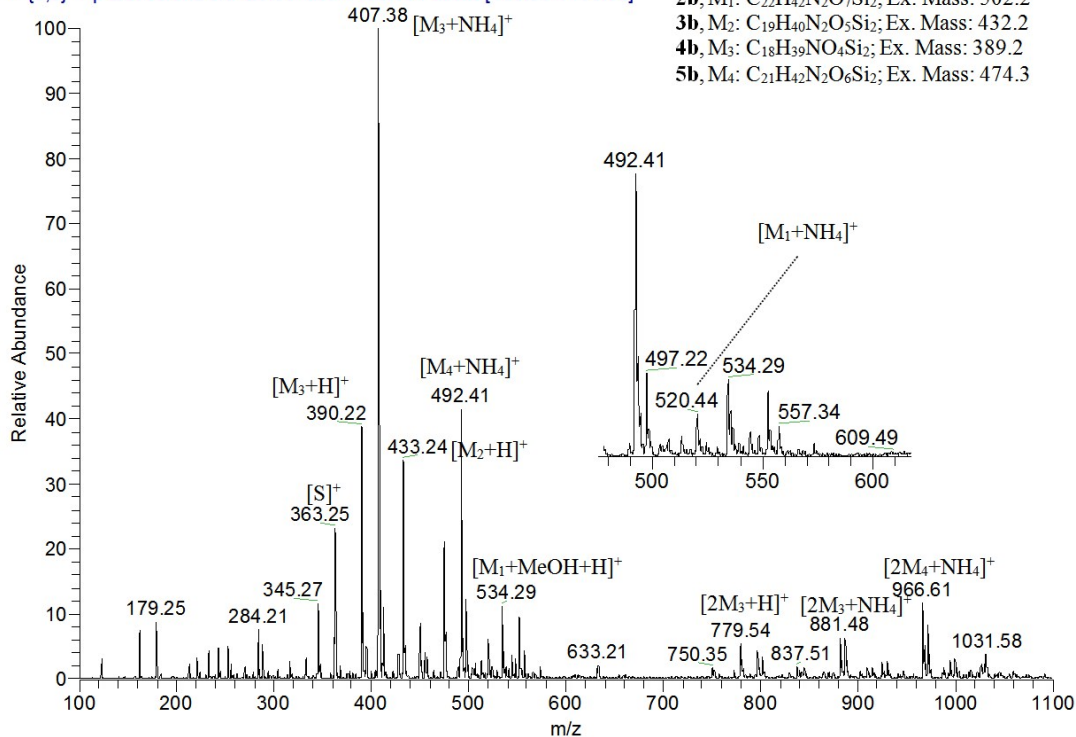


Figure S15: MS (ESI⁺) spectrum of crude ozonolysis product (**2b** & **5b**).

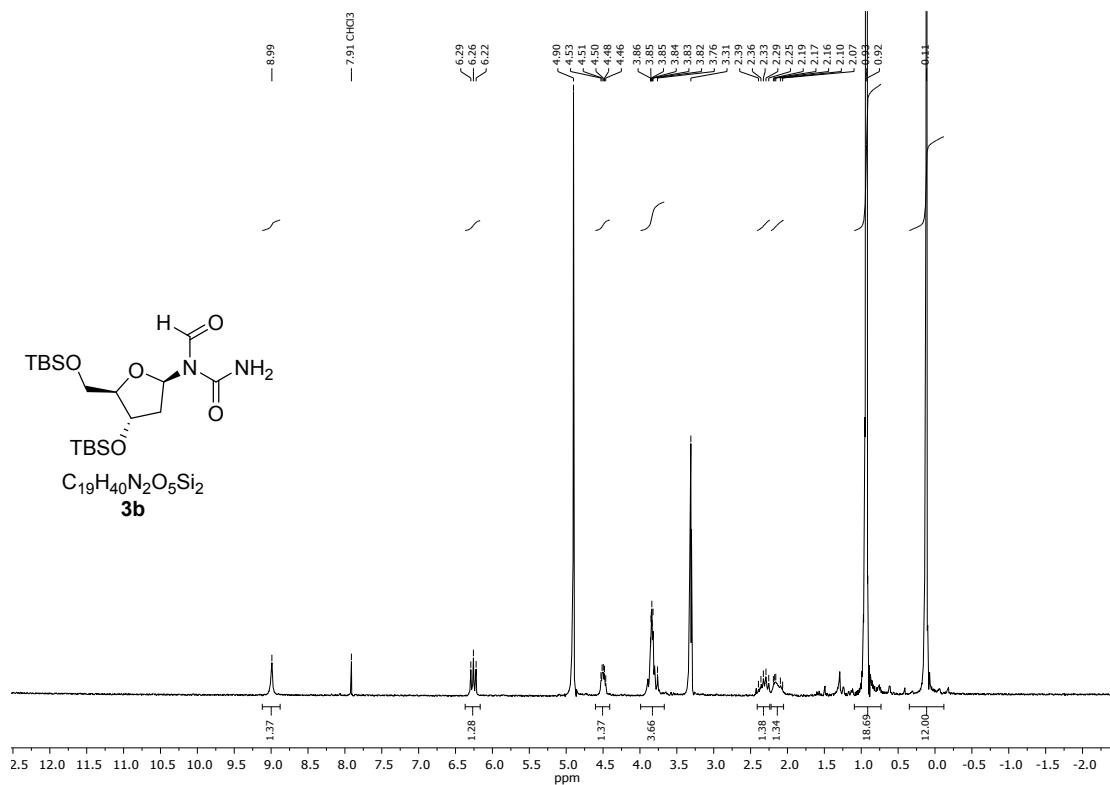


Figure S16: ¹H NMR spectrum of compound **3b** (200 MHz, CDCl₃).

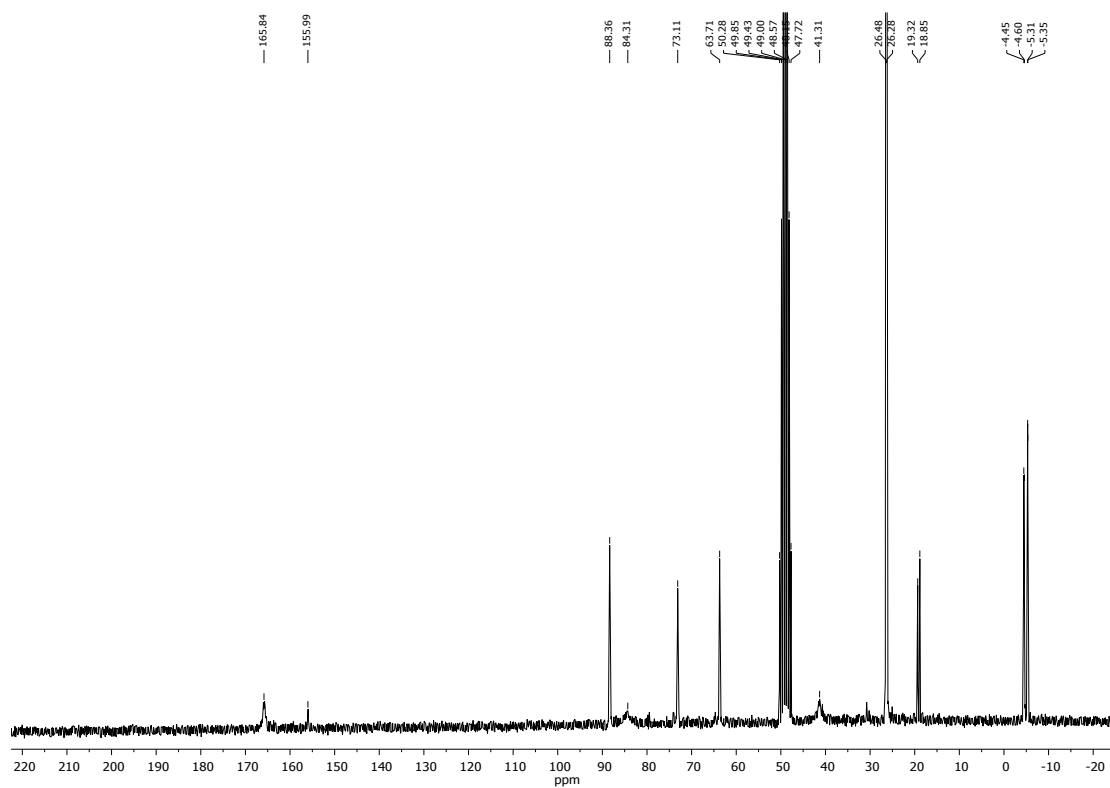


Figure S17: ¹³C NMR spectrum of **3b** (50 MHz, CDCl₃).

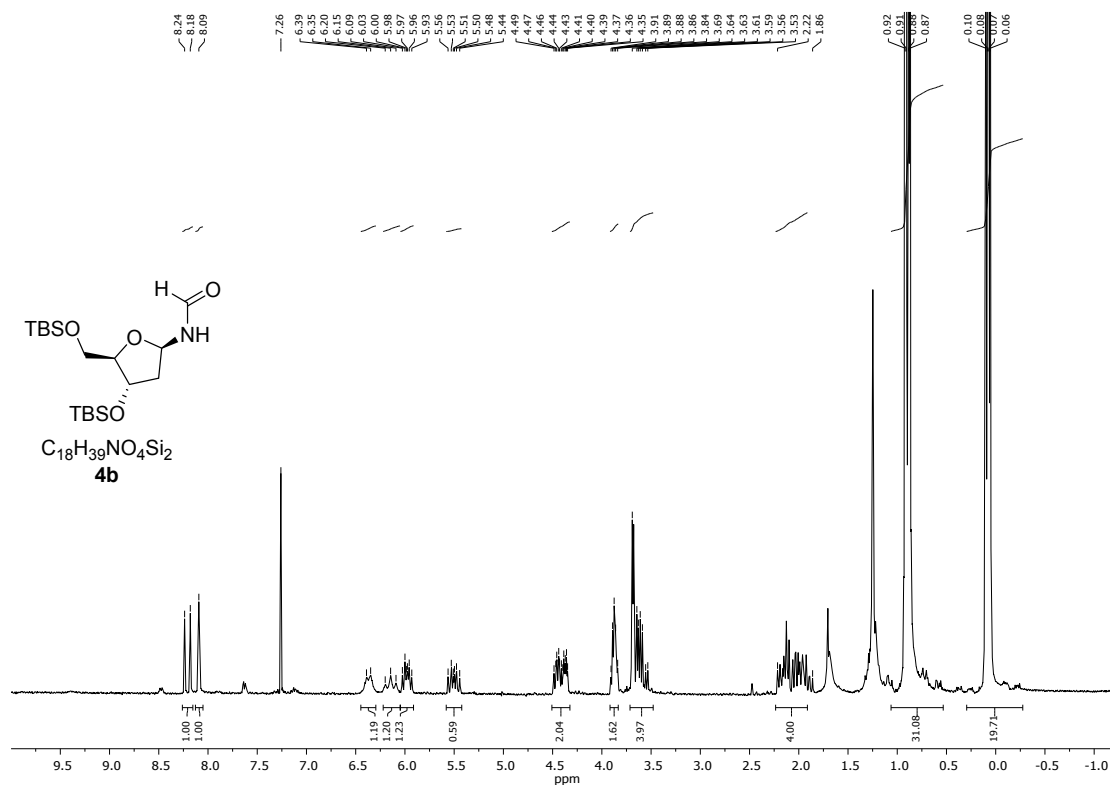


Figure S18: ¹H NMR spectrum of compound **4b** (200 MHz, CDCl₃).

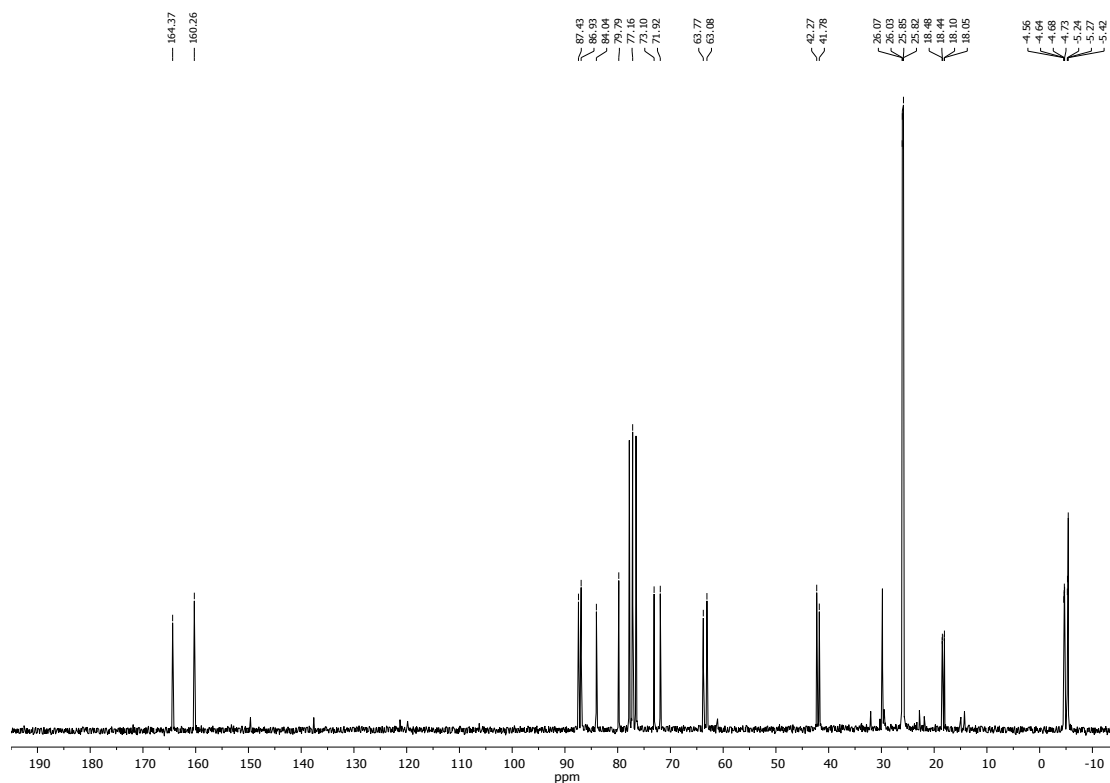


Figure S19: ¹³C NMR spectrum of **4b** (50 MHz, CDCl₃).

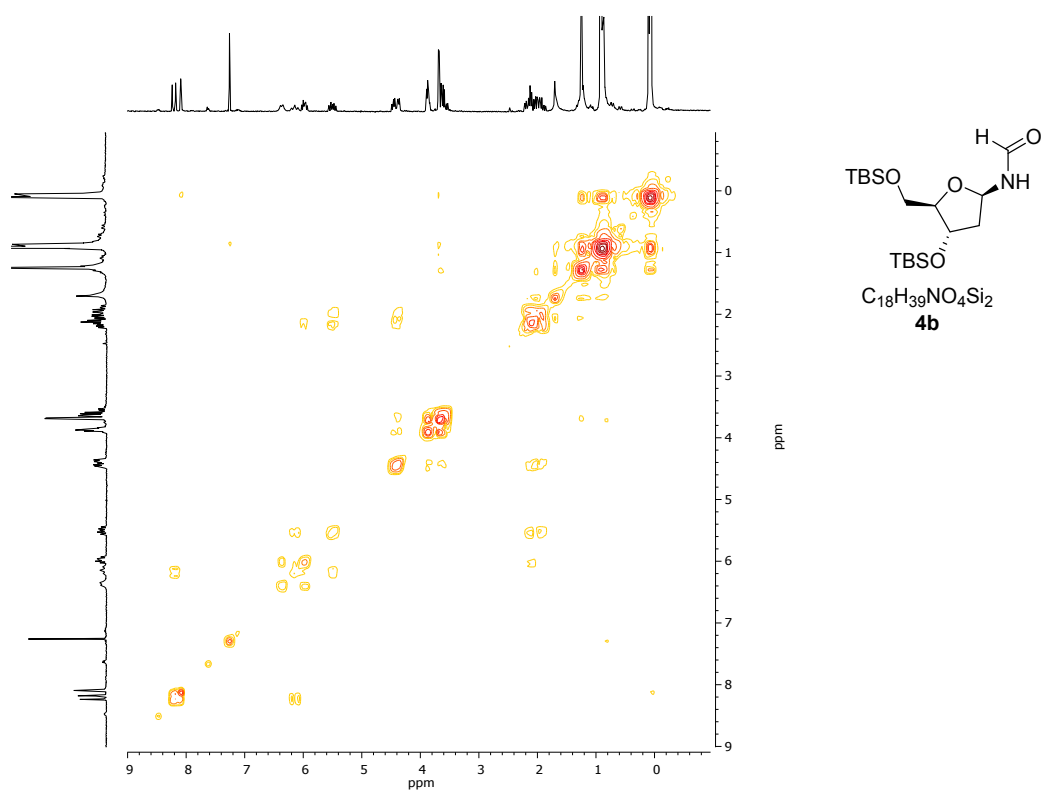


Figure S20: 2D-COSY spectrum of compound **4b** (200 MHz, CDCl₃).

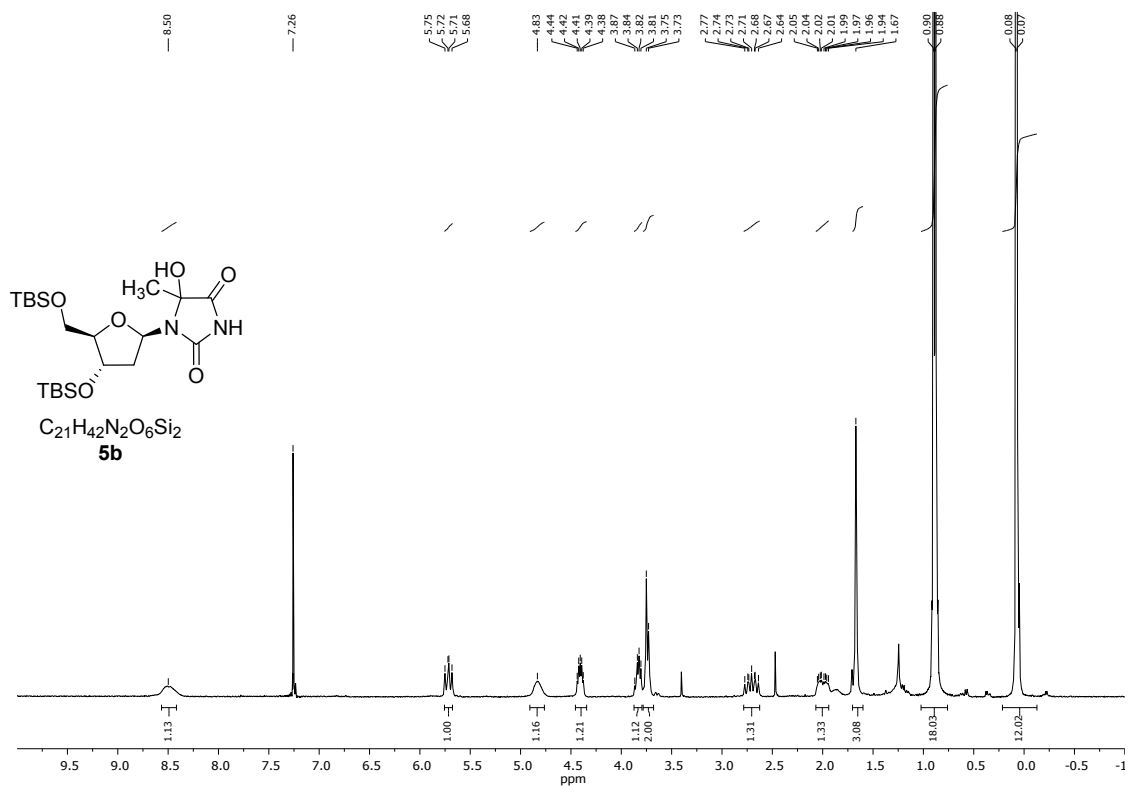


Figure S21: ^1H NMR spectrum of **5b** (200 MHz, CDCl_3).

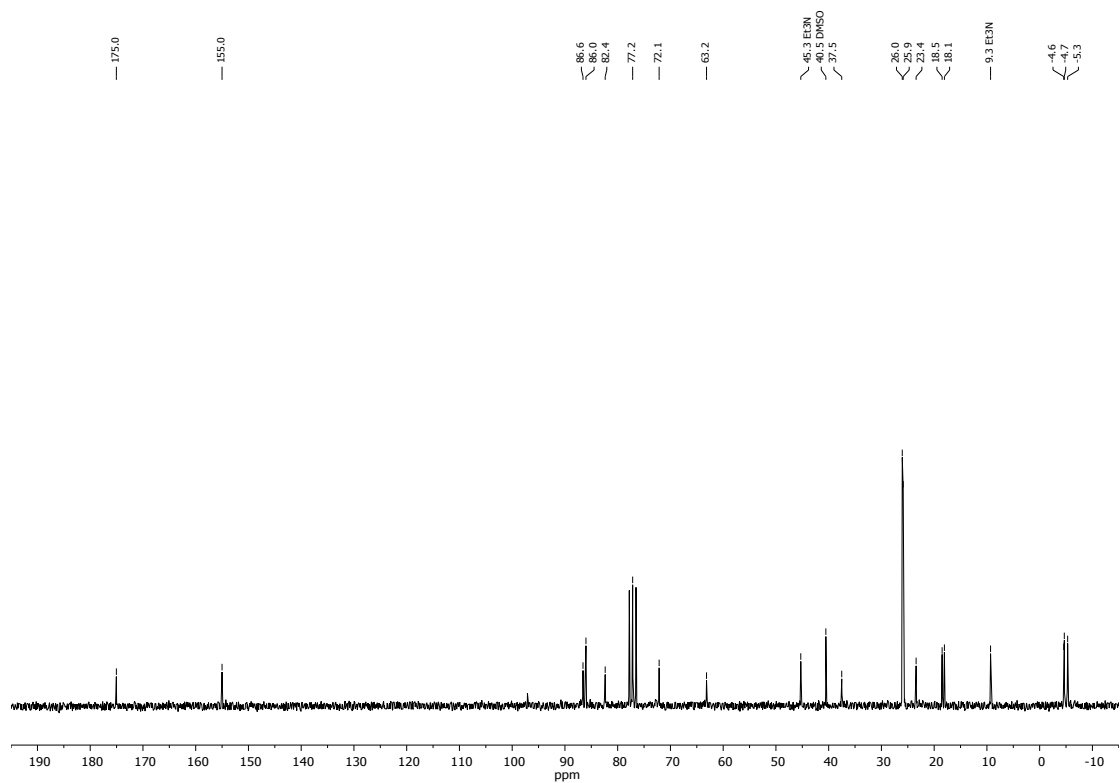


Figure S22: ^{13}C NMR spectrum of **5b** (50 MHz, CDCl_3).

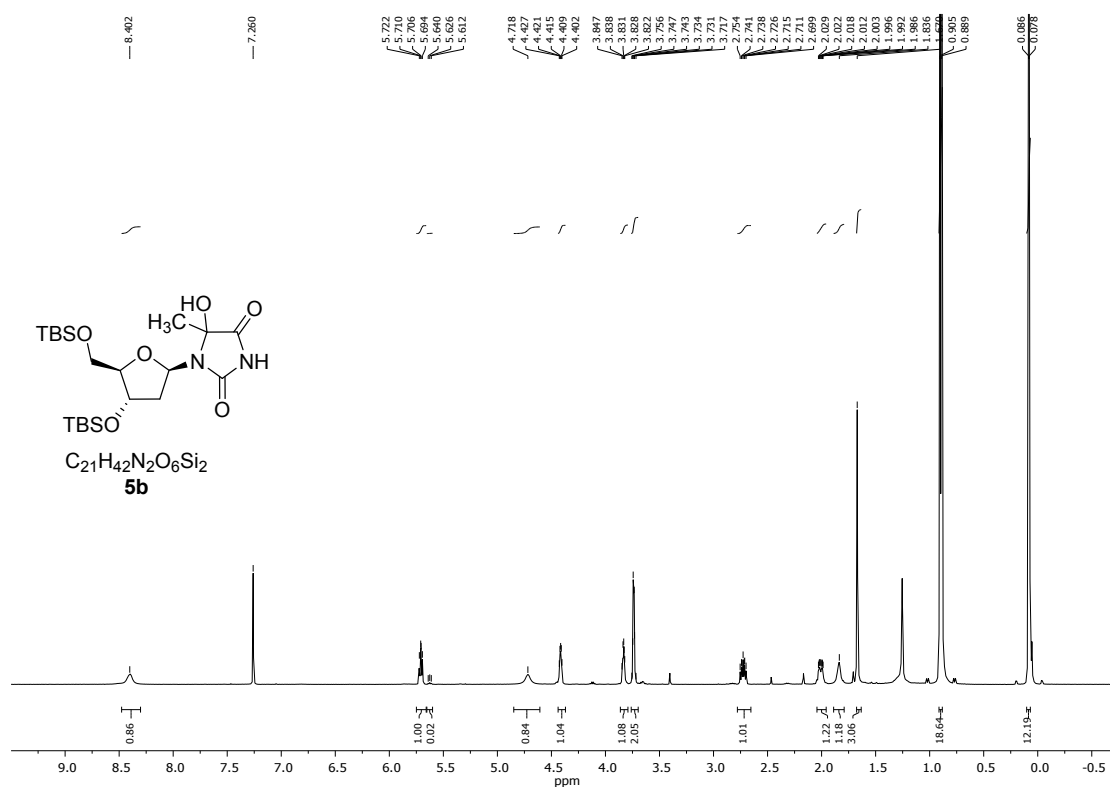


Figure S23: ^1H NMR spectrum of **5b** (500 MHz, CDCl_3).

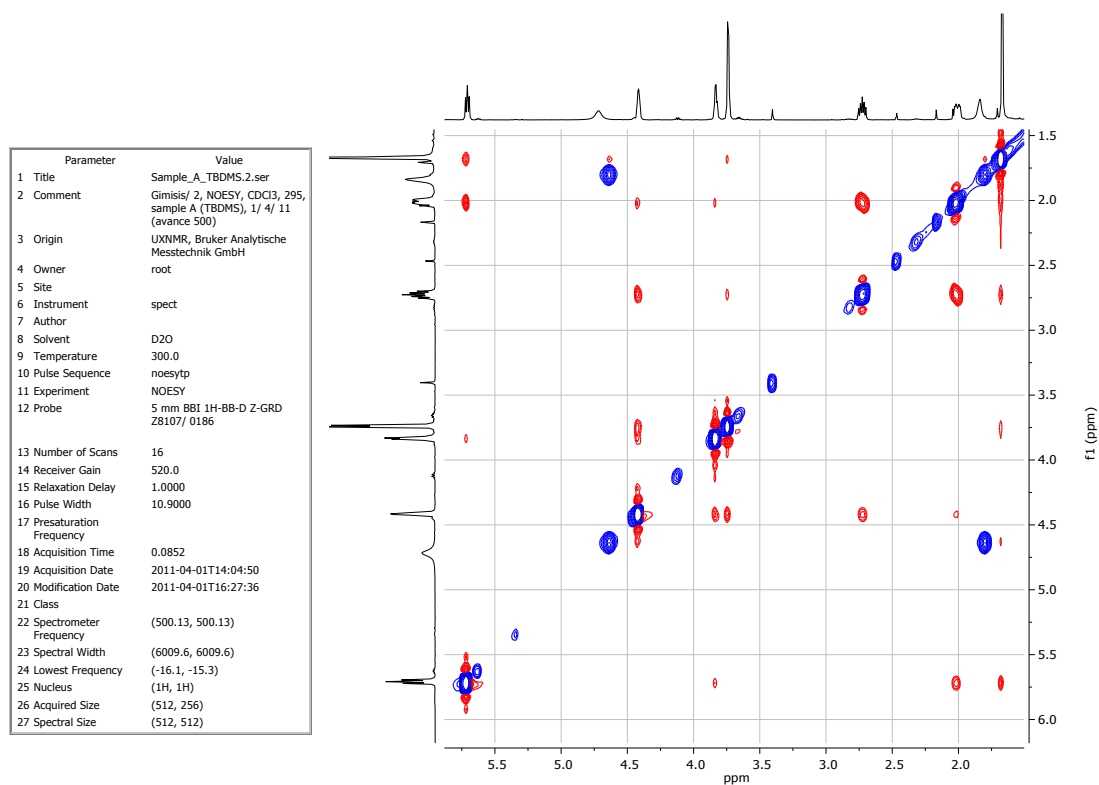


Figure S24: 2D-NOESY spectrum of **5b** (500 MHz, CDCl_3).

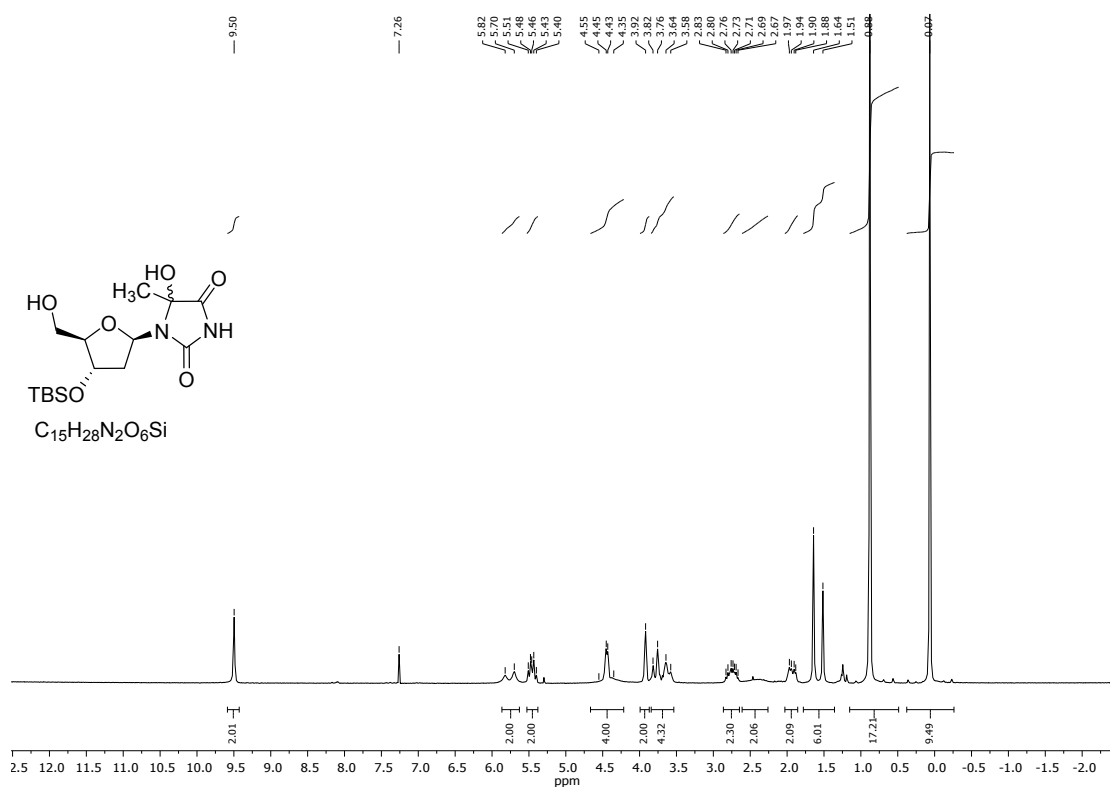


Figure S25: ^1H NMR spectrum of **5b'** (200 MHz, CDCl_3).

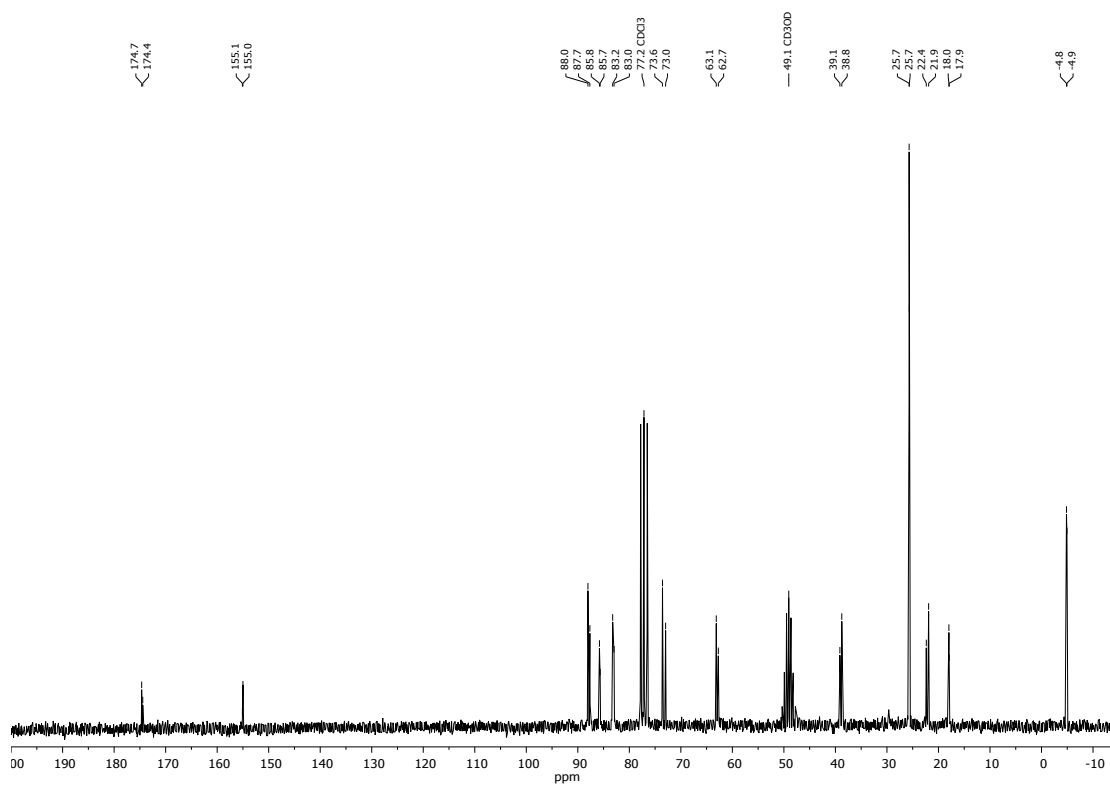


Figure S26: Figure S27: ^{13}C NMR spectrum of **5b'** (50 MHz, CDCl_3).

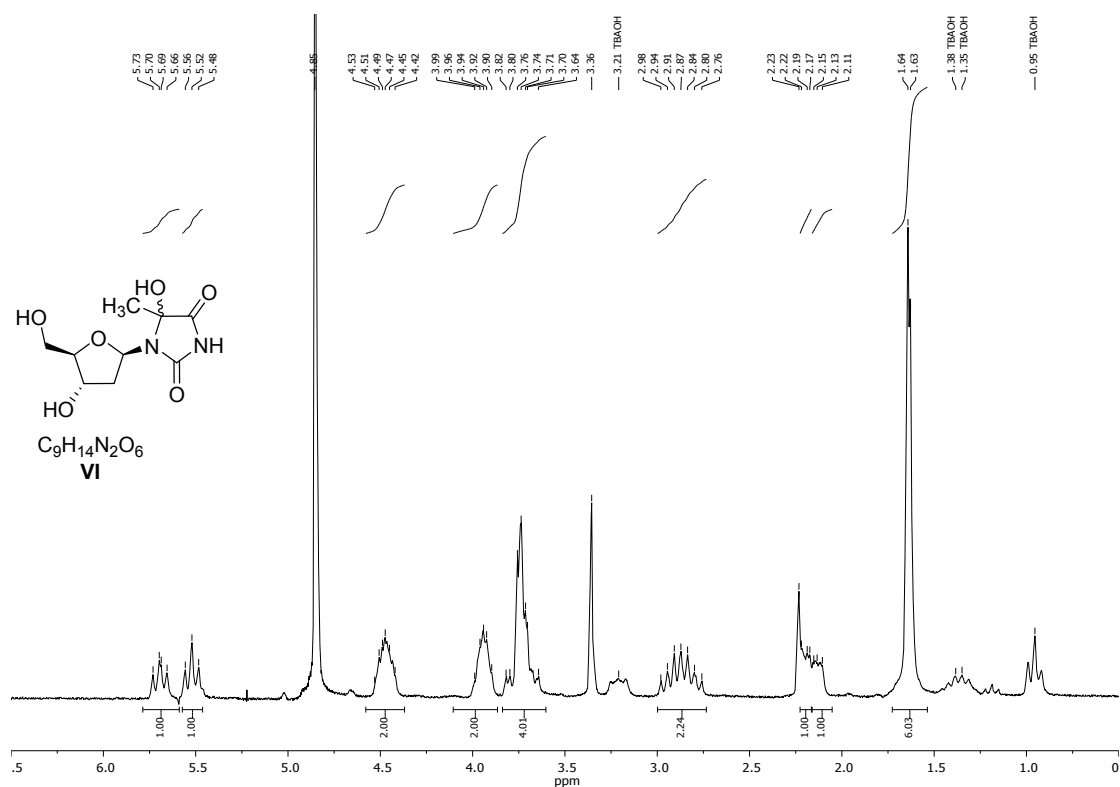


Figure S28: 1H NMR spectrum of VI (200 MHz, D_2O).

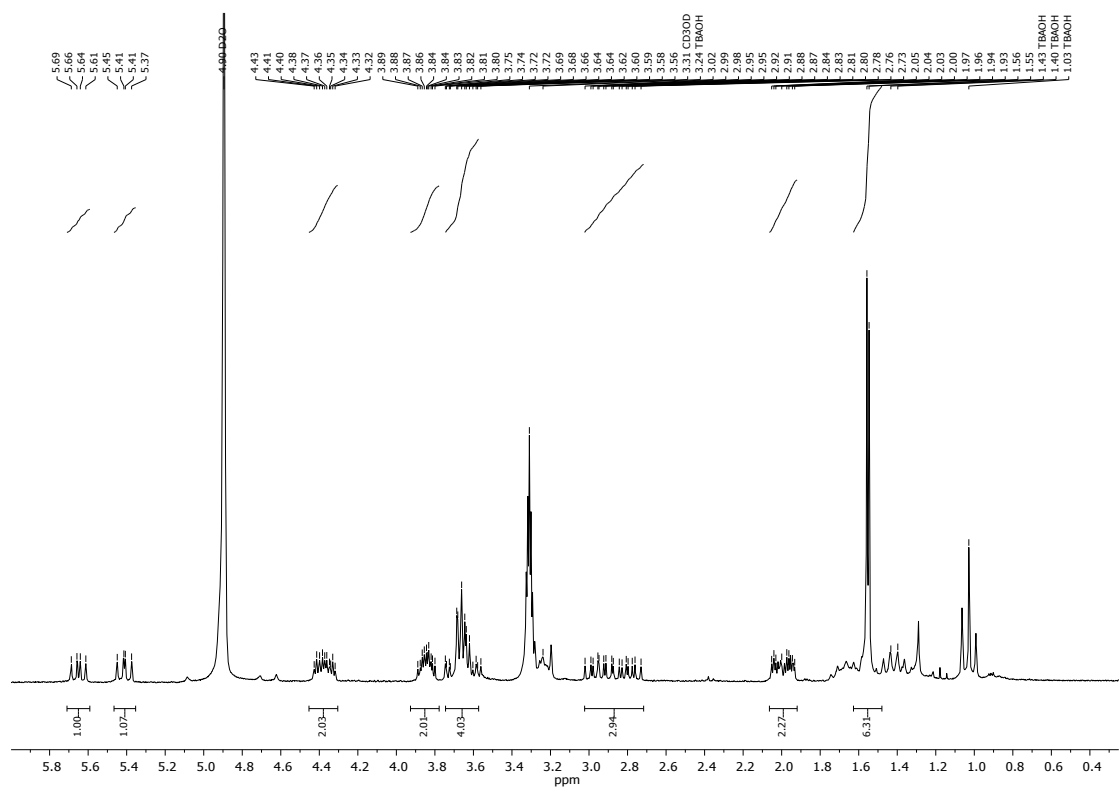


Figure S29: 1H NMR spectrum of VI (200 MHz, CD_3OD).

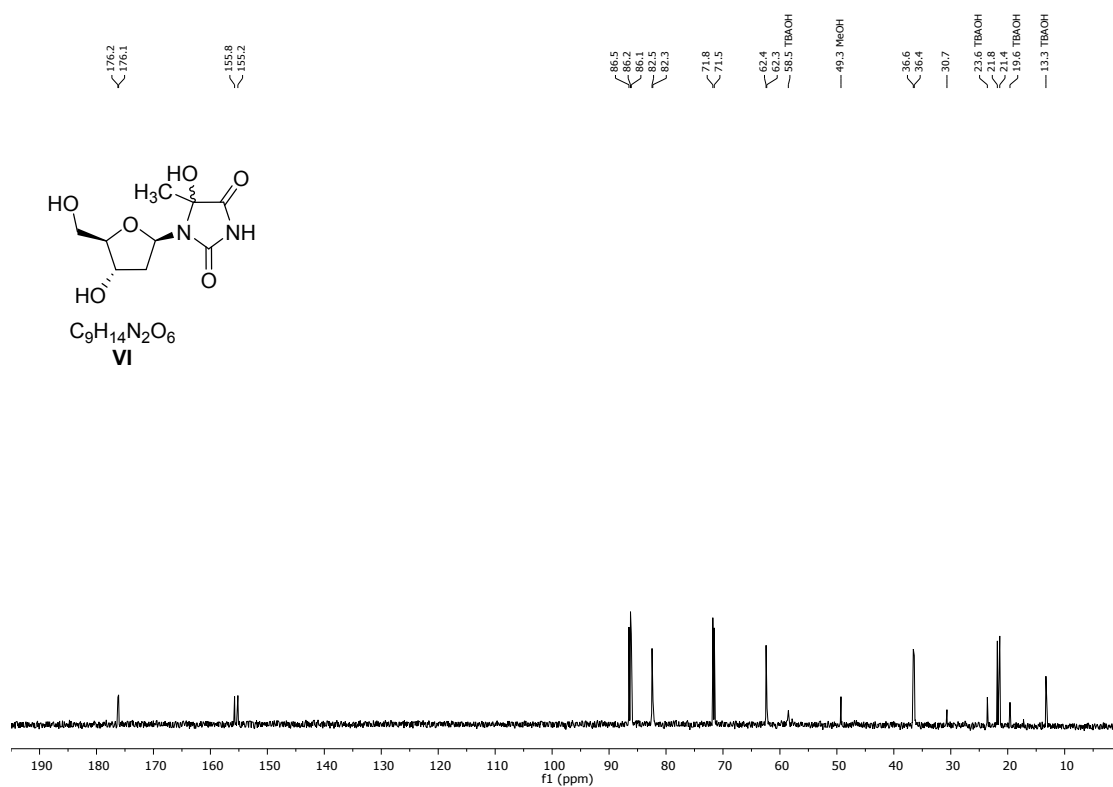


Figure S30: ^{13}C NMR spectrum of **5b** (50 MHz, $CDCl_3$).

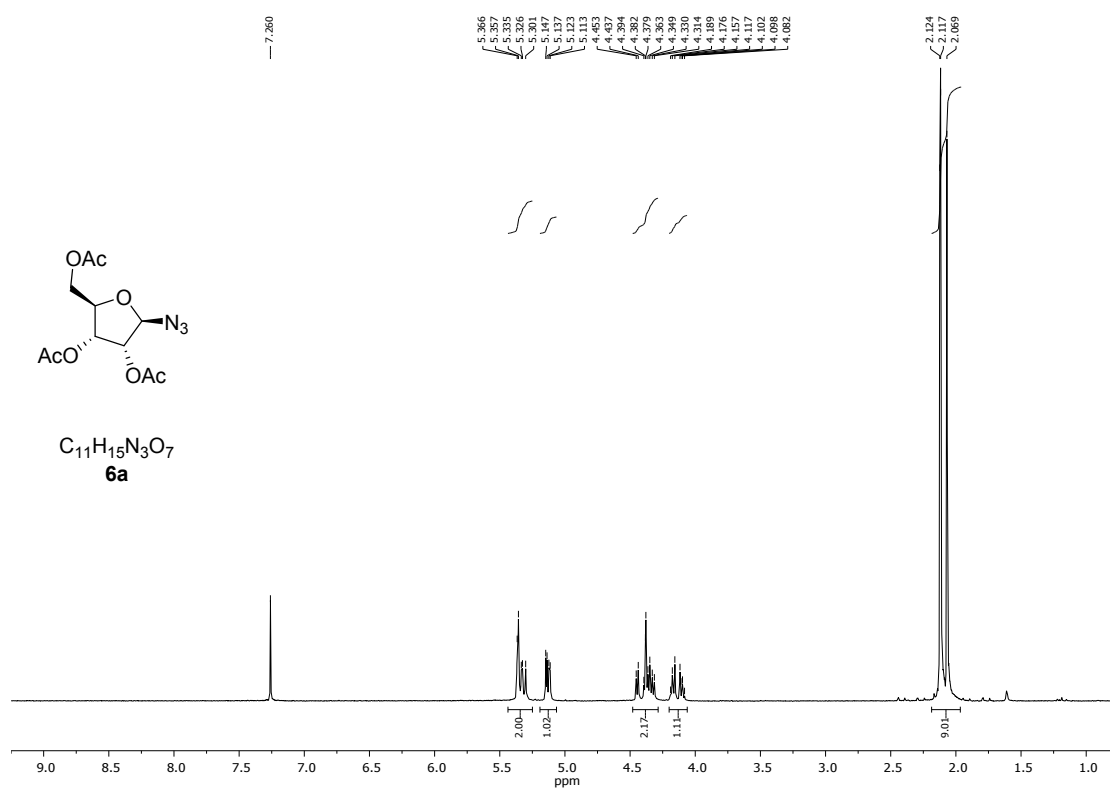


Figure S31: 1H NMR spectrum of **6a** (200 MHz, $CDCl_3$).

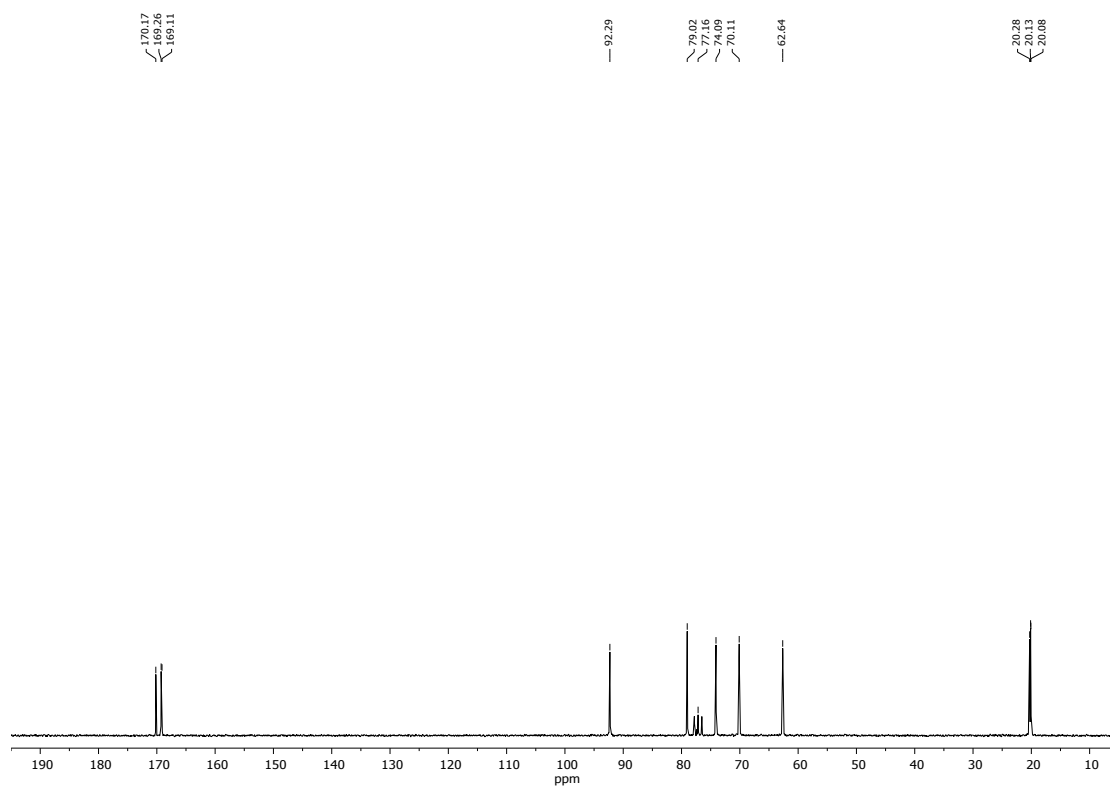


Figure S32: ^{13}C NMR spectrum of **6a** (50 MHz, $CDCl_3$).

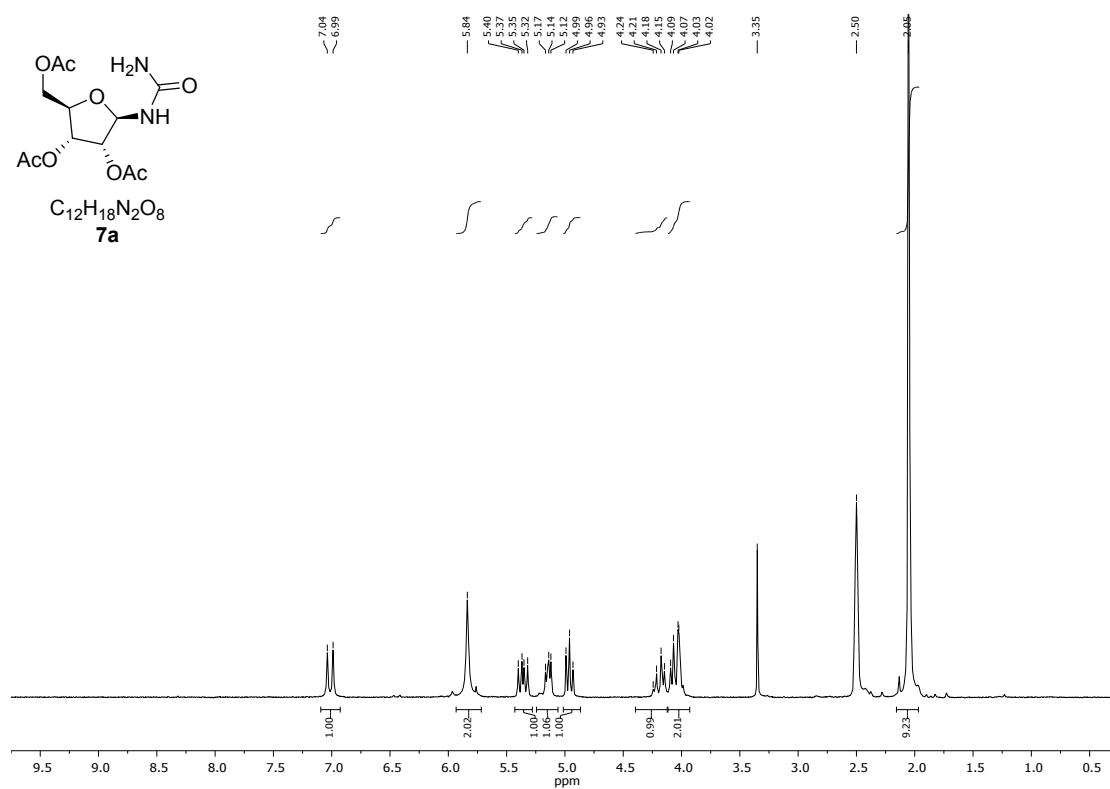


Figure S33: 1H NMR spectrum of **7a** (200 MHz, DMSO- d_6).

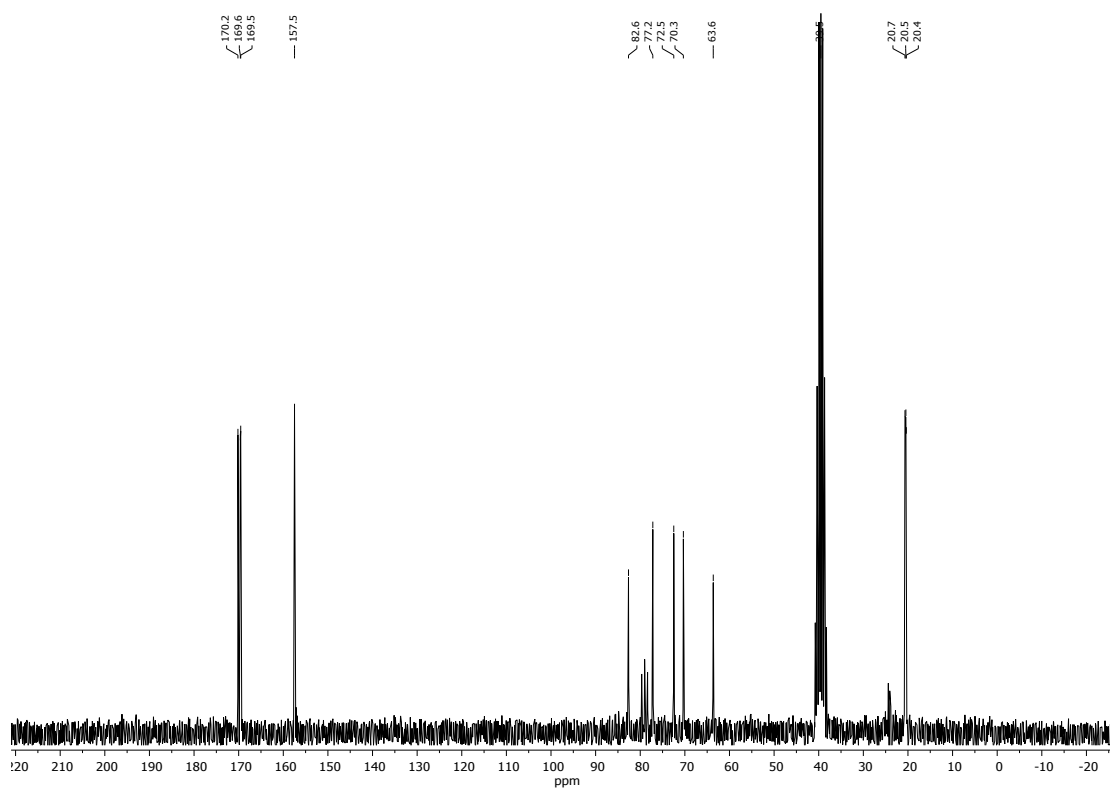


Figure S34: ^{13}C NMR spectrum of **7a** (50 MHz, DMSO- d_6).

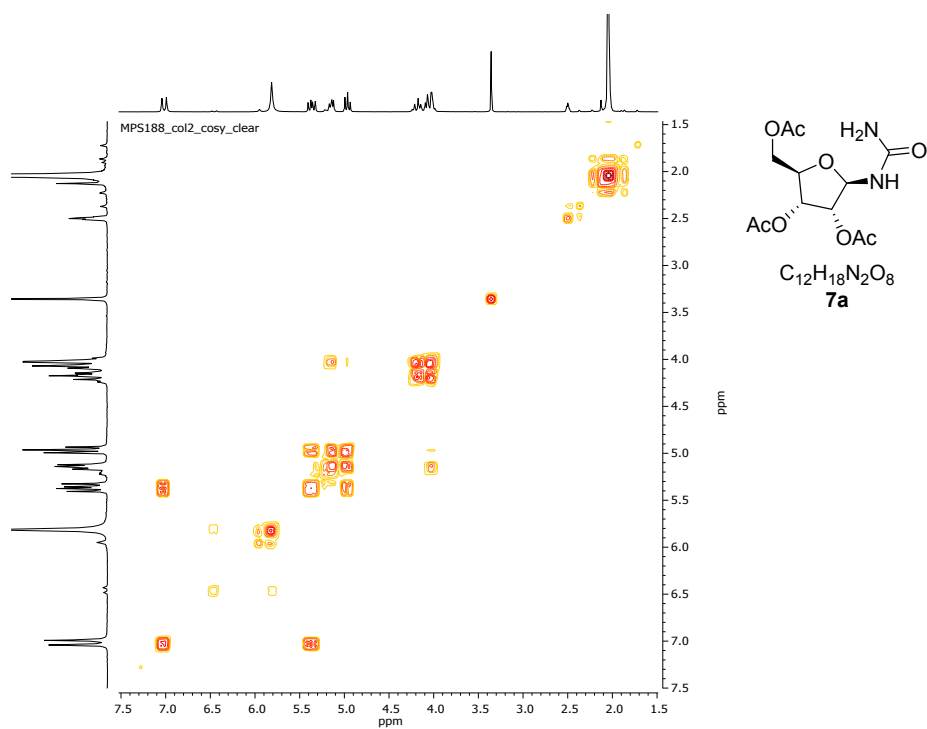


Figure S35: 2D COSY spectrum of **7a** (200 MHz, DMSO-d₆).

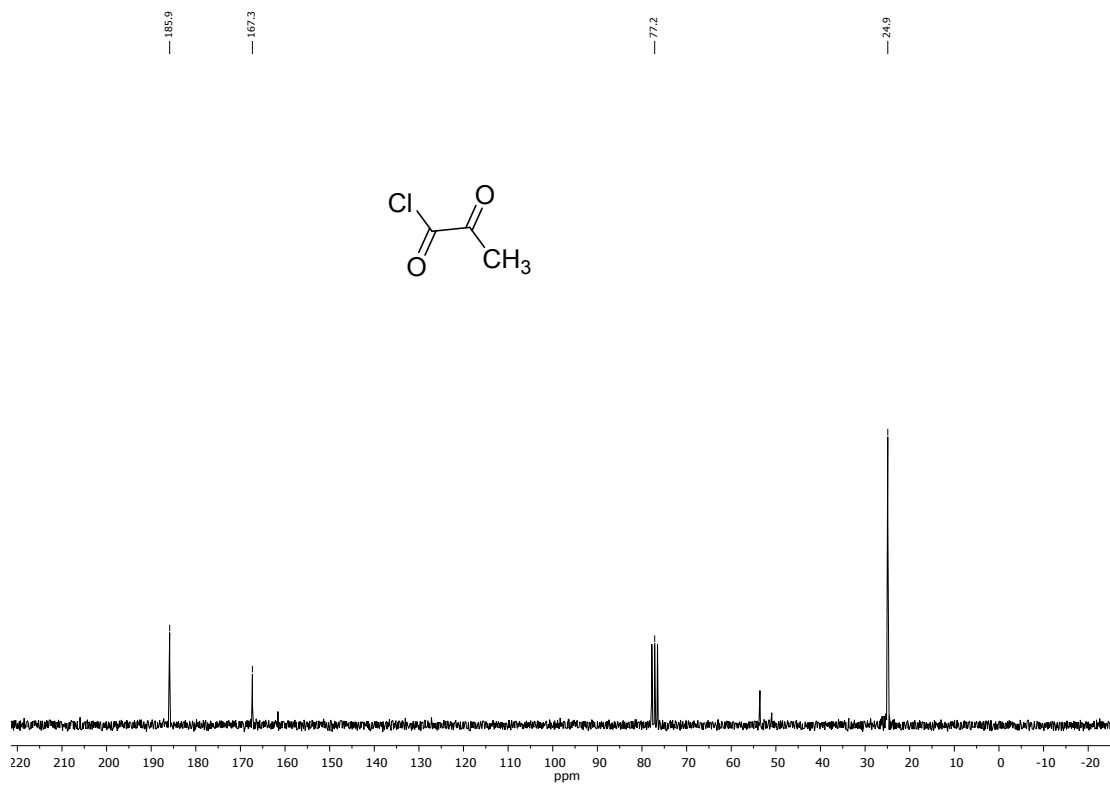


Figure S36: ¹³C NMR spectrum of pyruvoyl chloride (50 MHz, CDCl₃).

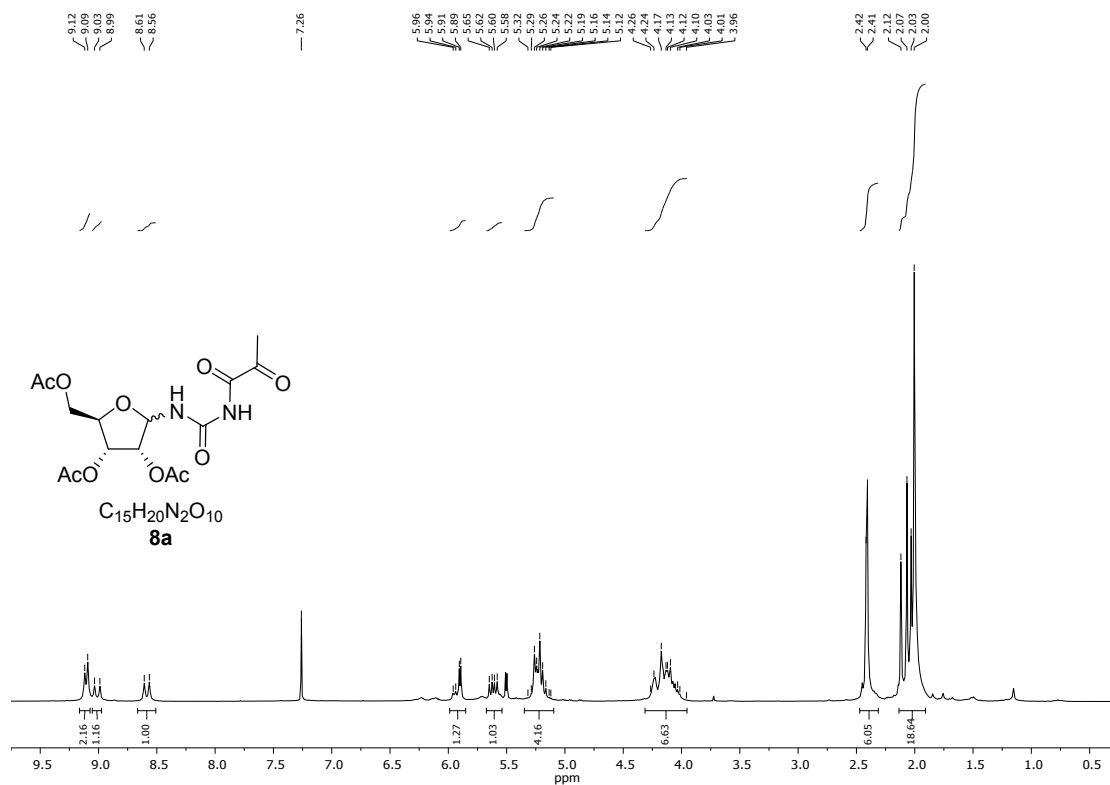


Figure S37: 1H NMR spectrum of **8a** (200 MHz, $CDCl_3$).

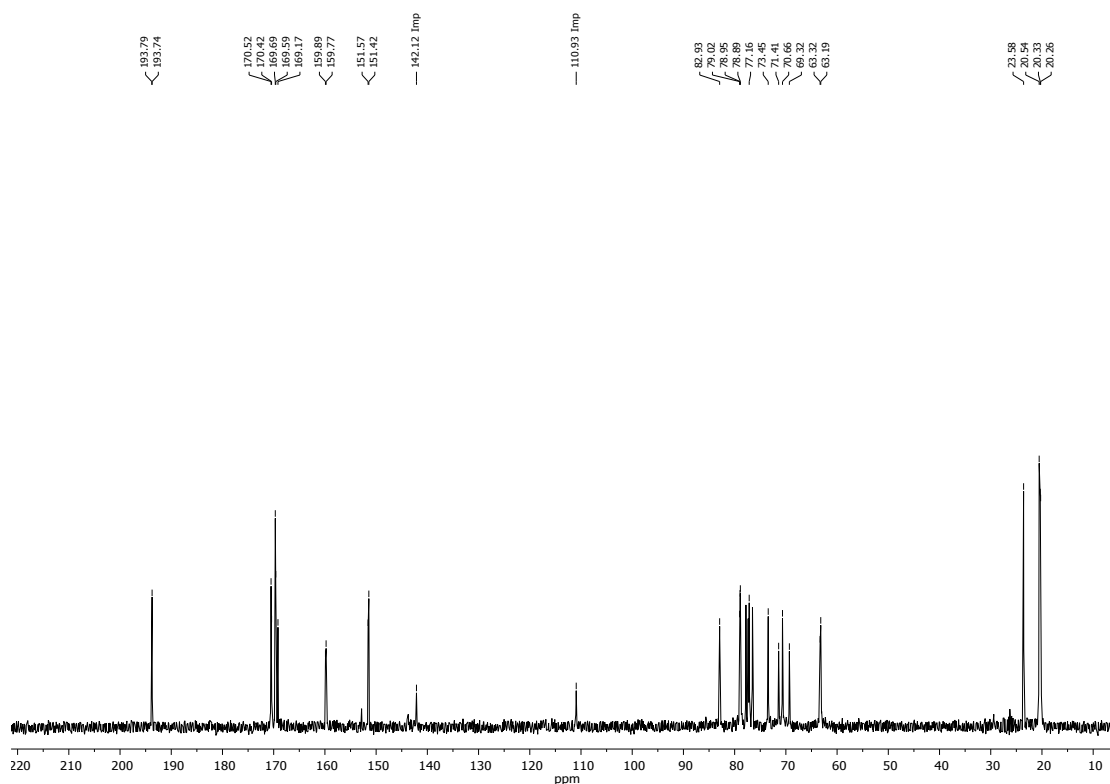


Figure S38: ^{13}C NMR spectrum of **8a** (50 MHz, $CDCl_3$).

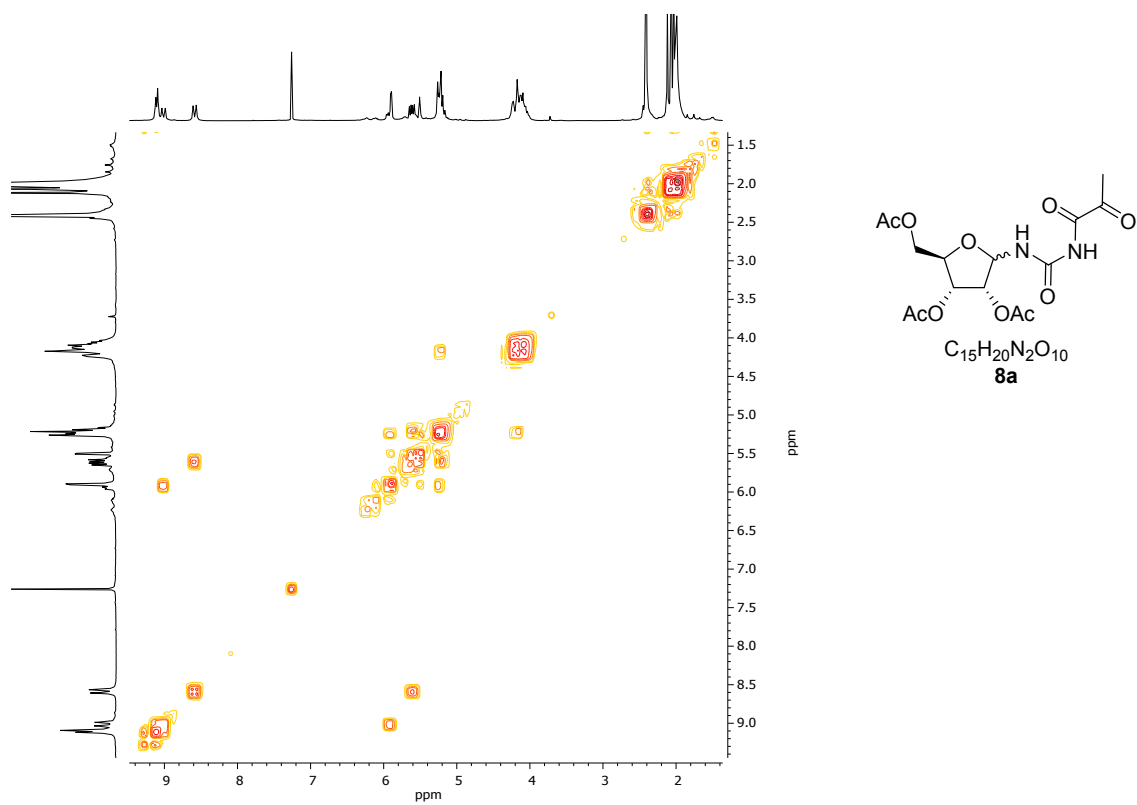


Figure S39: 2D-COSY spectrum of **8a** (200 MHz, $CDCl_3$).

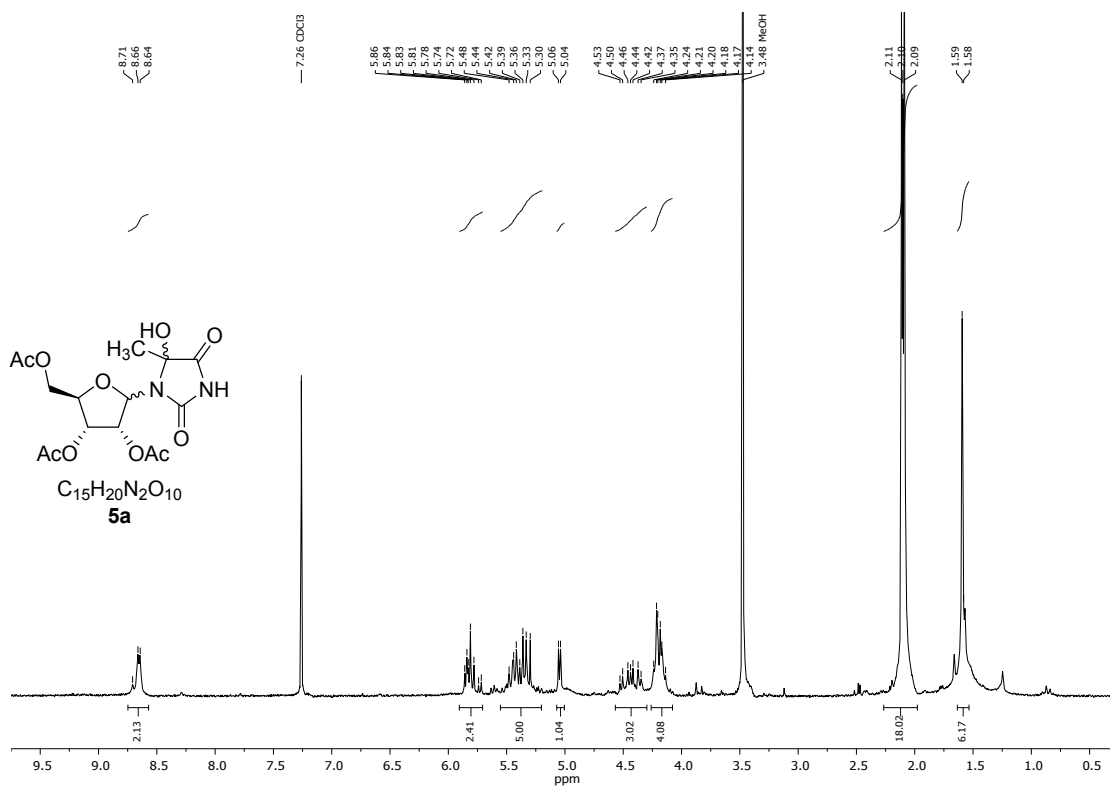


Figure S40: 1H NMR spectrum of **5a** (50 MHz, $CDCl_3$).

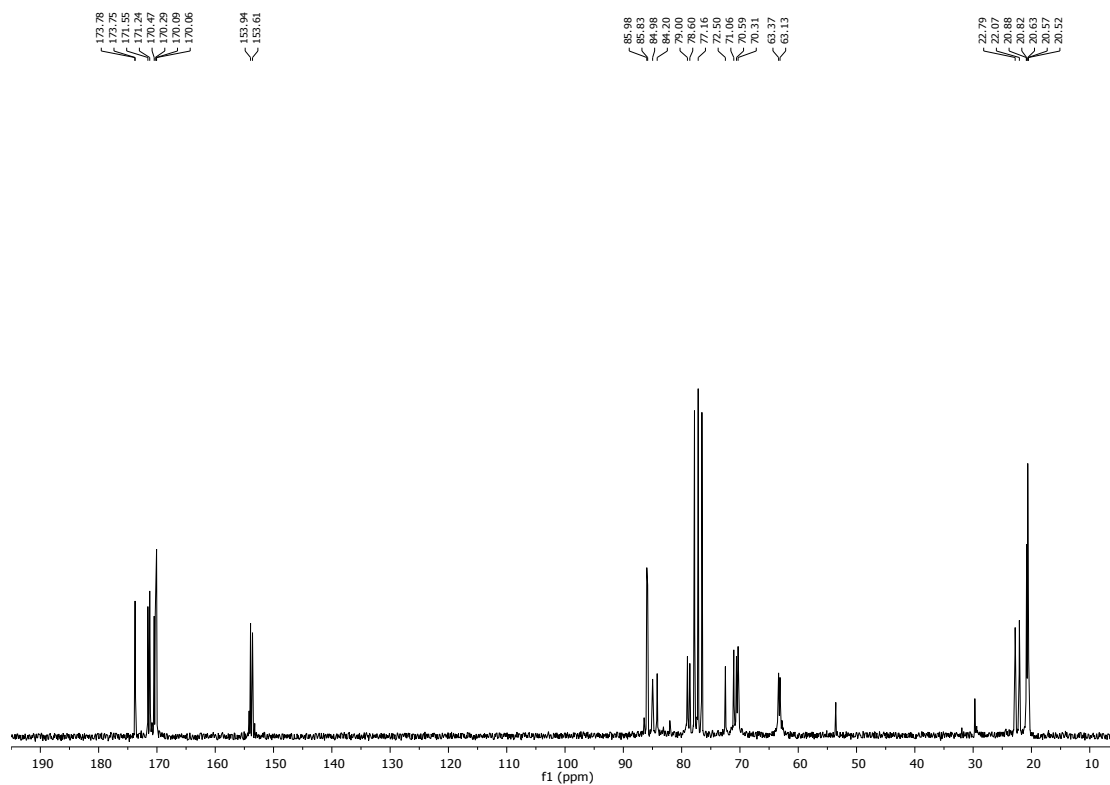


Figure S41: ^{13}C NMR spectrum of **5a** (50 MHz, $CDCl_3$).

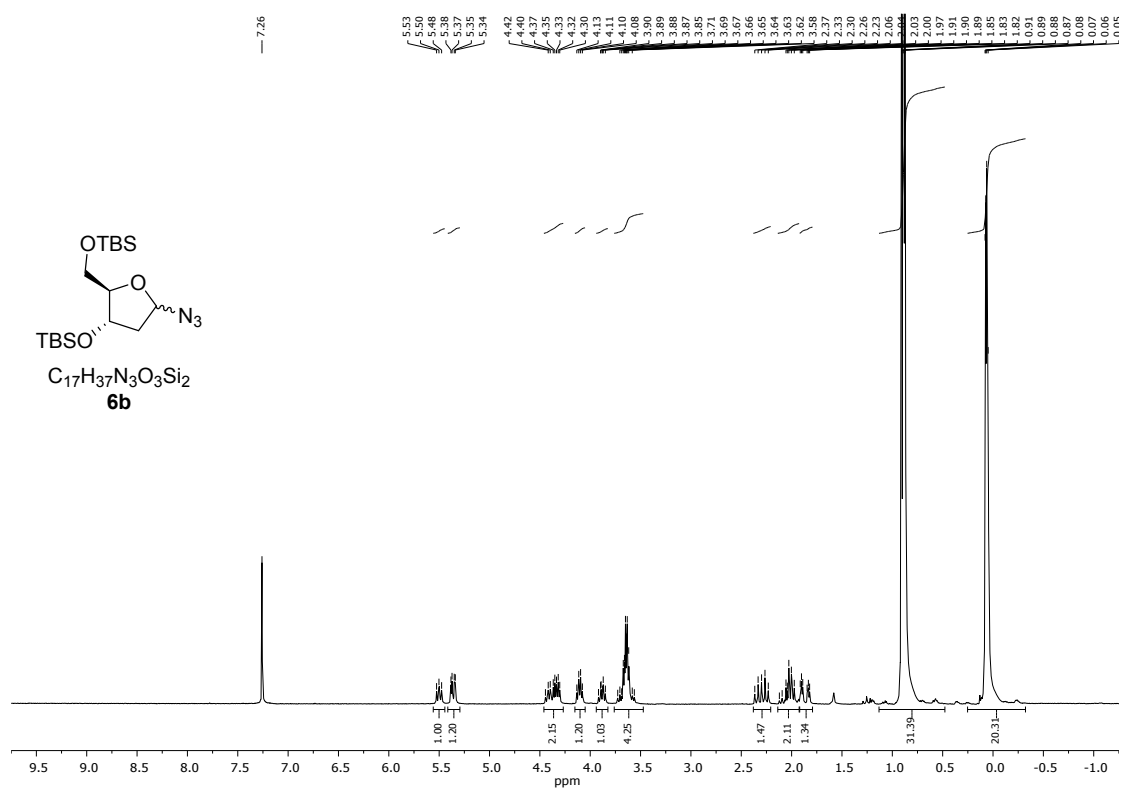


Figure S42: ^1H NMR spectrum of **6b** (200 MHz, CDCl_3).

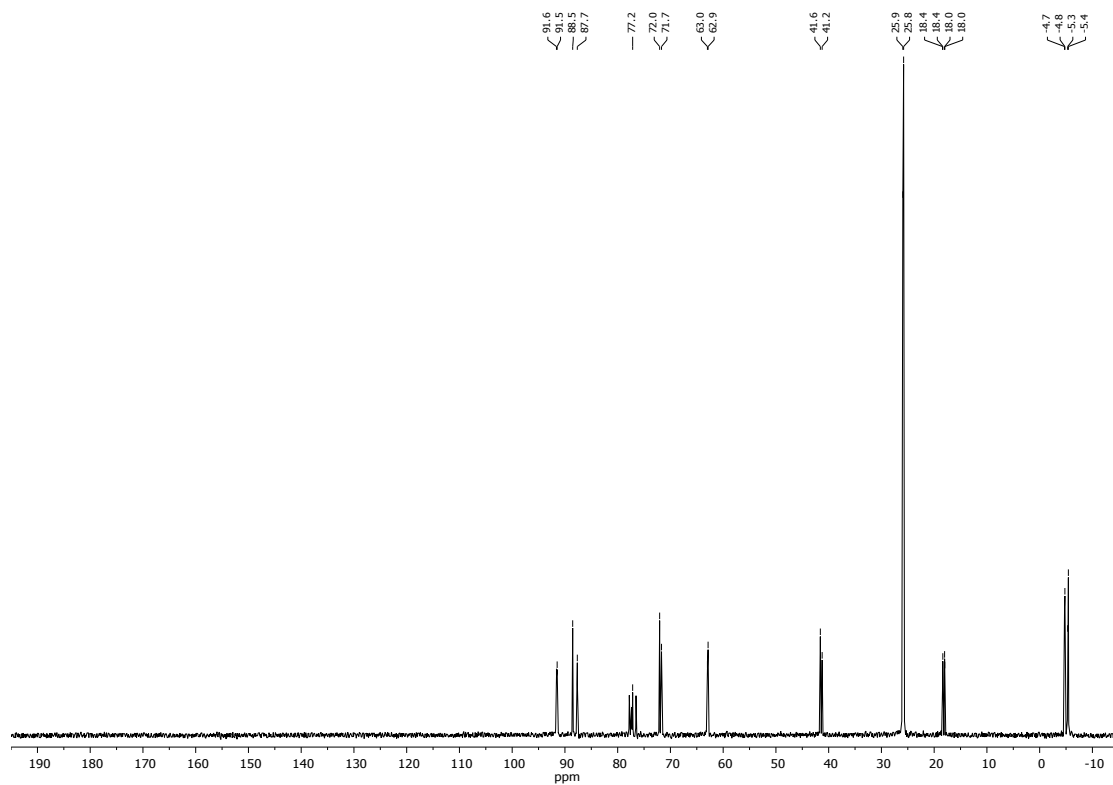


Figure S43: ^{13}C NMR spectrum of **6b** (50 MHz, CDCl_3).

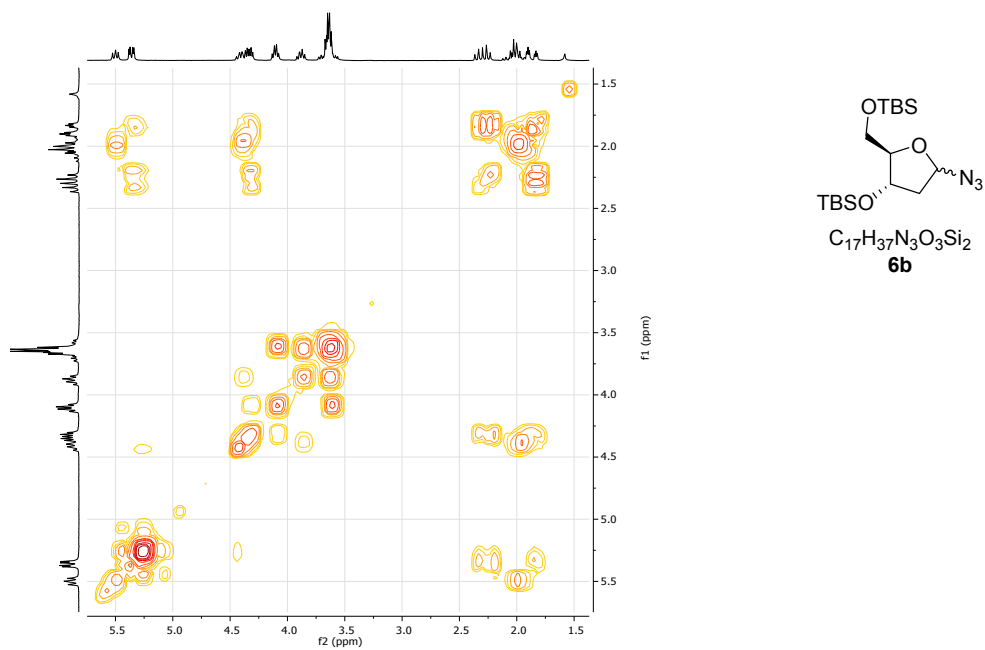


Figure S44: 2D-COSY spectrum of **6b** (200 MHz, $CDCl_3$).

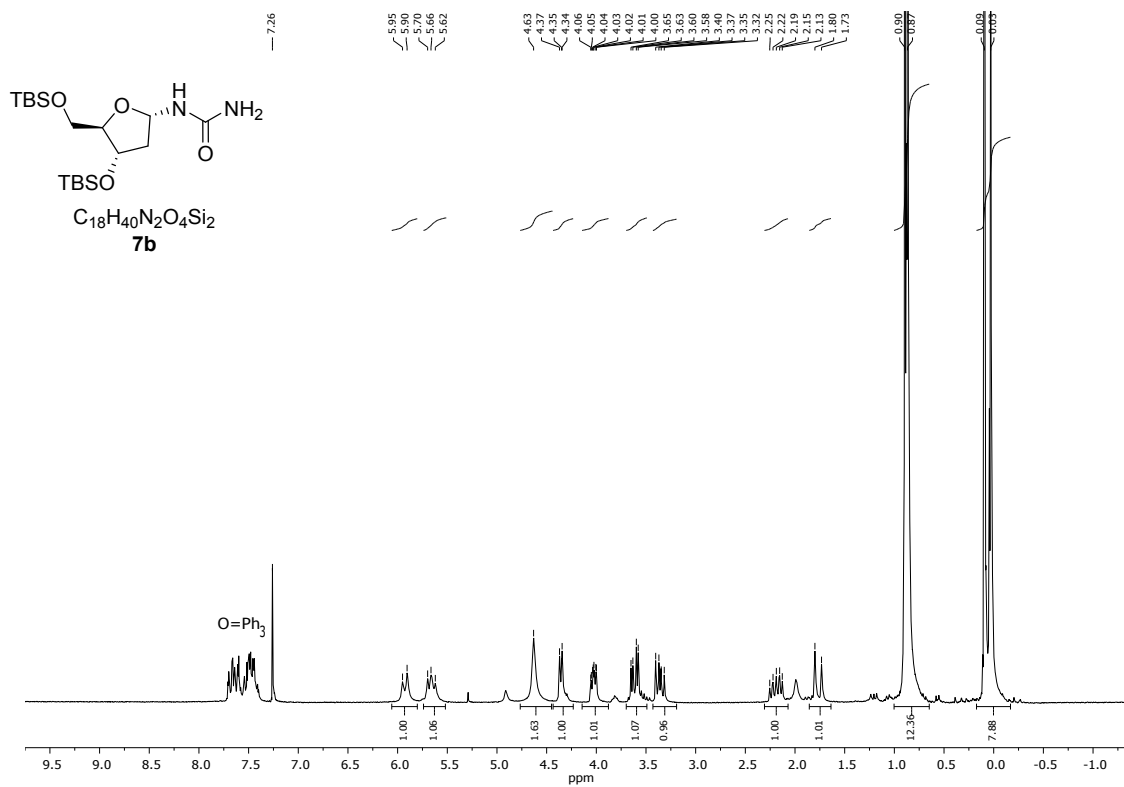


Figure S45: ^1H NMR spectrum of α -anomer of **7b** (200 MHz, CDCl_3).

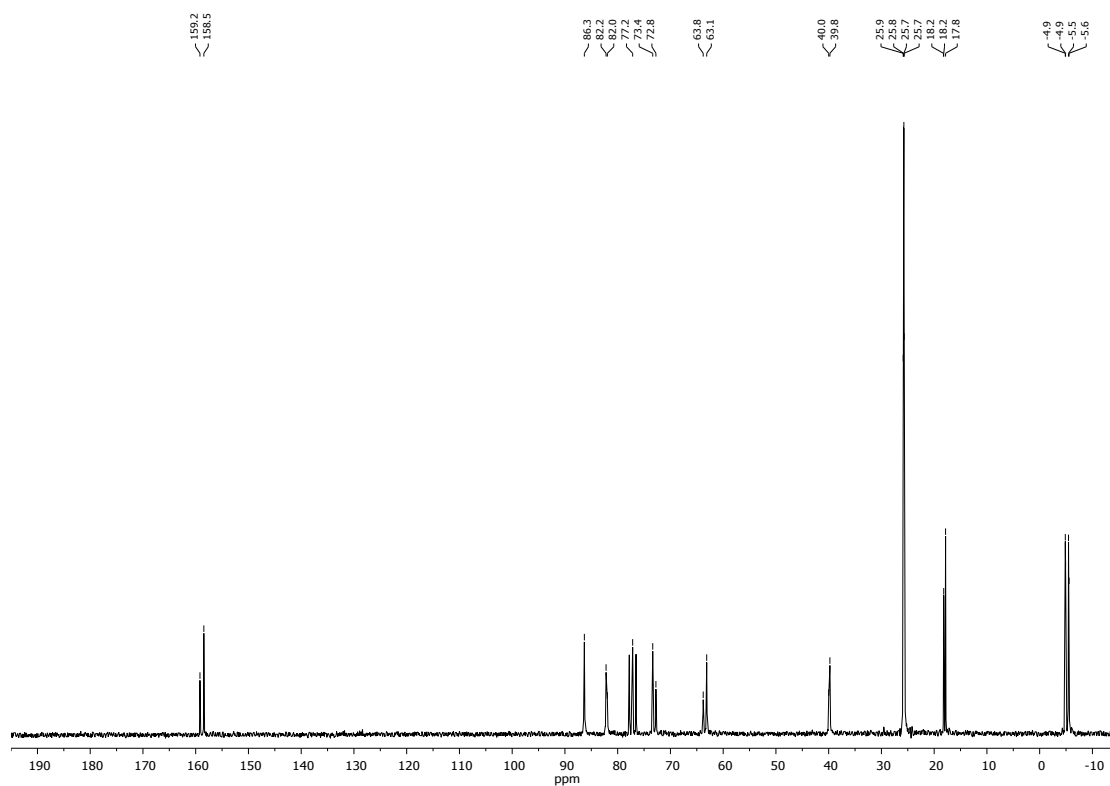
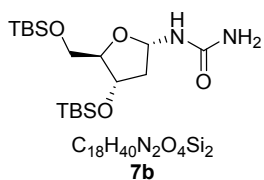


Figure S46: ^{13}C NMR spectrum of α -anomer of **7b** (50 MHz, CDCl_3).



Parameter	Value
1 Title	
2 Comment	Gimisis/ 14, NOESY, CDCl ₃ , 295, MPS187_col28, 4/ 6/ 13 (avance 500)
3 Origin	UXNMR, Bruker Analytische Messtechnik GmbH
4 Owner	root
5 Site	
6 Instrument	spect
7 Author	
8 Solvent	MeOH
9 Temperature	300.0
10 Pulse Sequence	noesytp
11 Experiment	NOESY
12 Probe	5 mm BBI 1H-BB-D Z-GRD Z8107/0186
13 Number of Scans	8
14 Receiver Gain	100.0
15 Relaxation Delay	1.0000
16 Pulse Width	9.6000
17 Presaturation Frequency	
18 Acquisition Time	0.1278
19 Acquisition Date	2013-06-04T17:53:42
20 Modification Date	2013-06-04T18:46:46
21 Class	
22 Spectrometer Frequency (500.13, 500.13)	
23 Spectral Width (4006.4, 4006.4)	
24 Lowest Frequency (-602.8, -602.8)	
25 Nucleus (1H, 1H)	
26 Acquired Size (512, 256)	
27 Spectral Size (512, 512)	

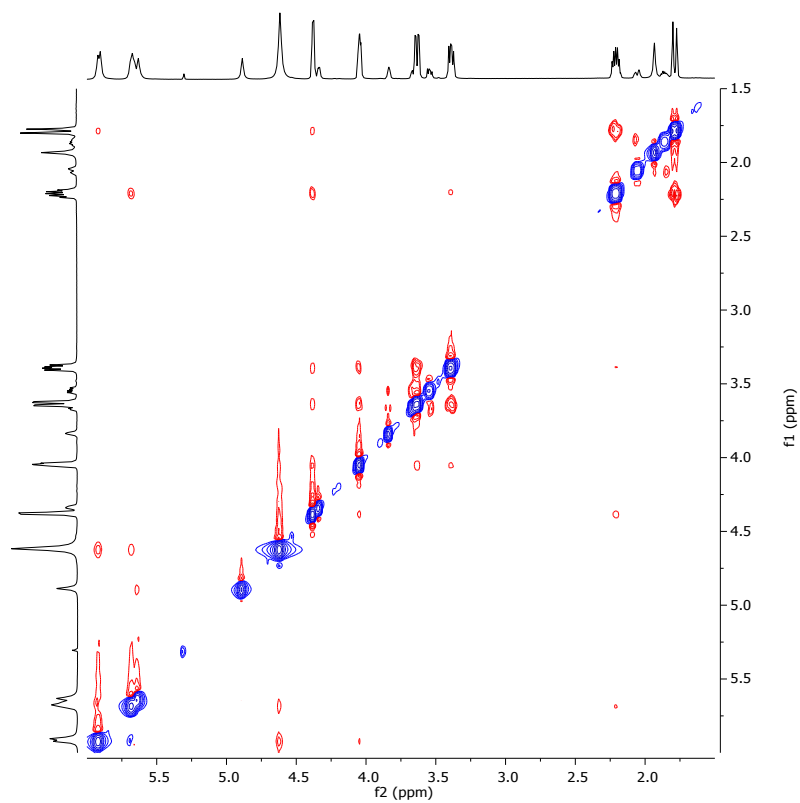


Figure S47: 2D-NOESY spectrum of α -anomer of **7b** (500 MHz, CDCl₃).

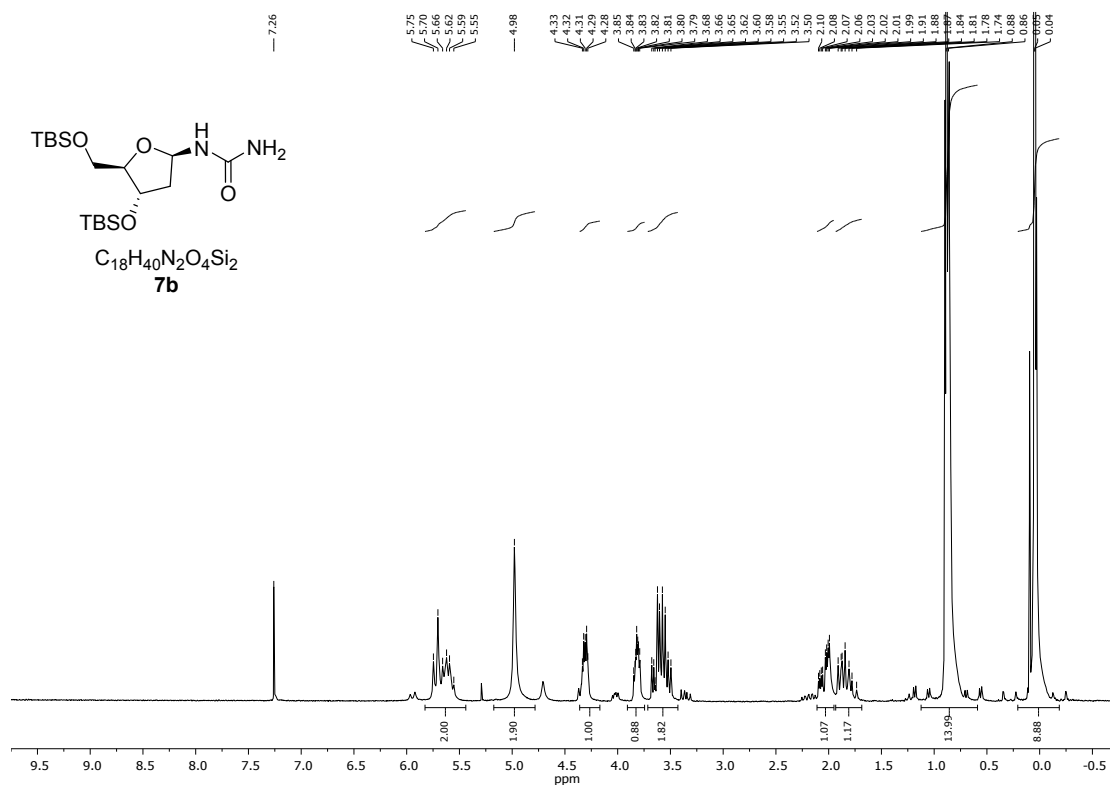


Figure S48: ^1H NMR spectrum of β -anomer of **7b** (200 MHz, CDCl_3).

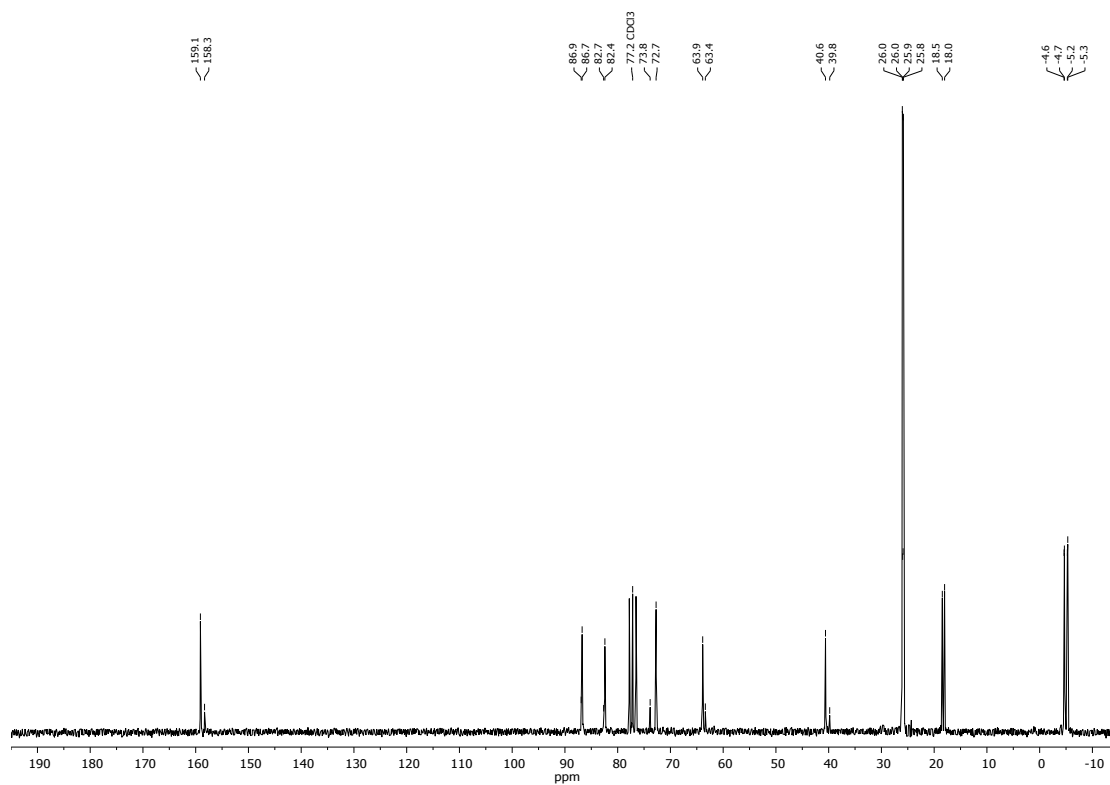
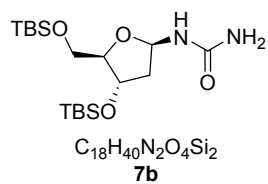


Figure S49: ^{13}C NMR spectrum of β -anomer of **7b** (50 MHz, CDCl_3).



Parameter	Value
1 Title	
2 Comment	Gimisis/ 18, NOESY, CDCl ₃ , 295, MPS187_col33_39, 7/ 6/ 13 (avance 500)
3 Origin	UXNMR, Bruker Analytische Messtechnik GmbH
4 Owner	root
5 Site	
6 Instrument	spect
7 Author	
8 Solvent	CDCl ₃
9 Temperature	300.0
10 Pulse Sequence	noesytp
11 Experiment	NOESY
12 Probe	5 mm BBI 1H-BB-D Z-GRD 28107/ 0186
13 Number of Scans	8
14 Receiver Gain	100.0
15 Relaxation Delay	1.0000
16 Pulse Width	9.6000
17 Presaturation Frequency	
18 Acquisition Time	0.0852
19 Acquisition Date	2013-06-07T15:40:11
20 Modification Date	2013-06-07T16:23:02
21 Class	
22 Spectrometer Frequency	(500.13, 500.13)
23 Spectral Width	(6009.6, 6009.6)
24 Lowest Frequency	(-1014.3, -1014.3)
25 Nucleus	(1H, 1H)
26 Acquired Size	(512, 217)
27 Spectral Size	(512, 512)

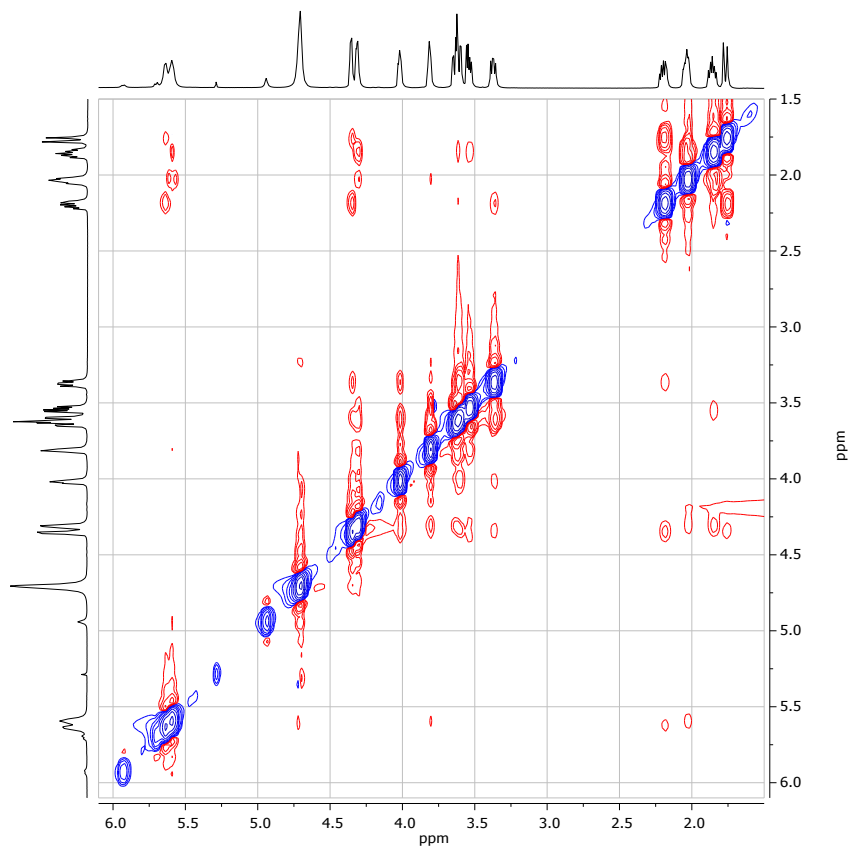


Figure S50: 2D-NOESY spectrum of β -anomer of **7b** (500 MHz, CDCl₃).

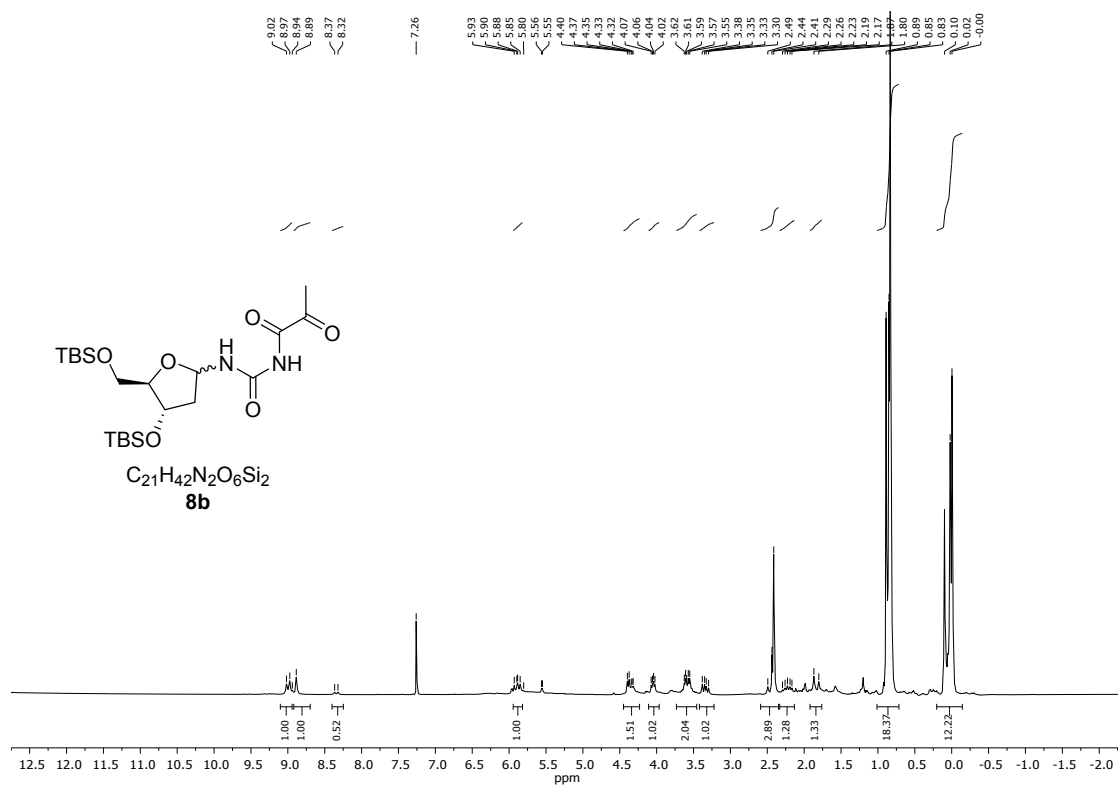


Figure S51: 1H NMR spectrum of **8b** (200 MHz, $CDCl_3$).

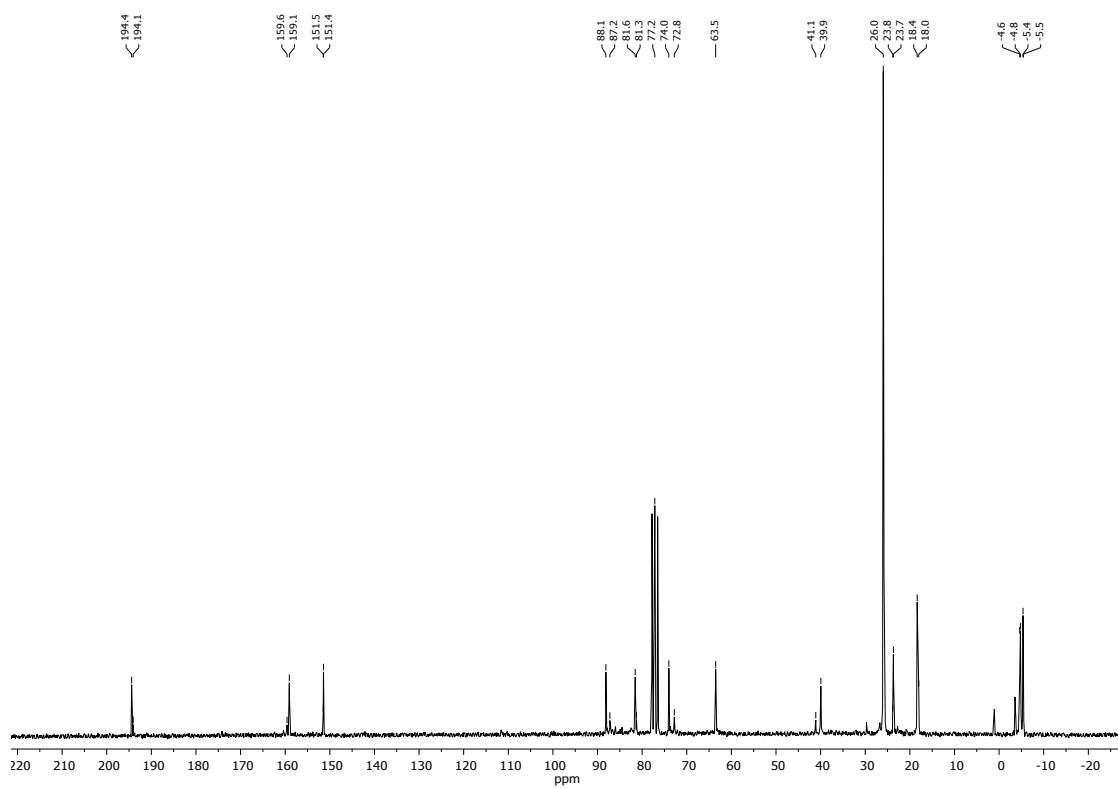


Figure S52: ^{13}C NMR spectrum of **8b** (50 MHz, $CDCl_3$).

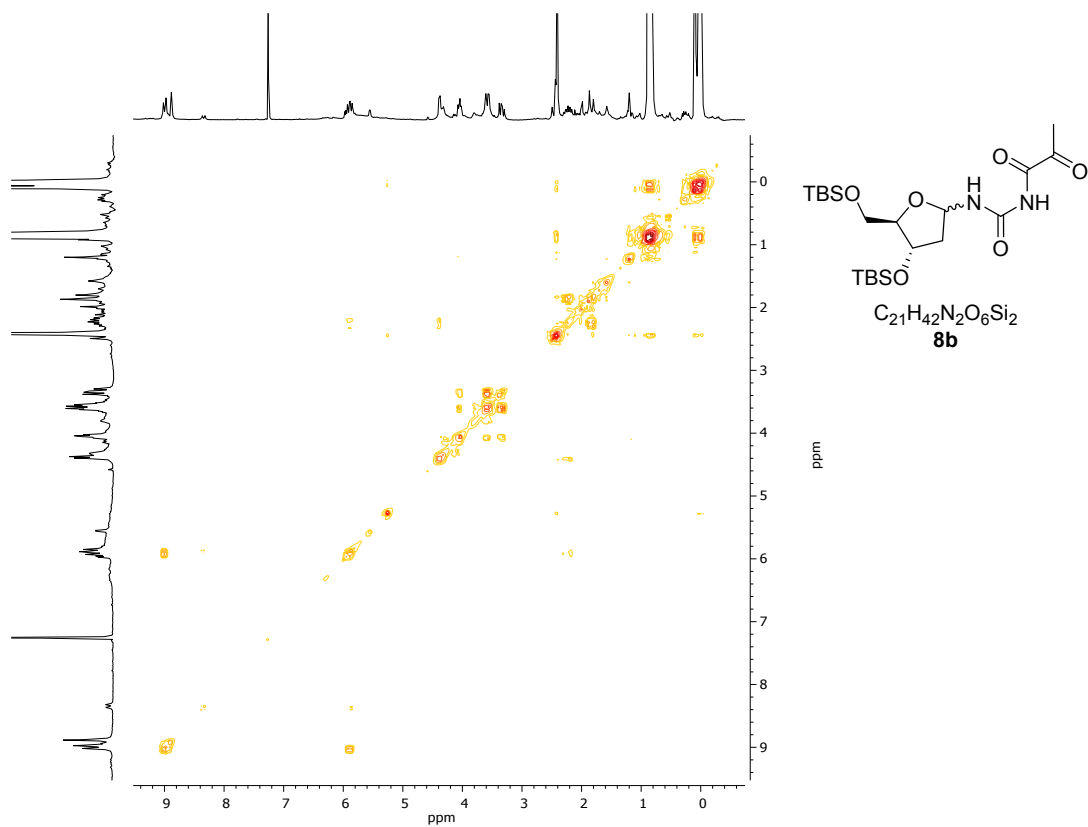


Figure S53: 2D-COSY spectrum of **8b** (200 MHz, $CDCl_3$).

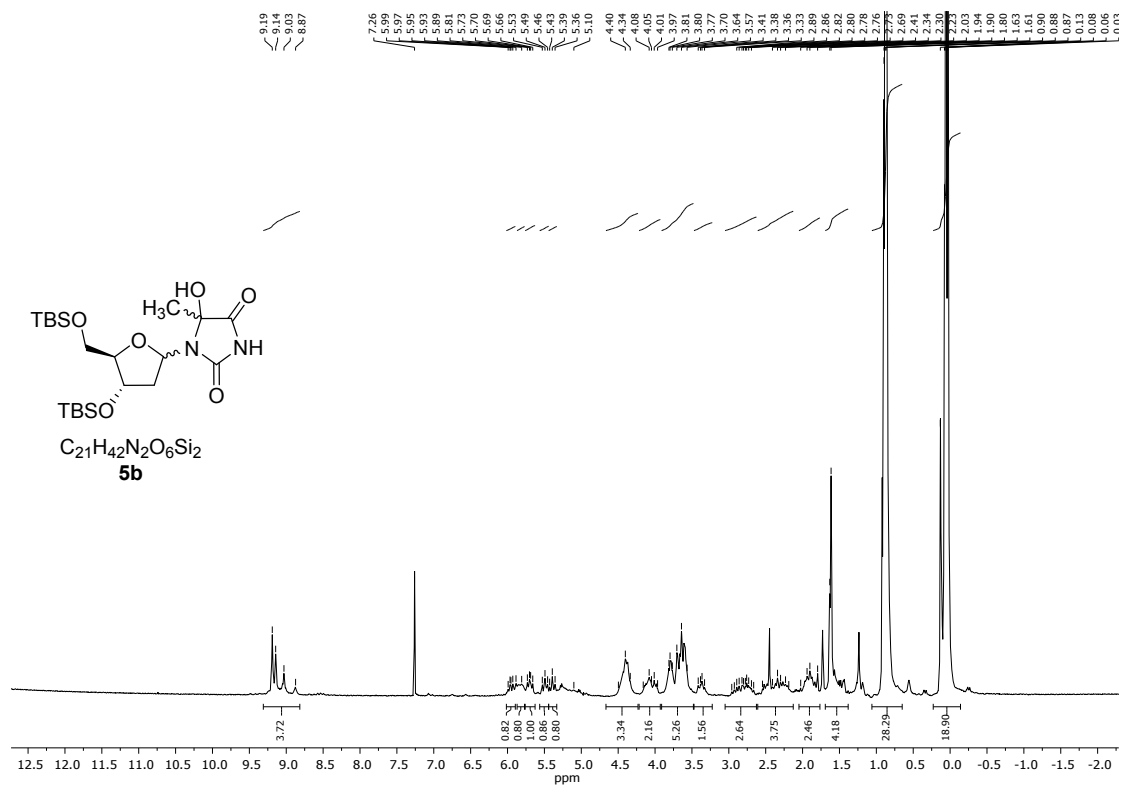


Figure S54: $^1\text{H NMR}$ spectrum of **5b** (200 MHz, CDCl_3).

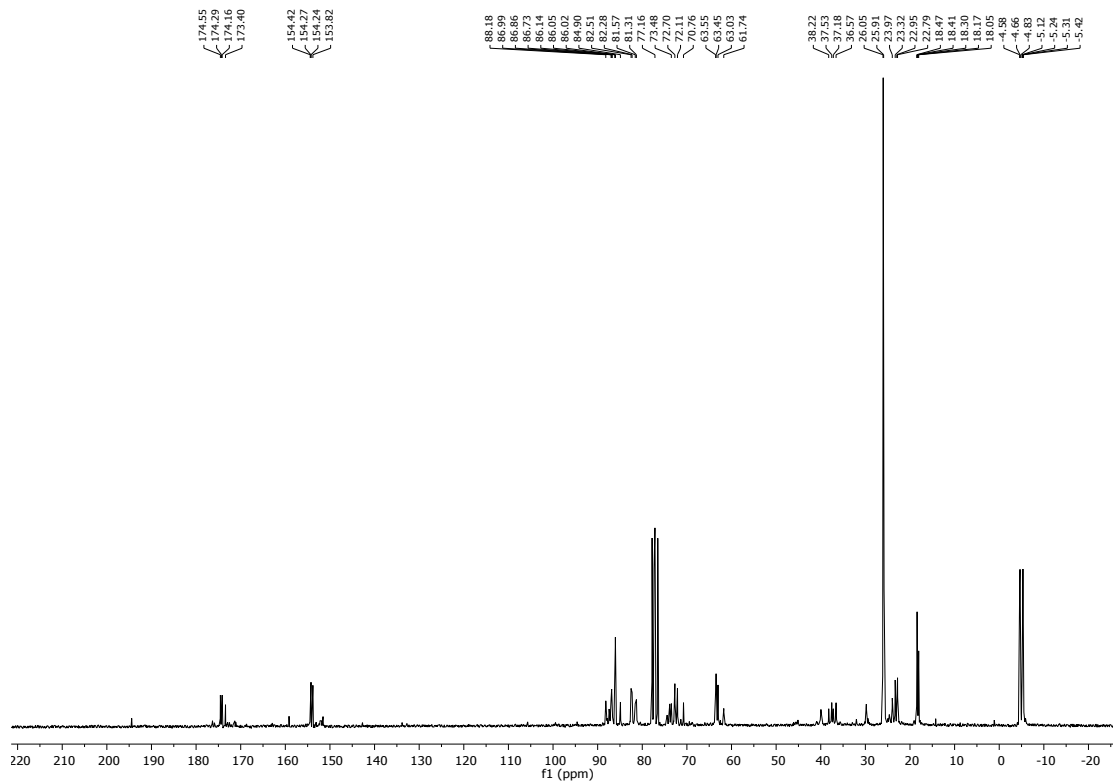


Figure S55: $^{13}\text{C NMR}$ spectrum of **5b** (50 MHz, CDCl_3).

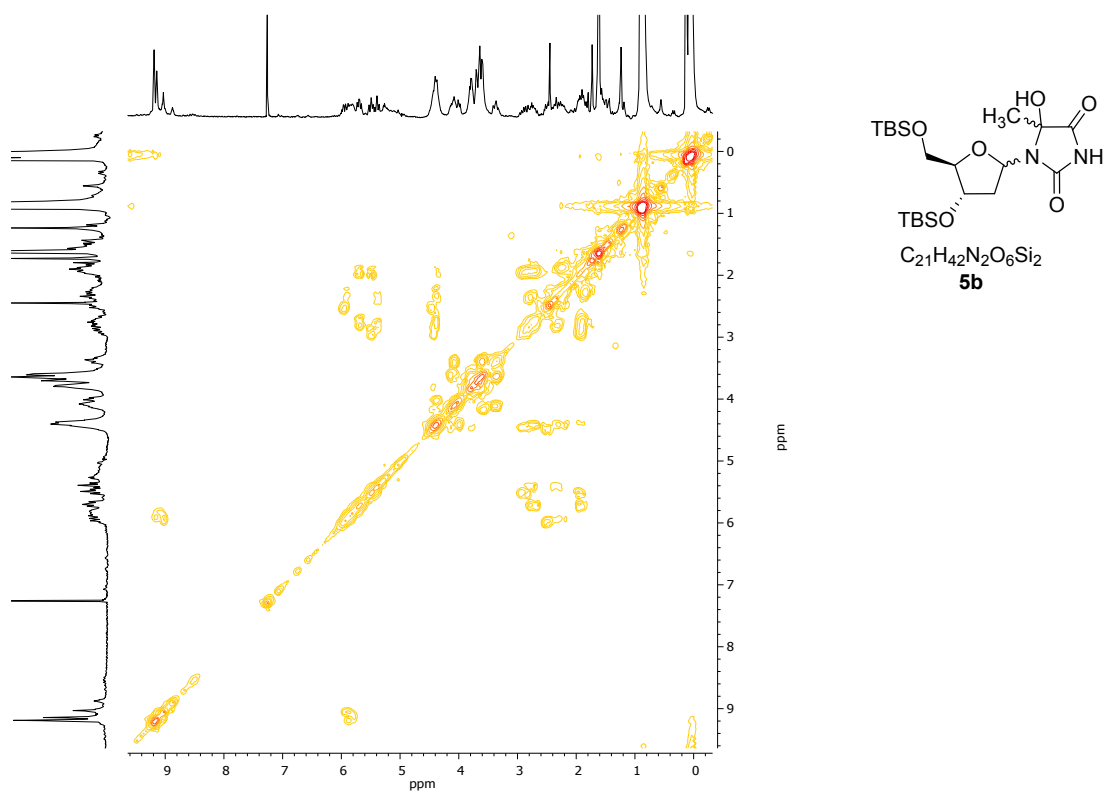


Figure S56: 2D-COSY spectrum of **5b** (200 MHz, CDCl₃).

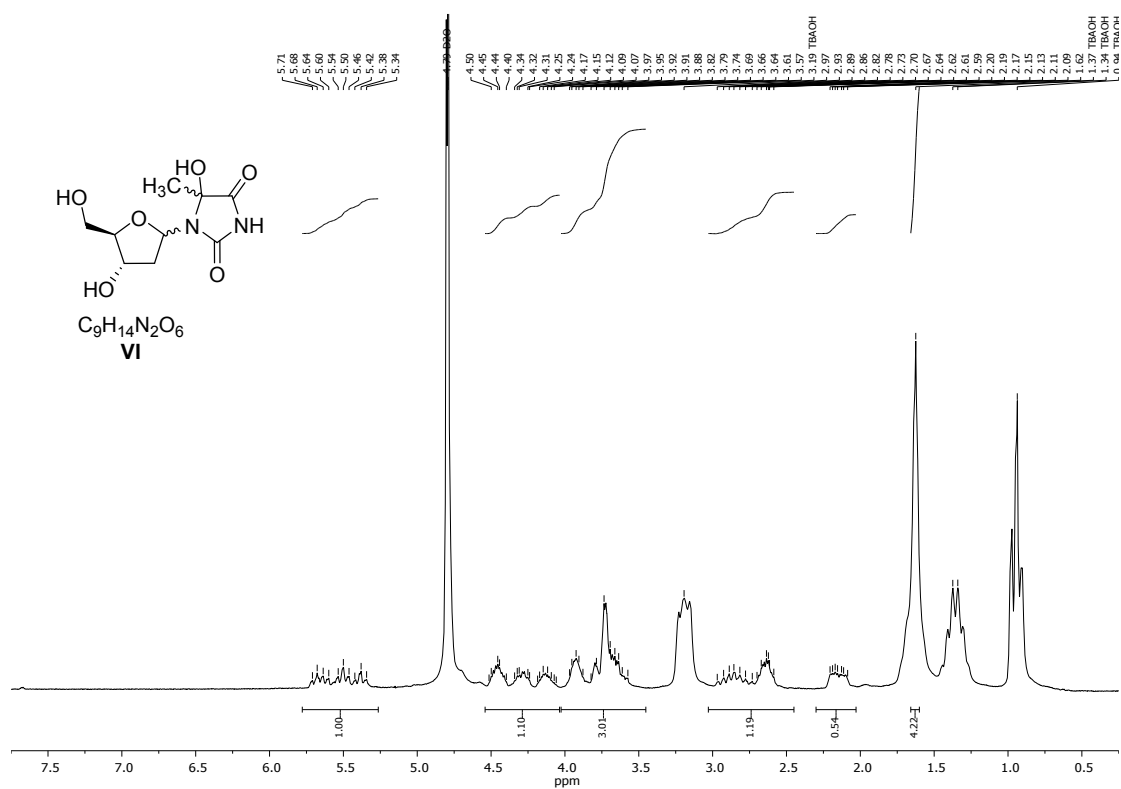


Figure S57: 1H NMR spectrum of VI (200 MHz, D_2O).

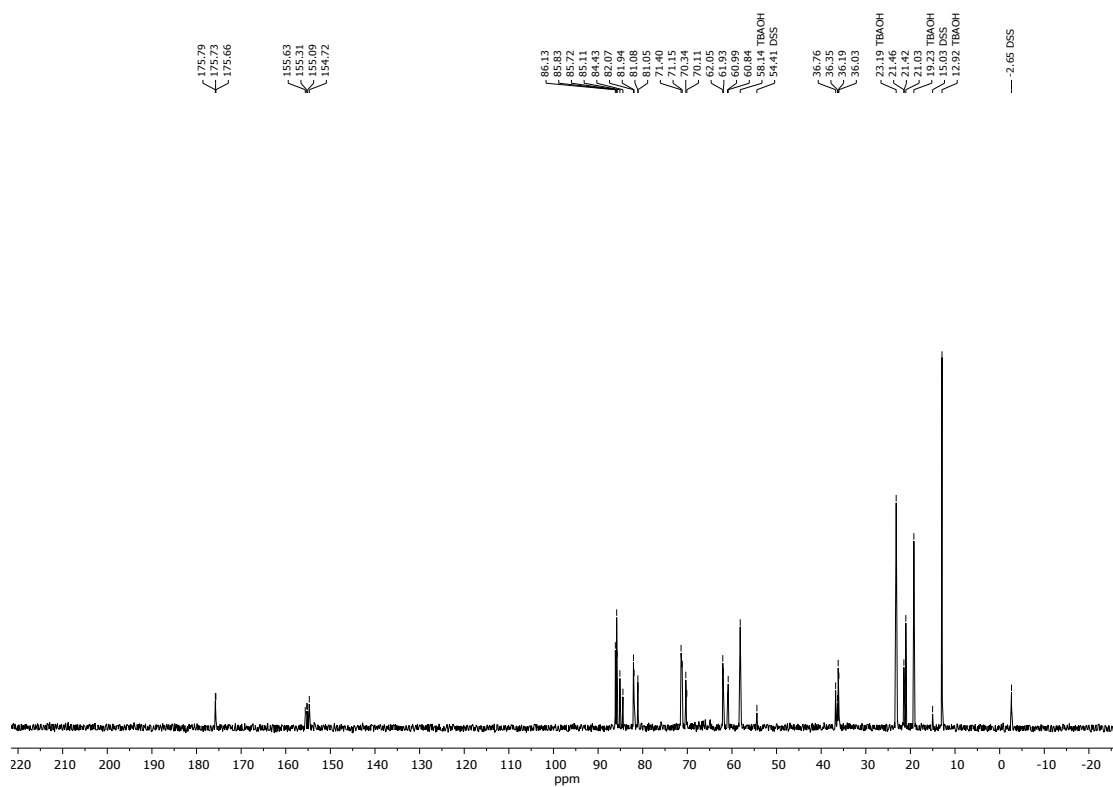


Figure S58: ^{13}C NMR spectrum of VI (50 MHz, D_2O).

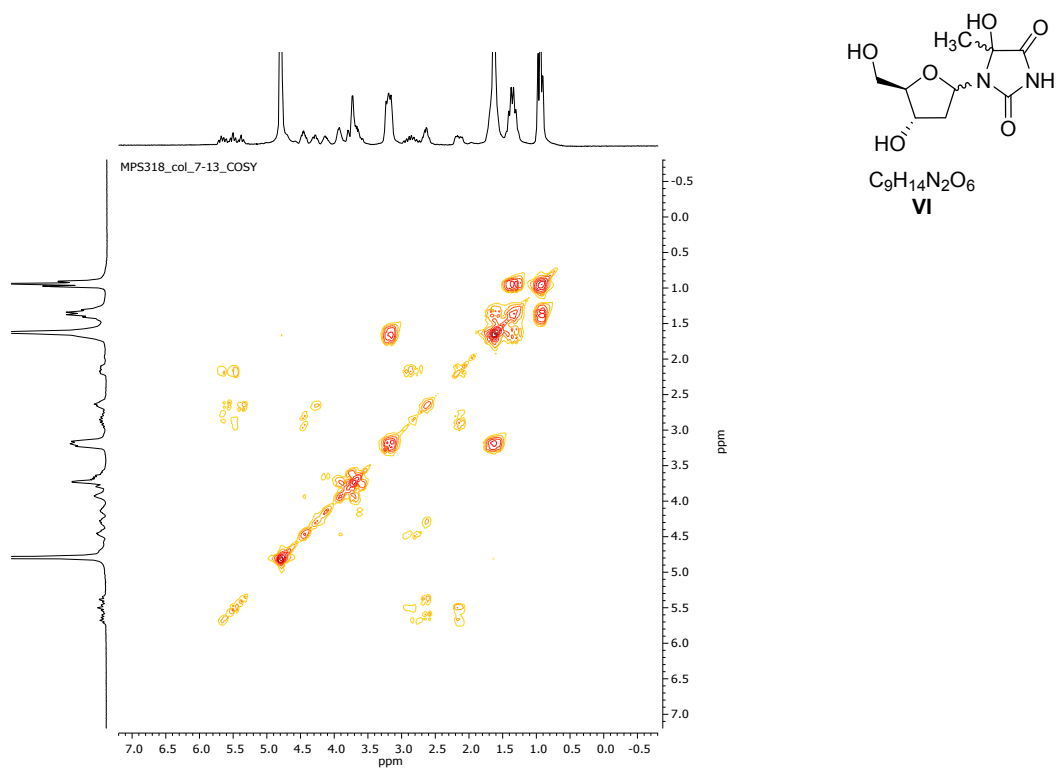


Figure S59: 2D-COSY spectrum of **VI** (200 MHz, D₂O).

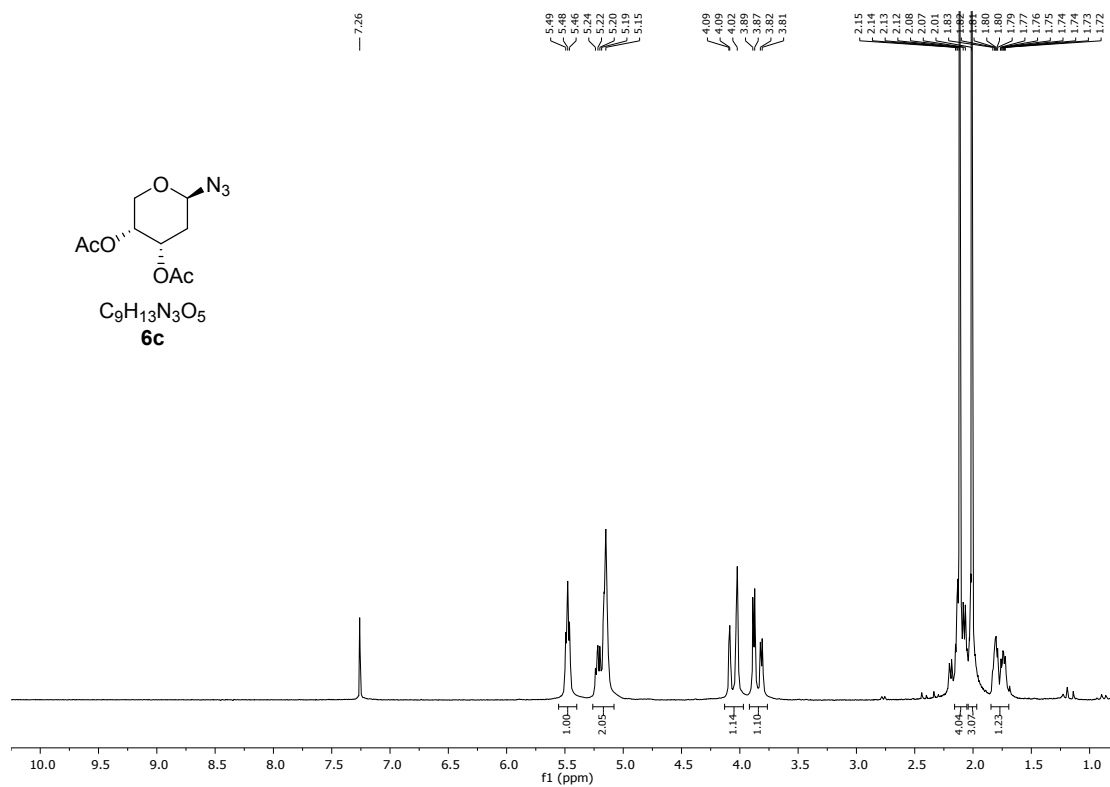


Figure S60: 1H NMR spectrum of **6c** (200 MHz, $CDCl_3$).

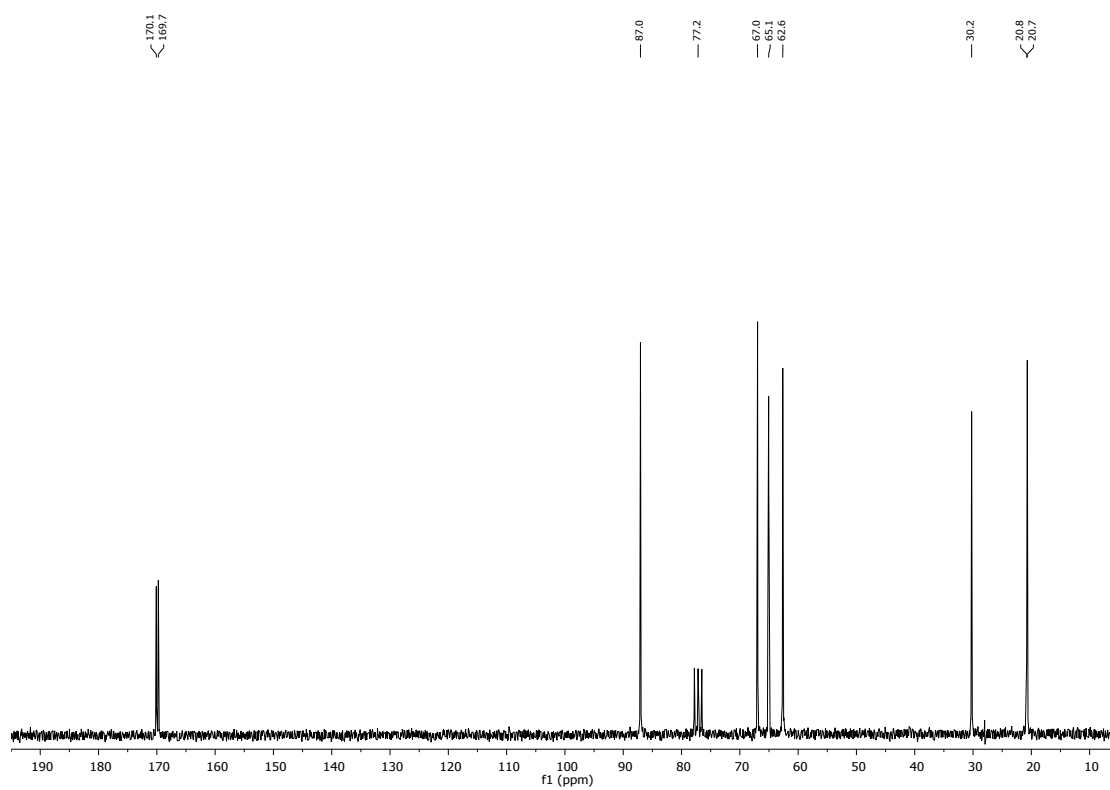


Figure S61: ^{13}C NMR spectrum of **6c** (50 MHz, $CDCl_3$).

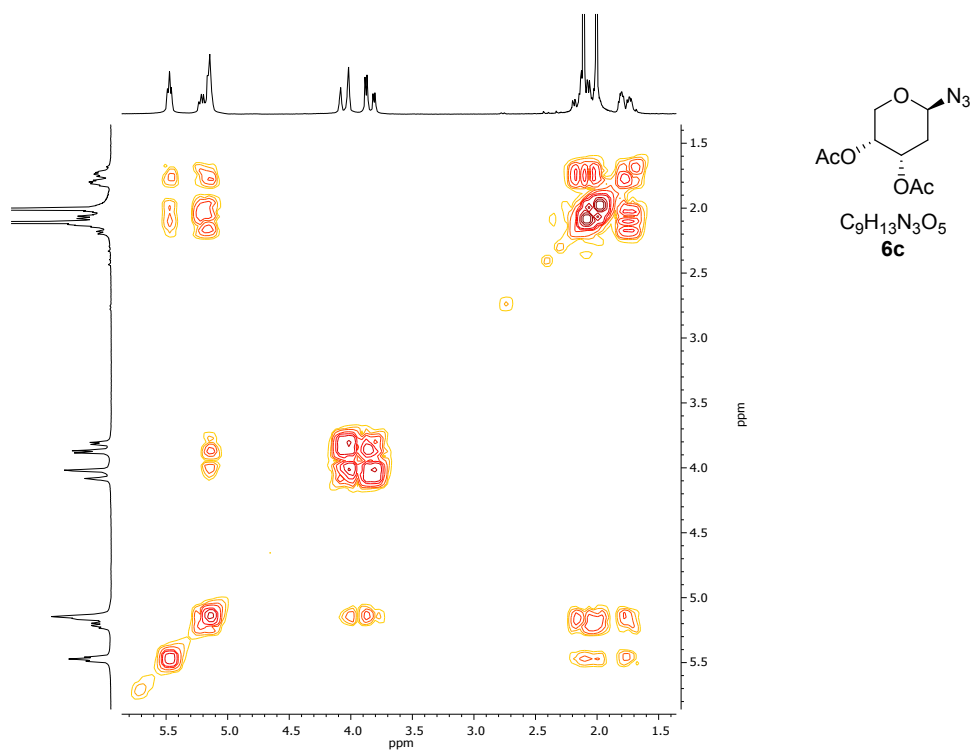


Figure S62: 2D-COSY spectrum of **6c** (200 MHz, $CDCl_3$).

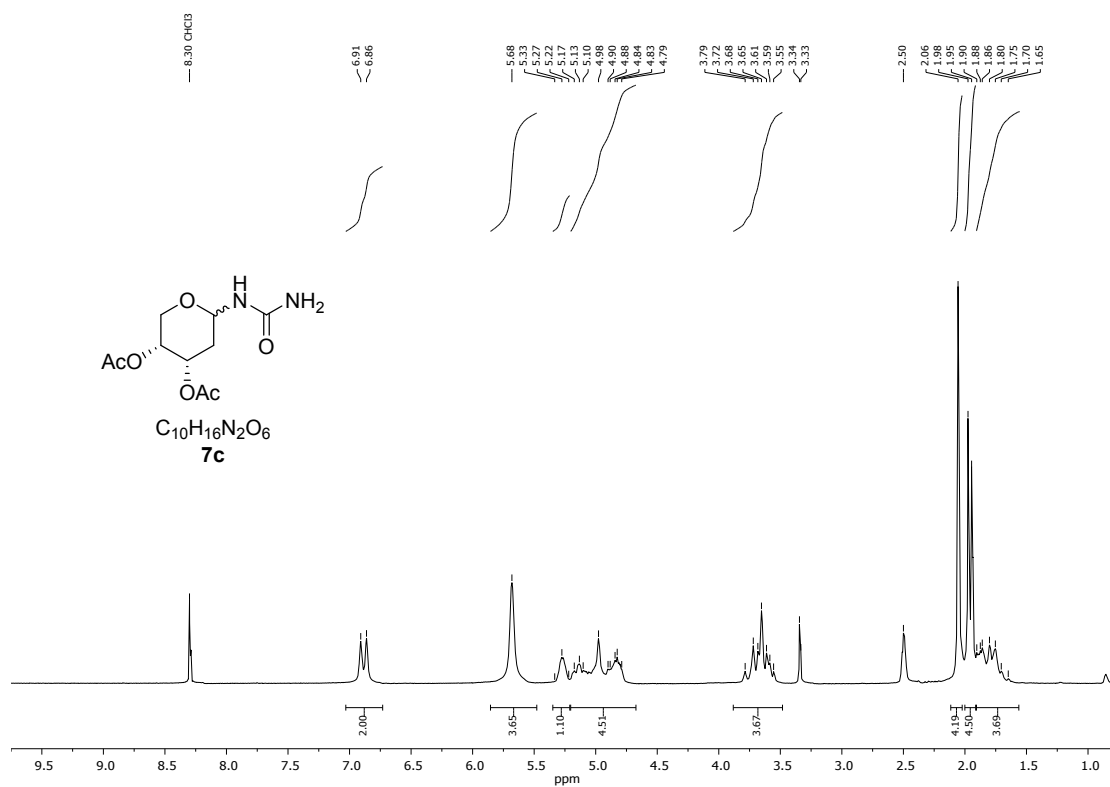


Figure S63: 1H NMR spectrum of **7c** (200 MHz, DMSO- d_6).

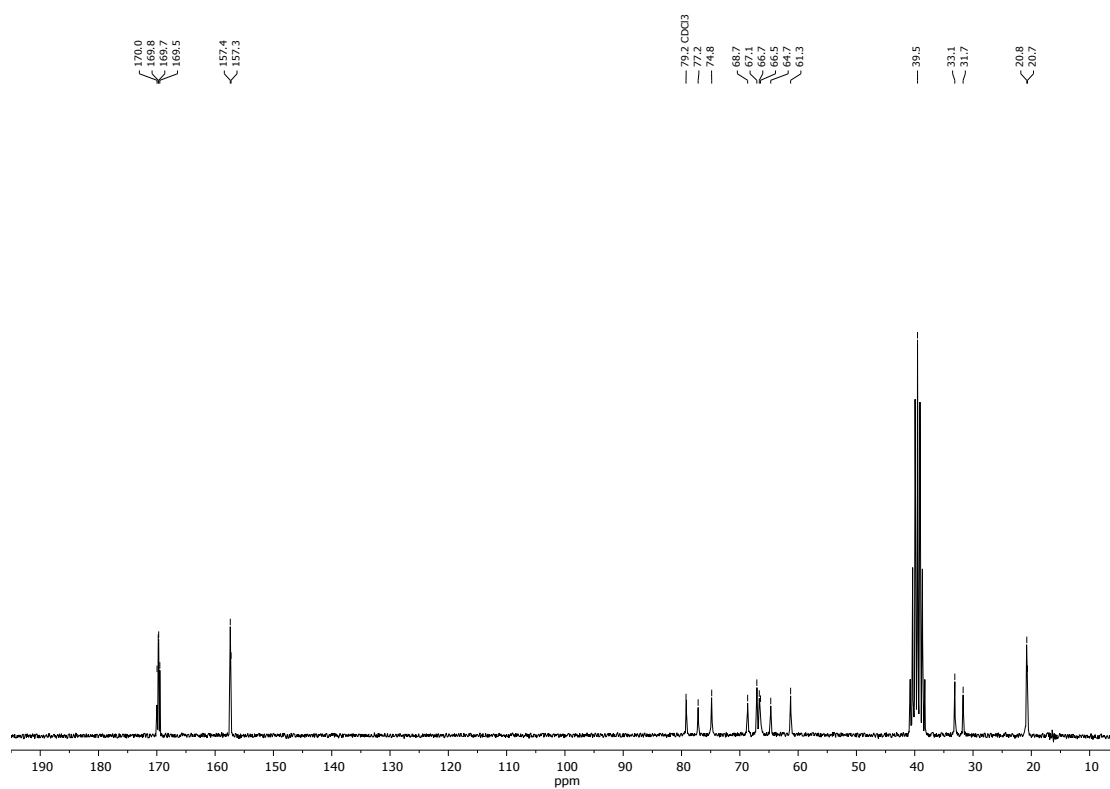


Figure S64: ^{13}C NMR spectrum of **7c** (200 MHz, DMSO- d_6).

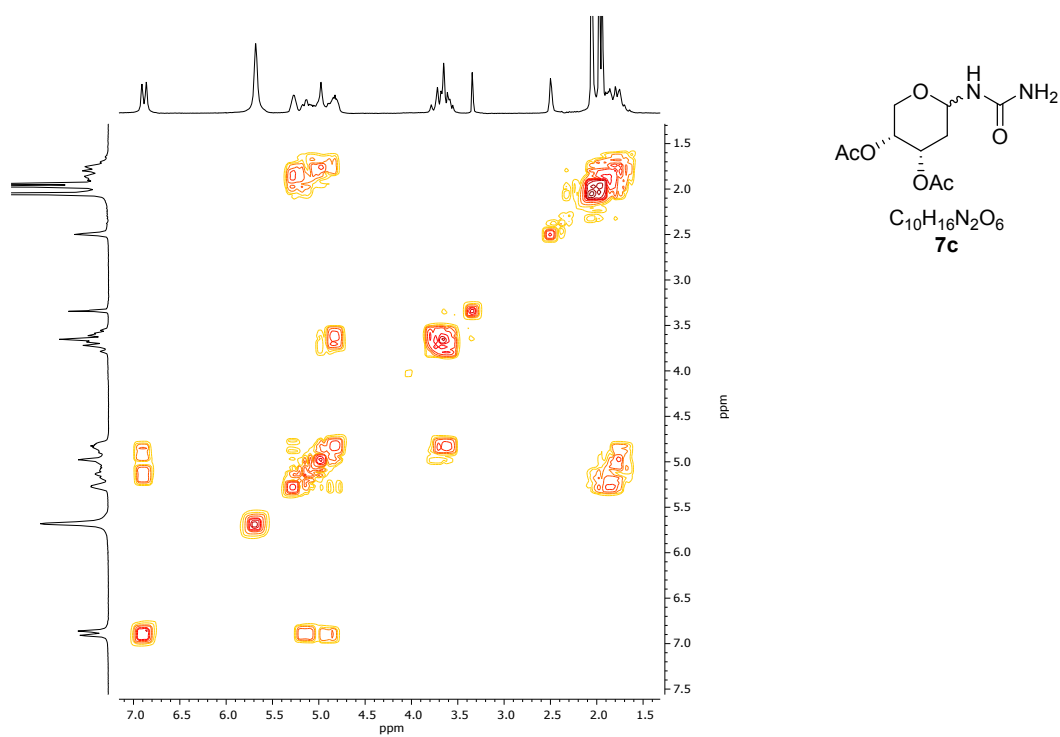


Figure S65: 1H NMR spectrum of **7c** (200 MHz, $DMSO-d_6$).

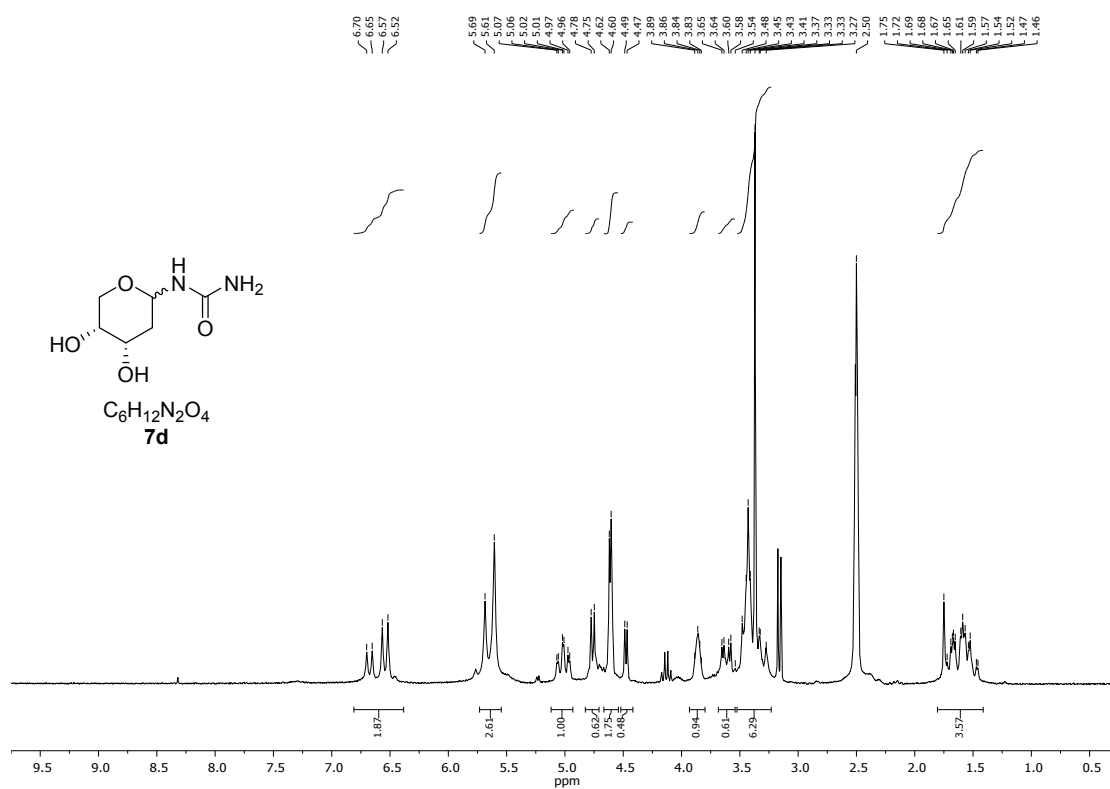


Figure S66: ¹H NMR spectrum of **7d** (200 MHz, DMSO-*d*₆).

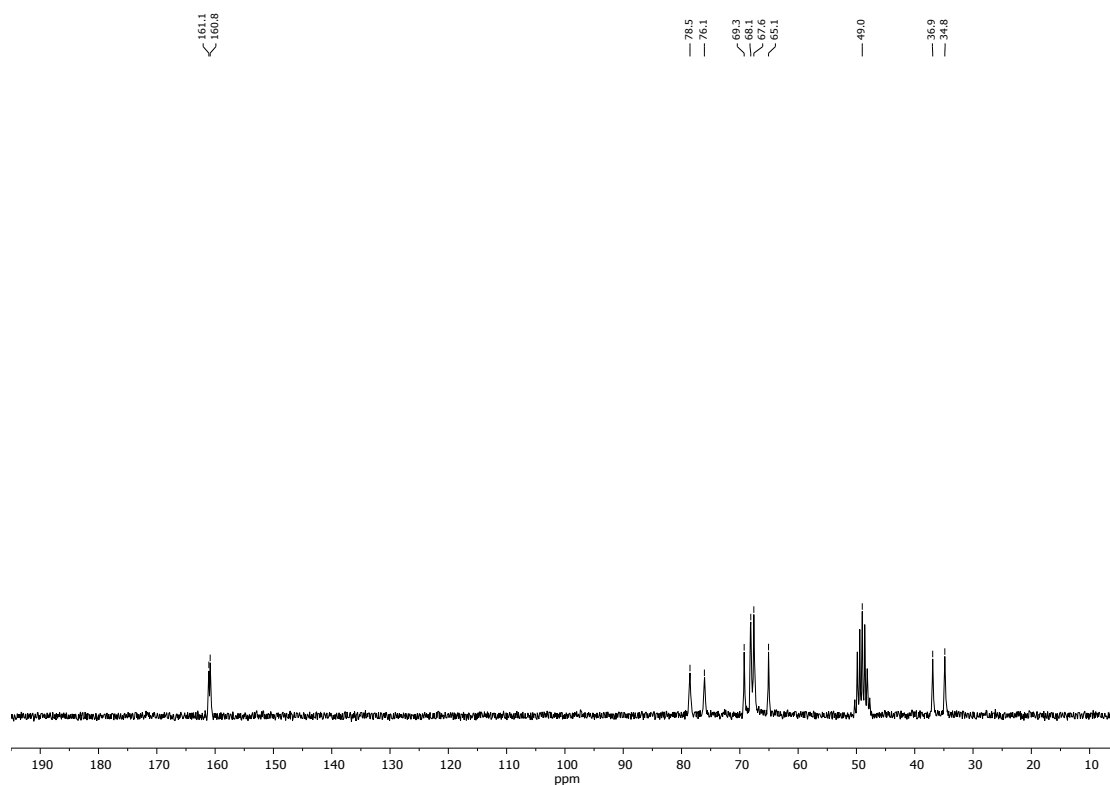


Figure S67: ¹³C NMR spectrum of **7d** (50 MHz, CD₃OD).

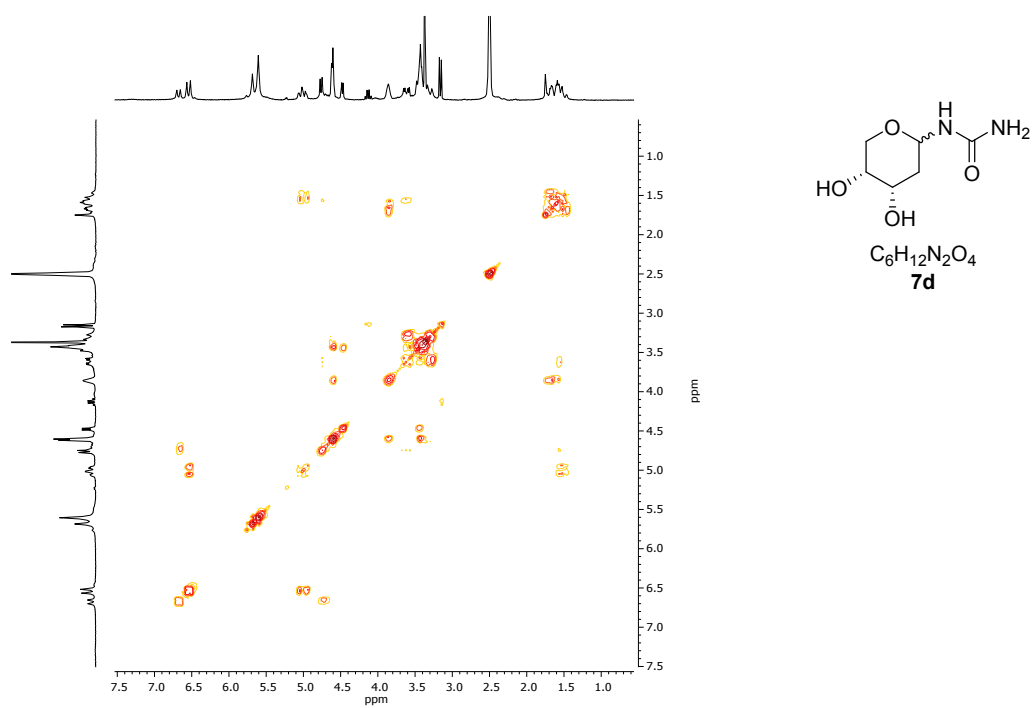


Figure S68: 2D-COSY spectrum of **7d** (200 MHz, DMSO-*d*₆).

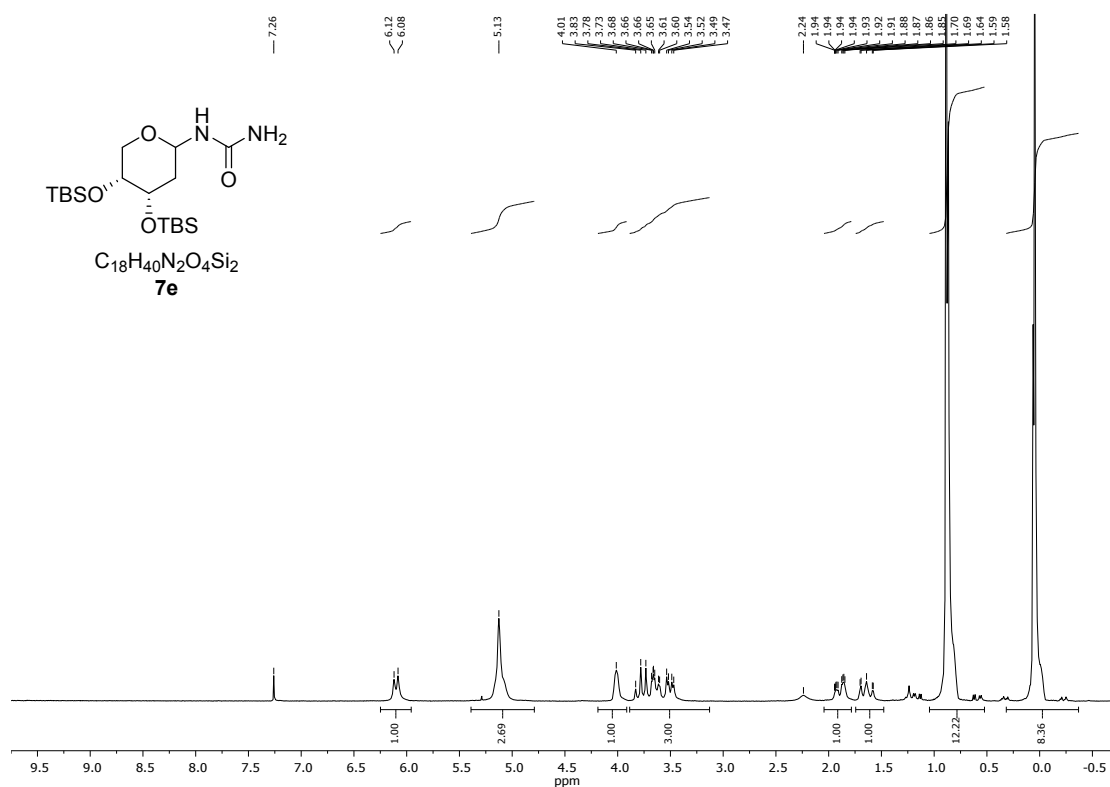


Figure S69: ^1H NMR spectrum of **7e** (200 MHz, CDCl_3).

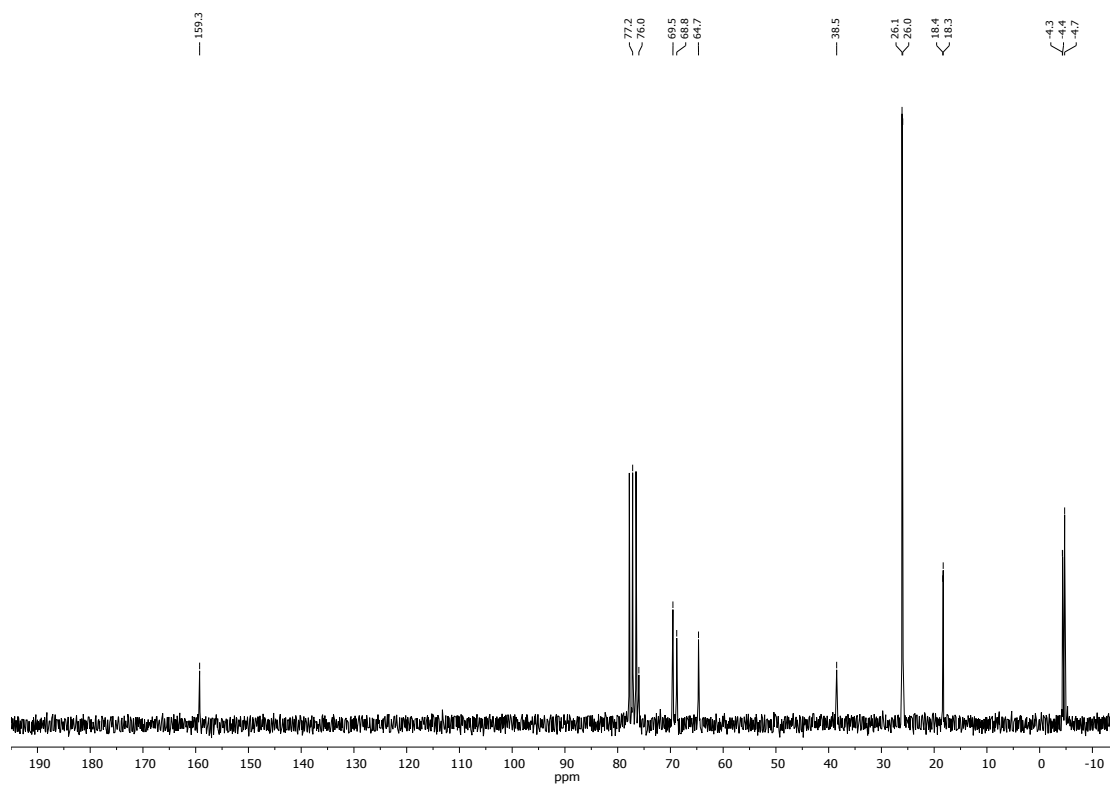


Figure S70: ^{13}C NMR spectrum of **7e** (50 MHz, CDCl_3).

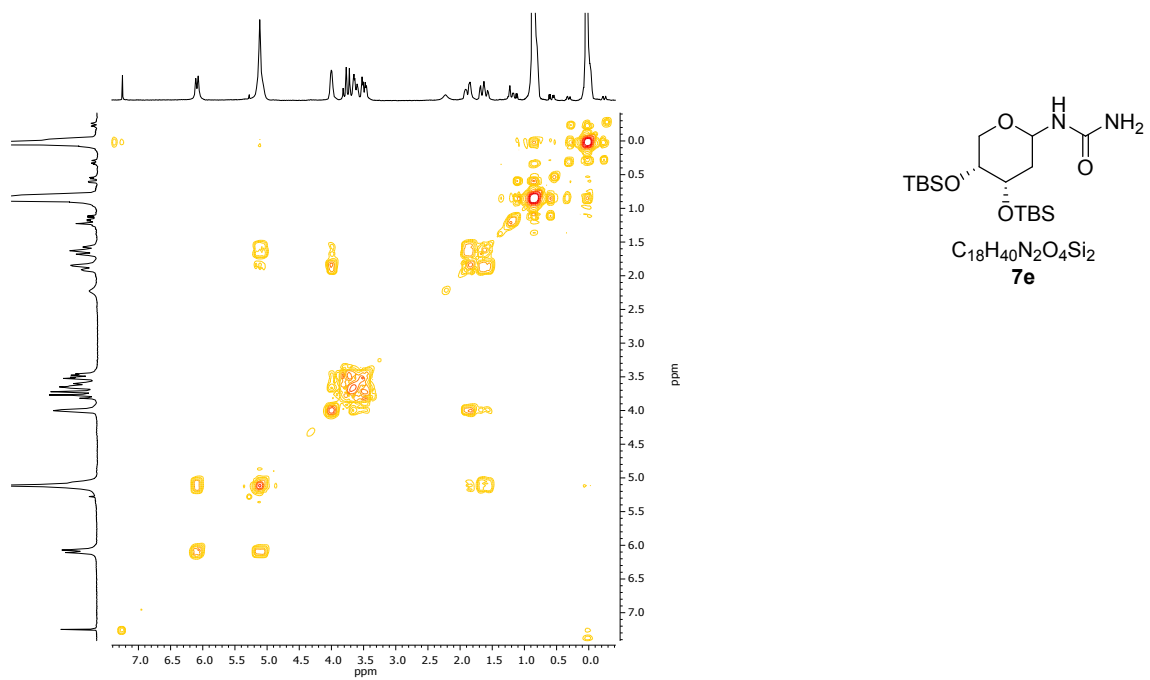


Figure S71: 2D-COSY spectrum of **7e** (200 MHz, $CDCl_3$).

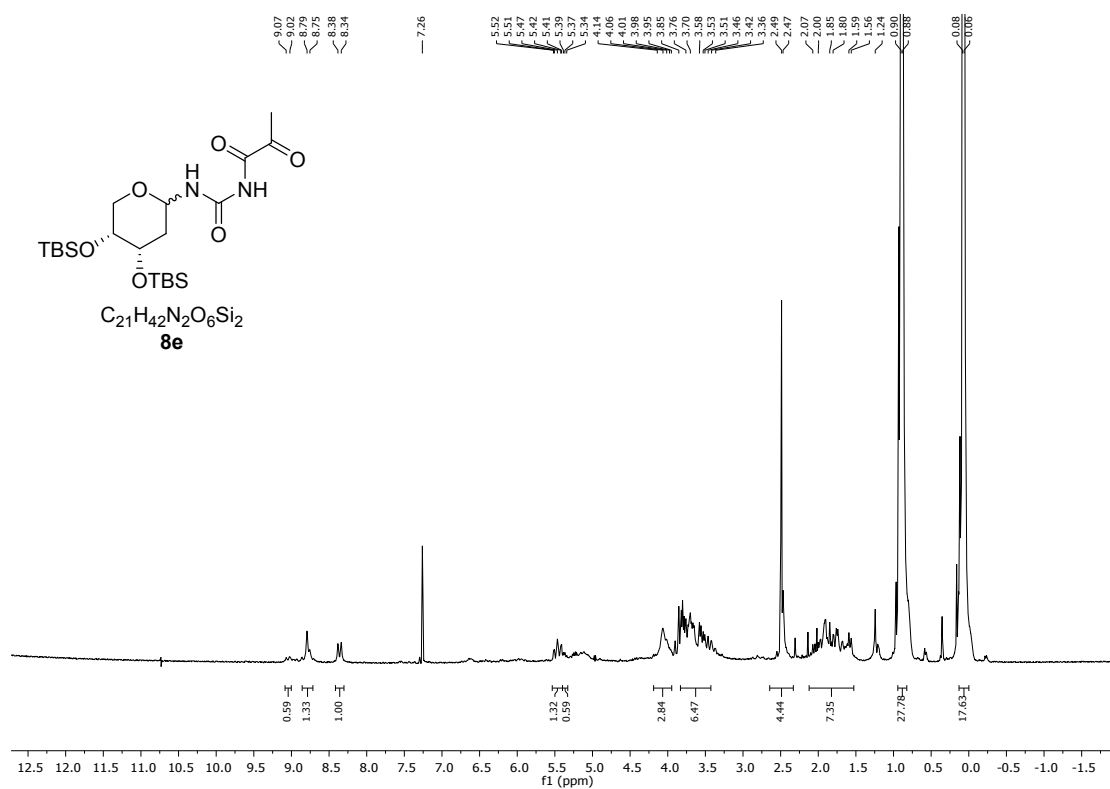


Figure S72: 1H NMR spectrum of **8e** (200 MHz, $CDCl_3$).

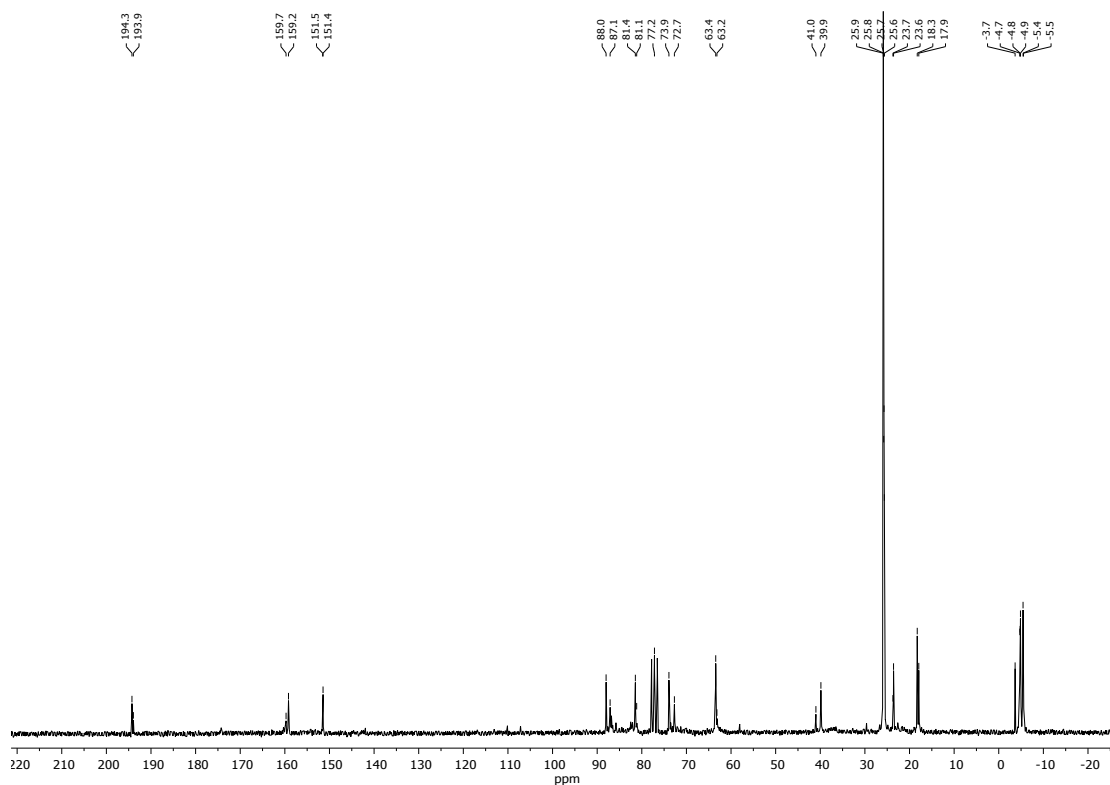


Figure S73: ^{13}C NMR spectrum of **8e** (50 MHz, $CDCl_3$).

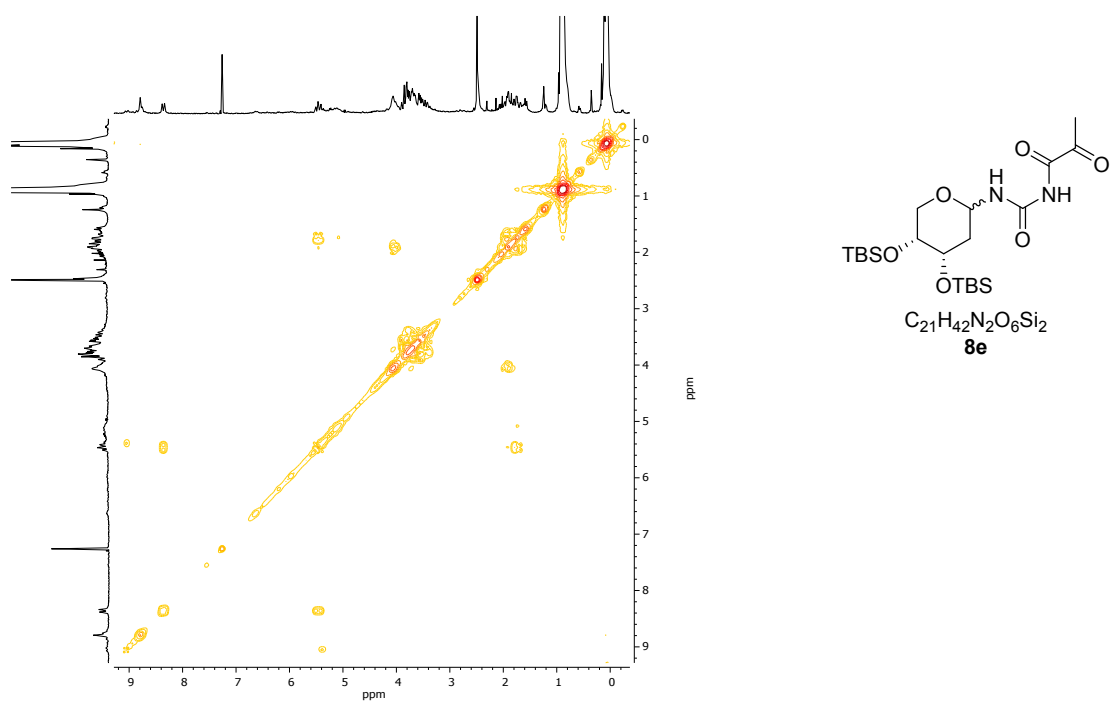


Figure S74: 2D-COSY spectrum of **8e** (200 MHz, $CDCl_3$).

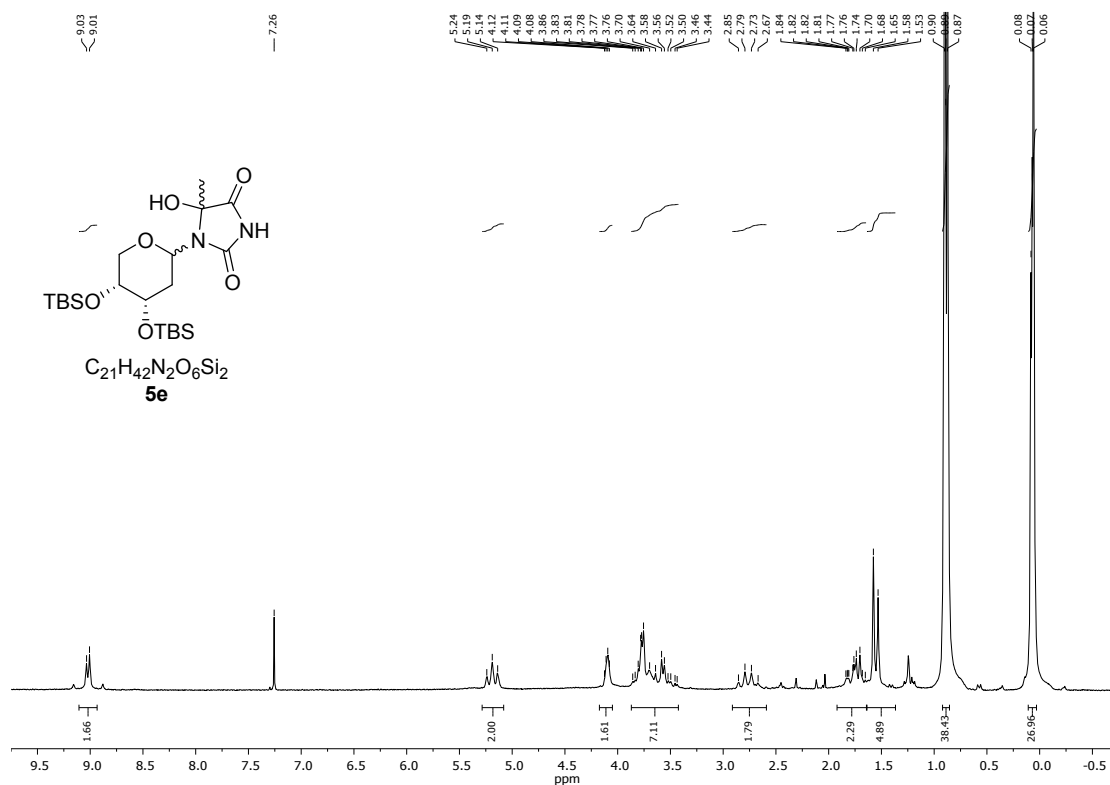


Figure S75: ^1H NMR spectrum of **5e** (200 MHz, CDCl_3).

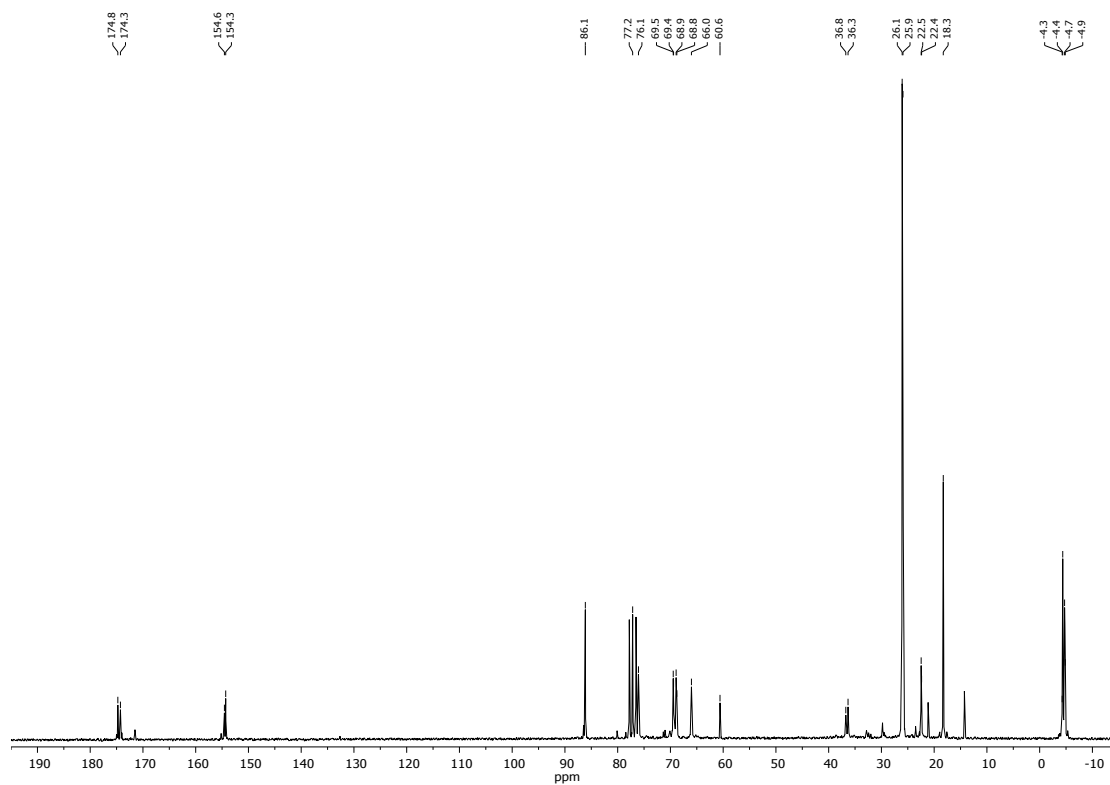


Figure S76: ^{13}C NMR spectrum of **5e** (50 MHz, CDCl_3).

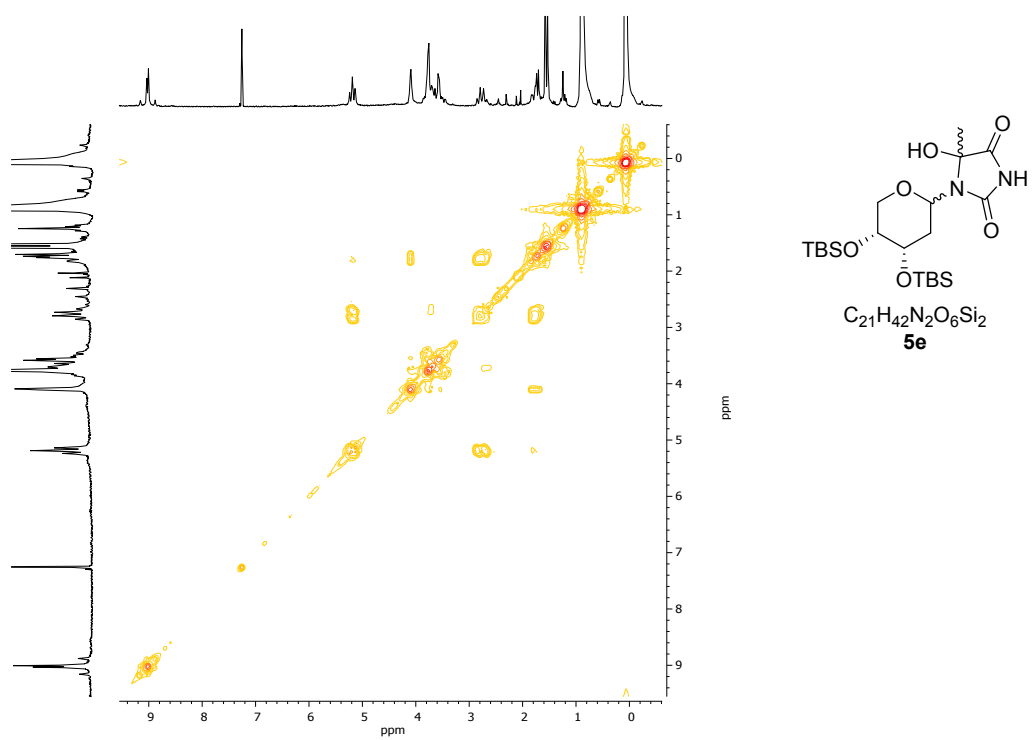


Figure S77: 2D-COSY spectrum of **5e** (200 MHz, $CDCl_3$).

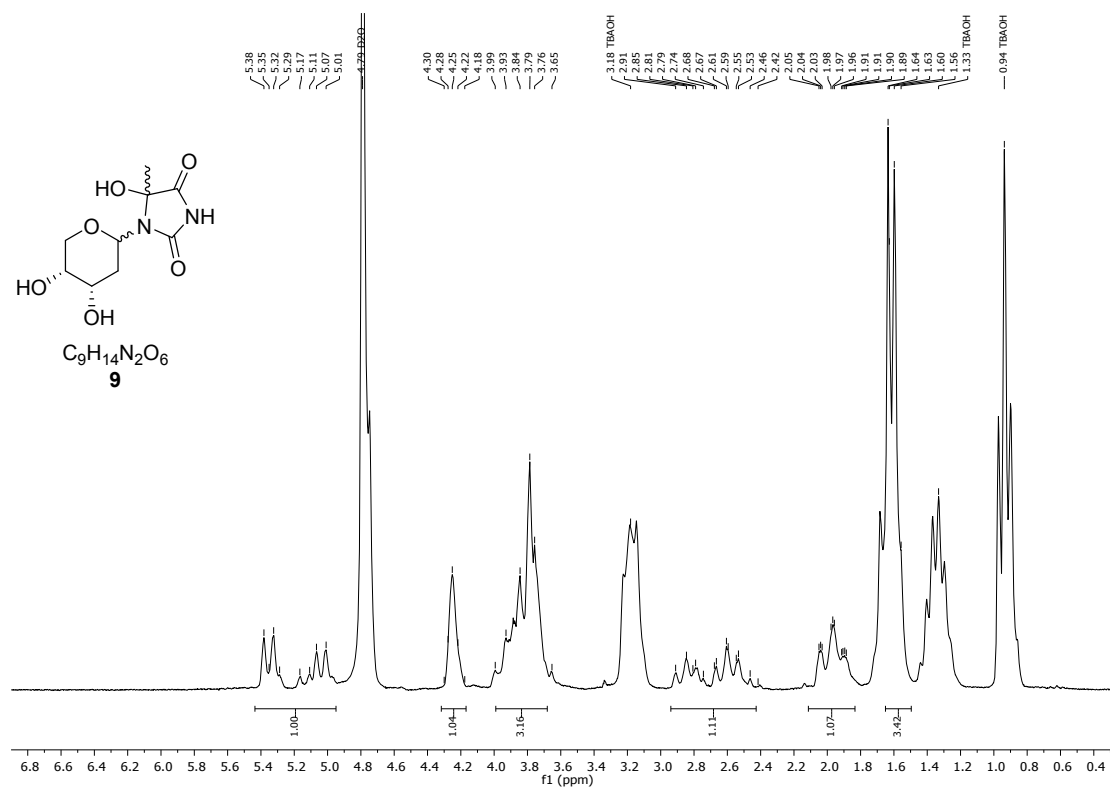


Figure S78: $^1\text{H-NMR}$ spectrum of **9** (200 MHz, D_2O).

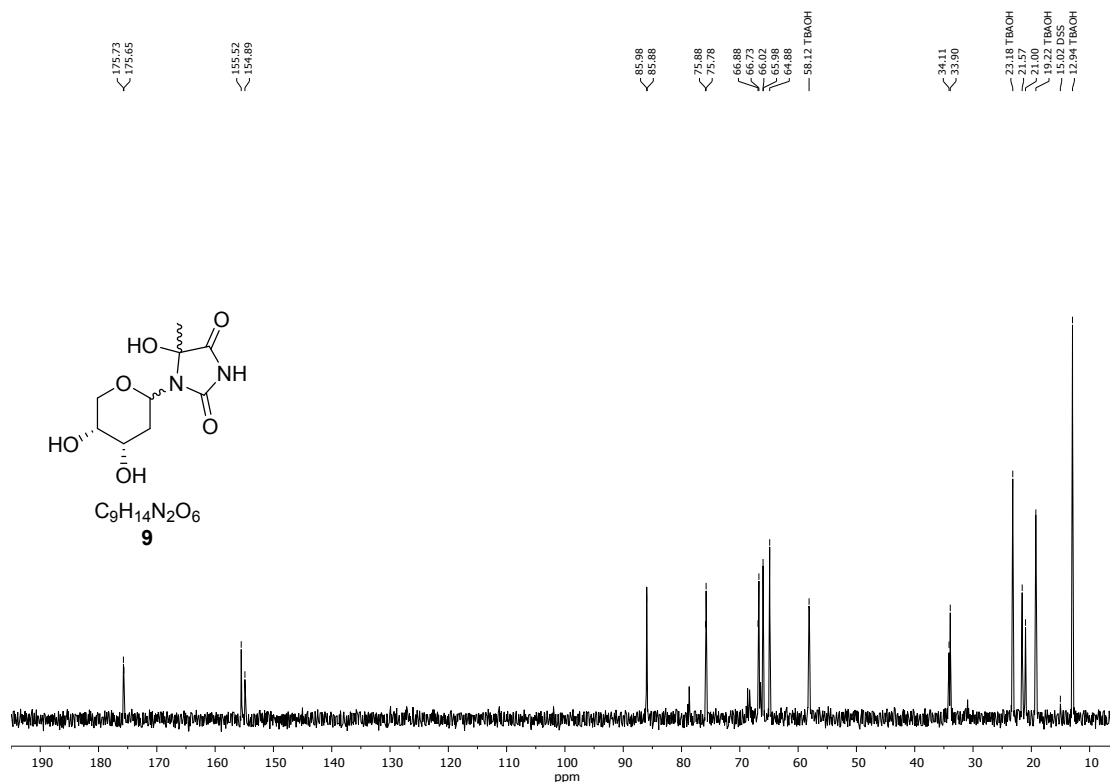


Figure S79: $^{13}\text{C-NMR}$ spectrum of **9** (50 MHz, D_2O).

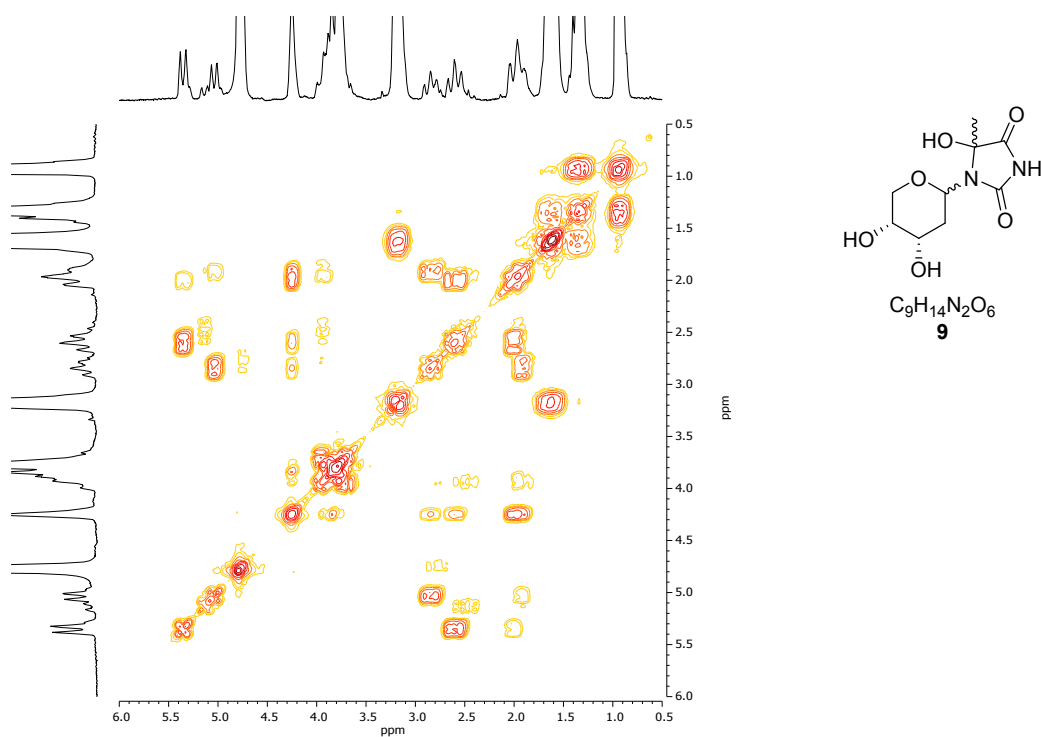


Figure S80: 2D-COSY spectrum of **9** (200 MHz, D₂O).