Follow the Silyl Cation: Insights into a Vorbrüggen Reaction

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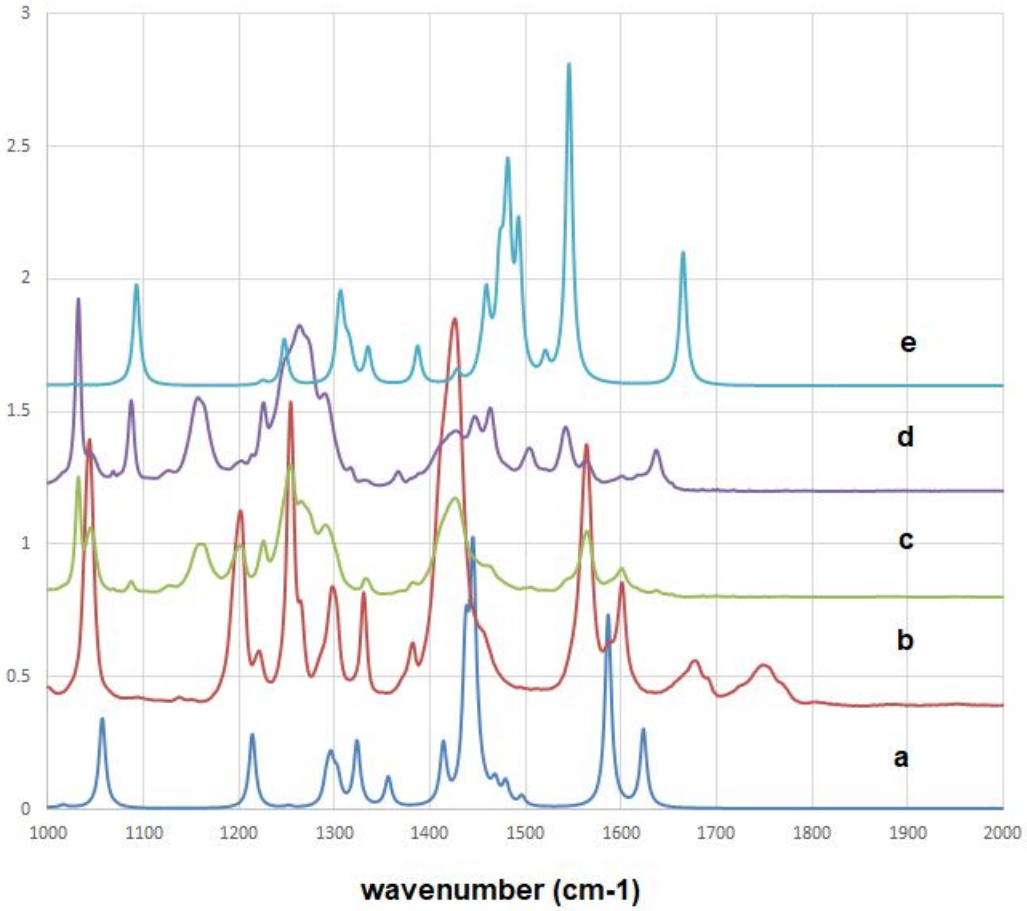
Figure S1. Comparison of Experimental and DFT IR Spectra of Compounds **8** and **9**.



a. Predicted IR spectra of **8** with Spatial Density Map (SMD) solvation in acetonitrile using a B3LYP/6-311+G(2d,p) optimized structure, b. Experimental IR spectra of authentic **8** in 20 mL/g d_3-MeCN at RT, c. Experimental IR spectra of thymine with 1.0 equiv HMDS and 1.0 equiv TMSOTf in 20 mL/g d_3-MeCN at RT, d. Experimental IR spectra of thymine with 1.0 equiv HMDS and 1.6 equiv TMSOTf in 20 mL/g d_3-MeCN at RT, e. Predicted IR spectra of **9** with Spatial Density Map (SMD) solvation in acetonitrile using a B3LYP/6-311+G(2d,p) optimized structure.

Table S1. ^{1}H and ^{13}C NMR Chemical Shifts of Silylated Thymines in d_3-MeCN (20 mL/g) at RT.

8 **9**

	8			**9**		
	^{1}H NMR (ppm)	^{13}C NMR (ppm)	^{13}C NMR (ppm, DFT-GIAO)[a]	^{1}H NMR (ppm)	^{13}C NMR (ppm)	^{13}C NMR (ppm, DFT-GIAO)[a]
1	NA	163.3	168.7	NA	160.3	165.8
2	7.96	160.3	165.5	7.9	151.8	155.4
3	NA	114.3	118.7	NA	117.3	122.5
4	NA	169.9	174.4	NA	173.7	177.4
5	1.93	12.9	13.5	2.09	12.8	13.7

a. ^{1}H and ^{13}C NMR chemical shift prediction for **8** and **9** with Spatial Density Map (SMD) solvation in acetonitrile using a B3LYP/6-311+G(2d,p) optimized structure referenced to TMS at the same level of theory.

Figure S2. Parity Plot of Experimental vs. DFT Calculated ^{13}C NMR shifts for Compounds **8** and **9**.

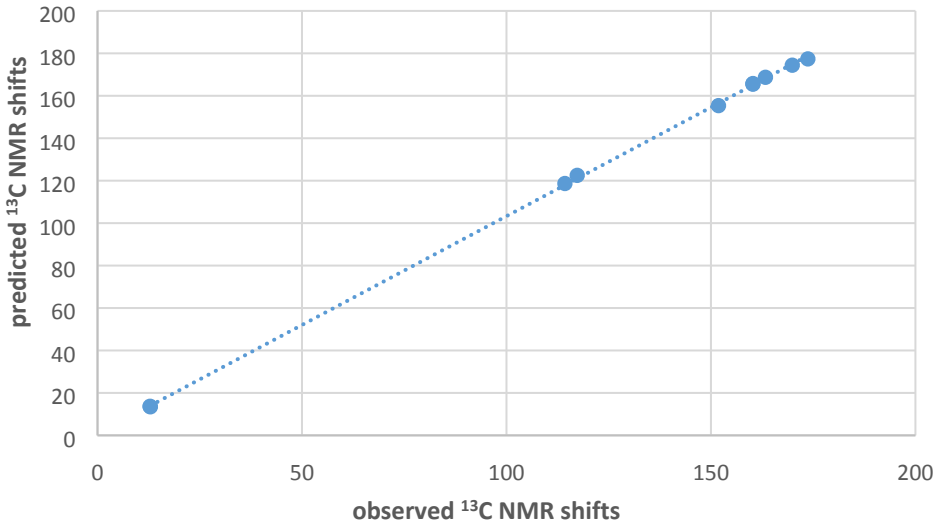
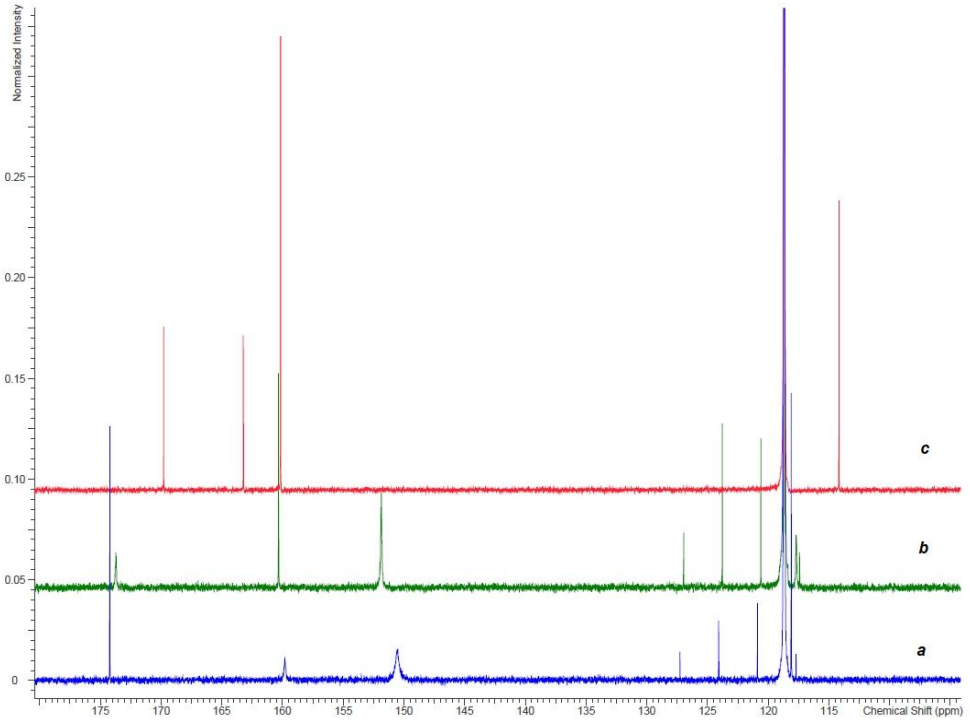
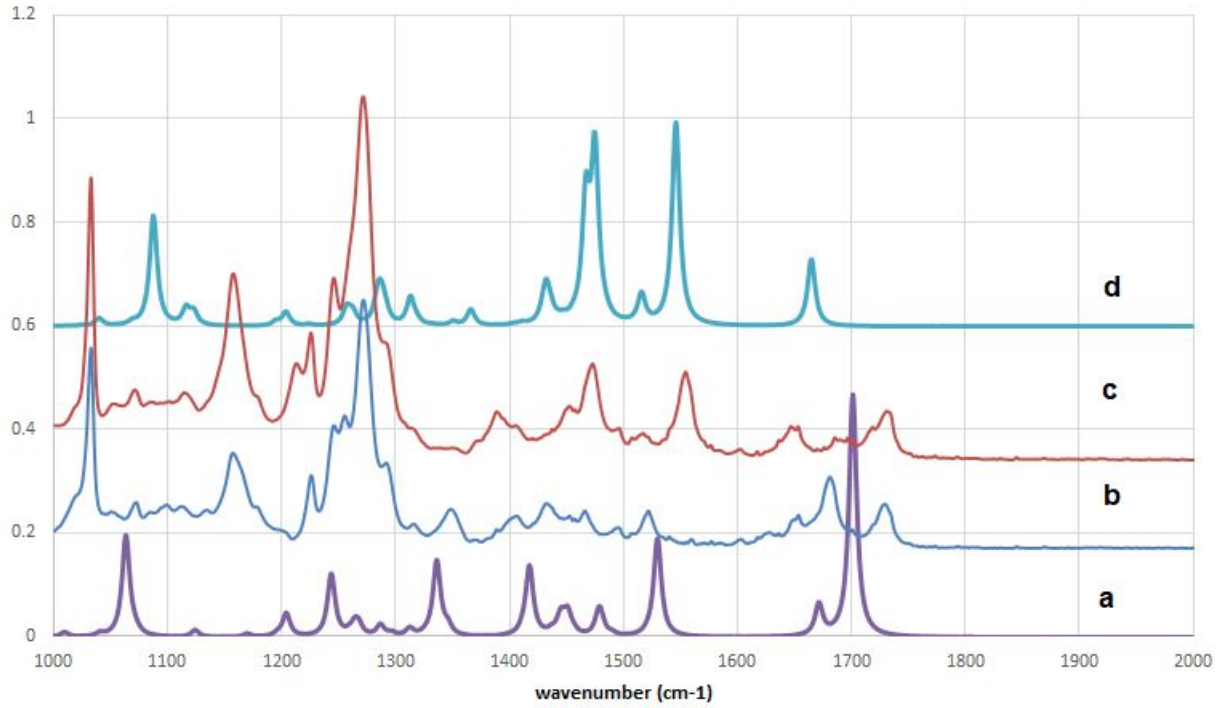


Figure S3. ^{13}C NMR spectra of Silylated Thymines.



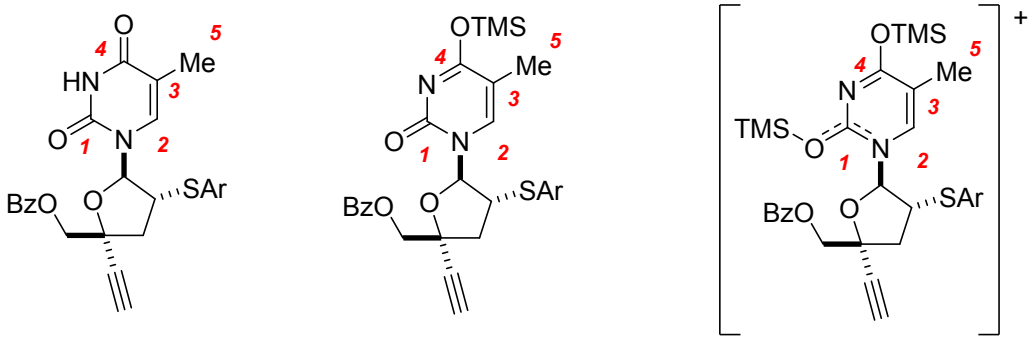
a. 1.07 g authentic bis-trimethylsilylthymine (3.96 mmol, 1 equiv) + 1.14 mL TMSOTf in 10 mL d_3-MeCN at RT, b. 500 mg thymine (3.96 mmol, 1.0 equiv) + 0.83 mL HMDS (3.96 mmol, 1.0 equiv) + 1.14 mL TMSOTf (6.34 mmol. 1.6 equiv) in 10 mL d_3-MeCN at RT, c. 107 mg authentic bis-trimethylsilylthymine (0.396 mmol, 1 equiv) in 1.0 mL d_3-MeCN at RT.

Figure S4. Comparison of Experimental and DFT IR Spectra of Compounds **10** and **11**.



a. Predicted IR spectra of **10** with Spatial Density Map (SMD) solvation in acetonitrile using a B3LYP/6-311+G(2d,p) optimized structure, b. Experimental IR spectra of **4** with 1.0 equiv DIPEA and 1.0 equiv TMSOTf in 20 mL/g d_3-MeCN at RT, c. Experimental IR spectra of **4** with 1.0 equiv DIPEA and 1.5 equiv TMSOTf in 20 mL/g d_3-MeCN at RT, d. Predicted IR spectra of **11** with Spatial Density Map (SMD) solvation in acetonitrile using a B3LYP/6-311+G(2d,p) optimized structure.

Table S2. ^{1}H and ^{13}C NMR Chemical Shifts of Silylated **4** in d_3-MeCN at RT.



4 **10** **11**

	4		**10**			**11**		
	^{1}H NMR (ppm)[a]	^{13}C NMR (ppm) [a]	^{1}H NMR (ppm)[a]	^{13}C NMR (ppm)[a]	^{13}C NMR (ppm DFT-GIAO)[b]	^{1}H NMR (ppm)[a]	^{13}C NMR (ppm)[a]	^{13}C NMR (ppm DFT-GIAO)[b]
1	NA	151.7	NA	156.3	159.9	NA	155.9	159.4
2	6.78	135.7	7.97	143.7	147.4	8.19	144.4	148.8
3	NA	112.4	NA	117.1	108.4	NA	119.3	122.9
4	NA	164.1	NA	172.5	175.7	NA	173.2	176.6
5	1.42	11.6	1.74	12.6	13.5	1.8	12.9	13.5

a. Due to the complex reaction mixture, ^{13}C NMR shifts were assigned from ^{1}H-^{13}C HMBC spectra (400 MHz ^{1}H NMR, d_3-MeCN) referenced to MeCN at 1.94 / 118.69 ppm, b. Predicted NMR spectra of **10** and **11** with Spatial Density Map (SMD) solvation in acetonitrile using a B3LYP/6-311+G(2d,p) optimized structure referenced to TMS at the same level of theory.

Figure S5. Parity Plot of Experimental versus DFT Calculated ^{13}C NMR shifts for Compounds **8** and **9**.

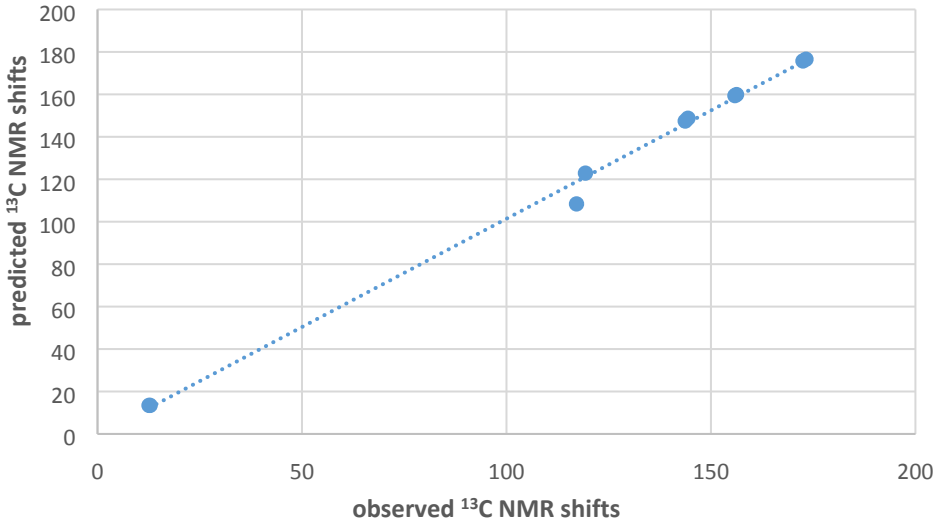


Figure S6. ^{1}H-^{13}C HMBC of Compound **10**.

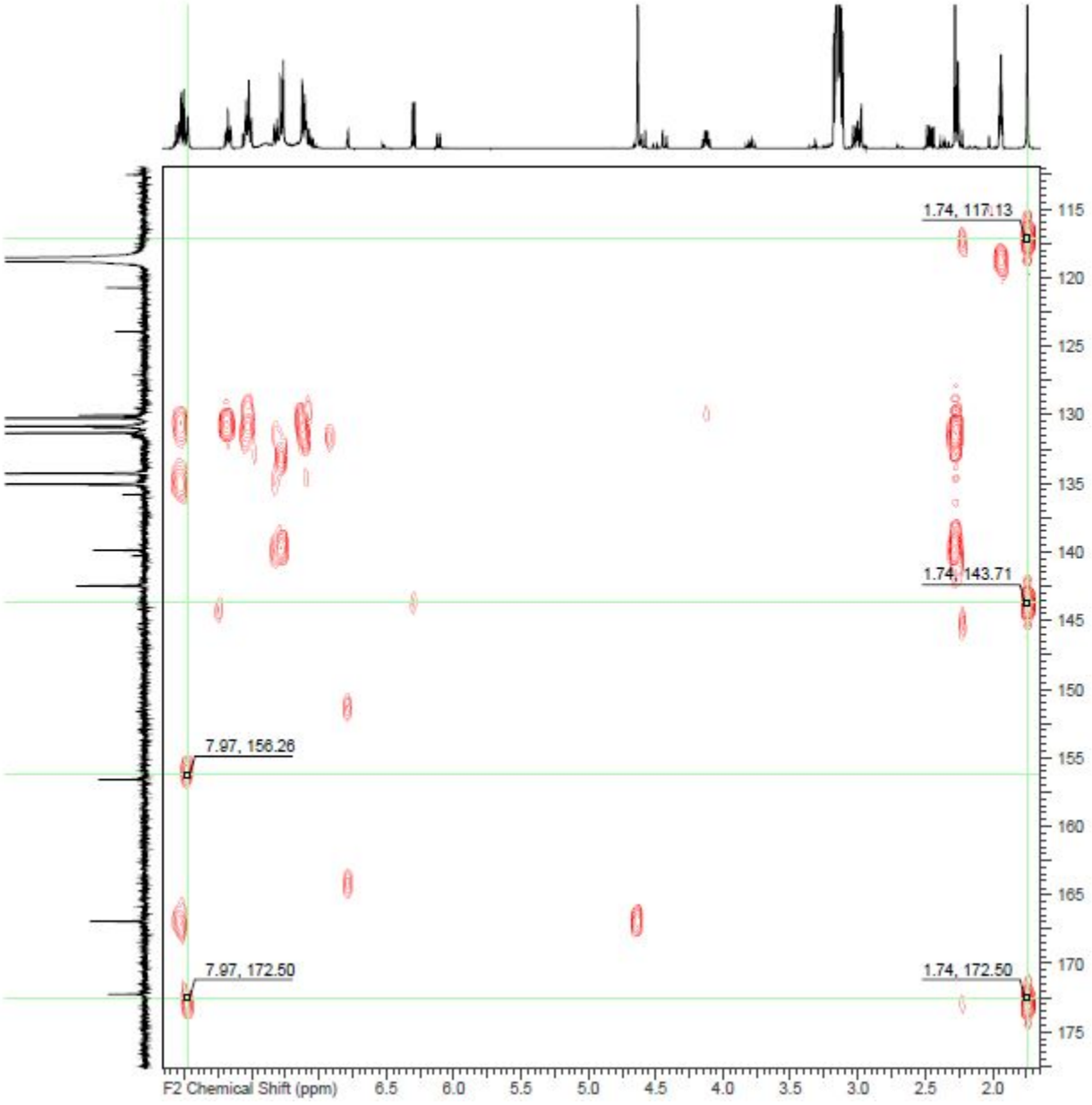


Figure S7. ^{1}H-^{13}C HMBC of Compound **11**.

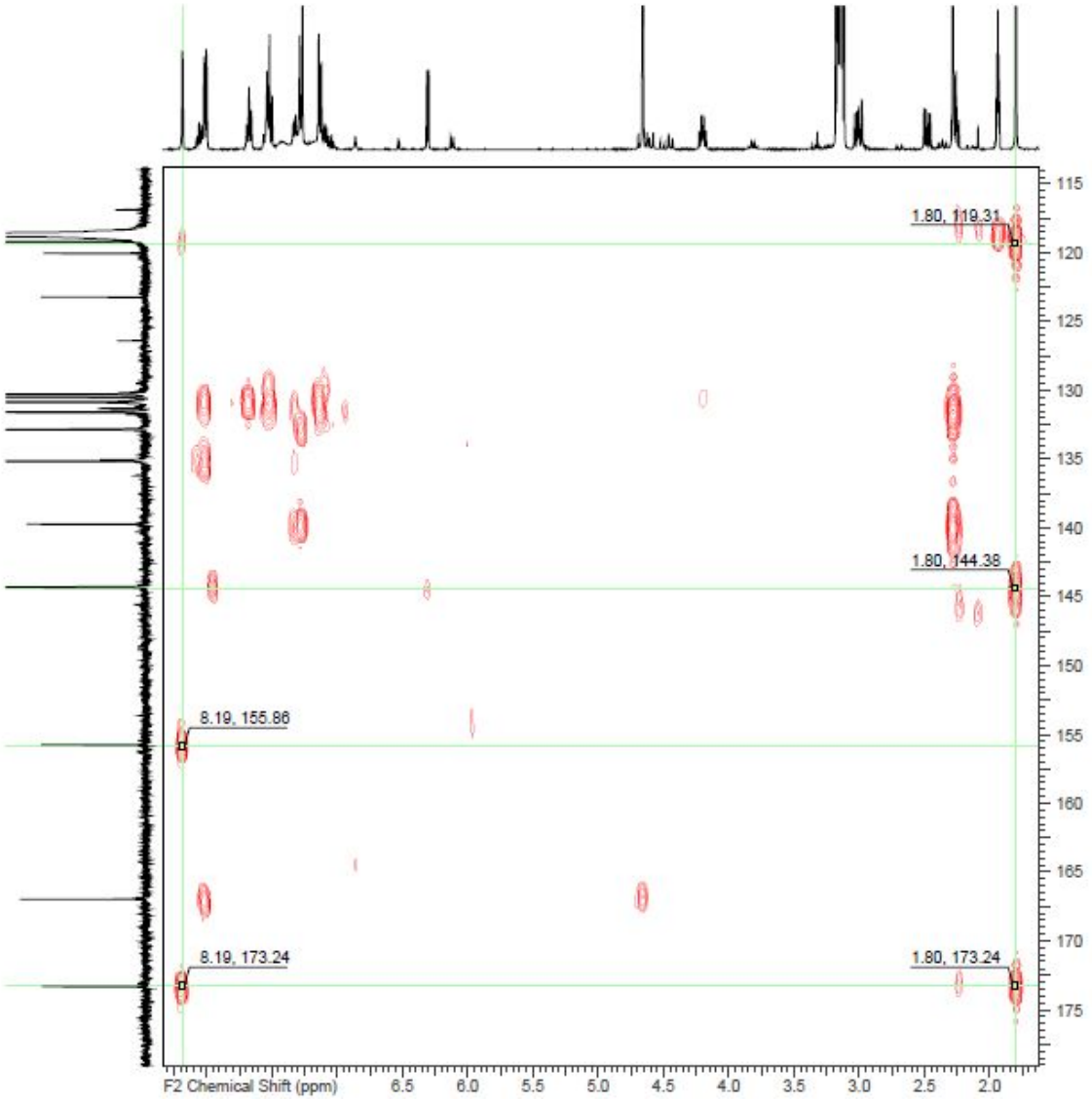
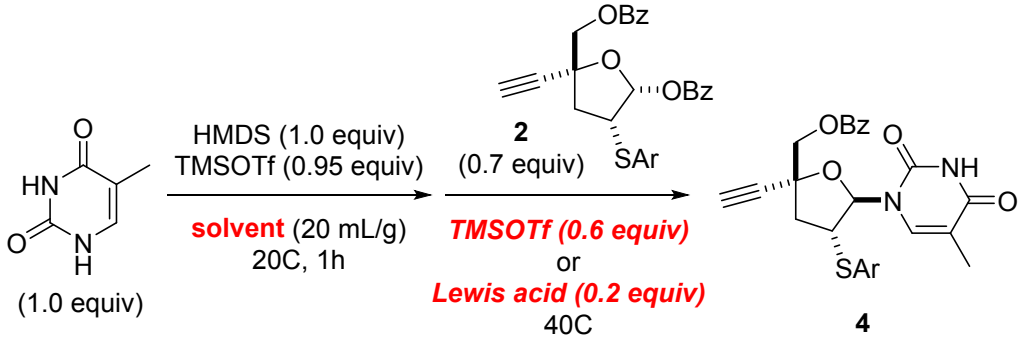


Table S3. Solvent and Lewis Acid Screening for the Reaction of **2**.



Lewis Acid	solvent	conv	dr	Lewis Acid	solvent	conv	dr
TMSOTf	$PhCH_3$	45.1	56.1	$Mg(OTf)_2$	$PhCF_3$	75.5	71.8
TMSOTf	THF	59.1	68.0	$Sc(OTf)_3$	DCE	82.3	76.7
TMSOTf	NMP	1.0	ND	$Sc(OTf)_3$	DME	64.3	74.0
TMSOTf	MeTHF	1.6	ND	$Sc(OTf)_3$	EtOAc	54.4	76.4
TMSOTf	MeCN	100.0	93.0	$Sc(OTf)_3$	MeCN	86.3	90.7
TMSOTf	EtOAc	61.0	66.1	$Sc(OTf)_3$	$PhCF_3$	78.4	71.8
TMSOTf	DMF	1.6	ND	$Sm(OTf)_3$	DCE	80.8	76.7
TMSOTf	DME	100.0	69.9	$Sm(OTf)_3$	DME	57.4	74.4
TMSOTf	DMA	1.5	ND	$Sm(OTf)_3$	EtOAc	72.6	75.0
TMSOTf	DCE	94.7	79.7	$Sm(OTf)_3$	MeCN	82.5	90.6
TMSOTf	CPME	0.3	50.0	$Sm(OTf)_3$	$PhCF_3$	78.5	71.7
TMSOTf	$PhCF_3$	88.9	71.6	$SnCl_2$	DCE	90.1	77.6
AgOTf	DCE	88.5	77.7	$SnCl_2$	DME	76.1	73.7
AgOTf	DME	69.0	73.5	$SnCl_2$	EtOAc	77.9	74.7
AgOTf	EtOAc	72.2	74.3	$SnCl_2$	MeCN	82.7	90.5
AgOTf	MeCN	75.2	90.3	$SnCl_2$	$PhCF_3$	87.3	72.9
AgOTf	$PhCF_3$	85.9	73.3	$SnCl_4$	DCE	87.5	77.6
$In(OTf)_3$	DCE	98.1	78.1	$SnCl_4$	DME	70.8	73.7
$In(OTf)_3$	DME	74.2	73.6	$SnCl_4$	EtOAc	76.2	74.3
$In(OTf)_3$	EtOAc	84.0	74.4	$SnCl_4$	MeCN	82.0	90.3
$In(OTf)_3$	MeCN	94.4	90.4	$SnCl_4$	$PhCF_3$	81.8	72.9
$In(OTf)_3$	$PhCF_3$	91.7	72.8	$Zn(OTf)_2$	DCE	98.6	78.3
$Mg(OTf)_2$	DCE	75.8	76.6	$Zn(OTf)_2$	DME	71.8	73.8
$Mg(OTf)_2$	DME	63.8	73.3	$Zn(OTf)_2$	EtOAc	78.3	74.4
$Mg(OTf)_2$	EtOAc	67.1	73.9	$Zn(OTf)_2$	MeCN	86.3	90.3
$Mg(OTf)_2$	MeCN	69.4	90.4	$Zn(OTf)_2$	$PhCF_3$	92.0	73.3

Table S4. HPLC concentration results for the reaction of **2** used for kinetic model building.

Fitting set 1: T = 21.8°C; MeCN: 24 mL
Input as dispensed: 7.77 mmol thymine; 5.44 mmol **2**; 12.4 mmol TMSOTf; 7.77 mmol HMDS

Time (min)	**2** (mol/L)	**4** (mol/L)	**6** (mol/L)	**7** (mol/L)
5	2.33E-01	1.09E-02	1.21E-04	1.22E-04
10	2.22E-01	2.35E-02	2.50E-04	1.17E-04
20	1.94E-01	4.45E-02	4.99E-04	1.65E-05
30	1.75E-01	6.61E-02	7.44E-04	3.66E-05
45	1.47E-01	9.18E-02	1.07E-03	9.06E-05
60	1.27E-01	1.09E-01	1.28E-03	1.57E-04
120	7.80E-02	1.59E-01	1.88E-03	4.55E-04
180	5.58E-02	1.77E-01	2.10E-03	7.42E-04

Fitting set 2: T = 20.0°C; MeCN: 24 mL
Input as dispensed: 7.77 mmol thymine; 5.44 mmol **2**; 14.0 mmol TMSOTf; 7.77 mmol HMDS

Time (min)	**2** (mol/L)	**4** (mol/L)	**6** (mol/L)	**7** (mol/L)
5	2.20E-01	1.66E-02	1.81E-04	4.58E-05
10	2.04E-01	3.61E-02	3.98E-04	6.71E-05
20	1.64E-01	7.69E-02	9.04E-04	3.78E-05
30	1.29E-01	1.06E-01	1.27E-03	1.03E-04
45	9.71E-02	1.37E-01	1.64E-03	2.15E-04
67	7.07E-02	1.62E-01	1.97E-03	3.62E-04
120	3.86E-02	1.92E-01	2.35E-03	6.05E-04
180	1.82E-02	2.13E-01	2.62E-03	8.28E-04

Fitting set 3: T = 20.0°C; MeCN: 24 mL
Input as dispensed: 7.77 mmol thymine; 3.89 mmol **2**; 12.4 mmol TMSOTf; 7.77 mmol HMDS

Time (min)	**2** (mol/L)	**4** (mol/L)	**6** (mol/L)	**7** (mol/L)
2.5	1.33E-01	7.29E-03	1.11E-04	1.16E-04
5	1.30E-01	1.55E-02	2.02E-04	3.44E-05
20	1.03E-01	5.26E-02	6.26E-04	1.09E-04
30	8.90E-02	6.95E-02	8.33E-04	1.17E-04
45	7.43E-02	8.85E-02	1.04E-03	1.13E-04
60	5.55E-02	9.53E-02	1.12E-03	1.50E-04
120	2.99E-02	1.37E-01	1.71E-03	5.22E-04

Fitting set 4: T = 41.6°C; MeCN: 24 mL
Input as dispensed: 7.77 mmol thymine; 5.44 mmol **2**; 12.4 mmol TMSOTf; 7.77 mmol HMDS

Time (min)	**2** (mol/L)	**4** (mol/L)	**6** (mol/L)	**7** (mol/L)
1	1.97E-01	3.54E-02	3.86E-04	0.00E+00

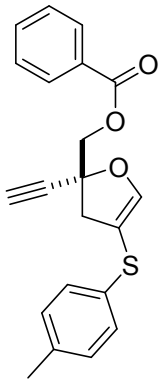
2.5	1.48E-01	8.09E-02	9.77E-04	6.43E-05
5	1.01E-01	1.26E-01	1.55E-03	2.68E-04
7.5	7.35E-02	1.50E-01	1.88E-03	4.70E-04
10	5.72E-02	1.65E-01	2.07E-03	6.74E-04
15	3.63E-02	1.86E-01	2.38E-03	9.57E-04
22.5	2.00E-02	2.02E-01	2.58E-03	1.18E-03
32.5	9.74E-03	2.10E-01	2.70E-03	1.42E-03
50	3.31E-03	2.19E-01	2.86E-03	1.70E-03

Fitting set 5: T = 42.4°C; MeCN: 24 mL
Input as dispensed: 7.77 mmol thymine; 5.44 mmol **2**; 10.9 mmol TMSOTf; 7.77 mmol HMDS

Time (min)	**2** (mol/L)	**4** (mol/L)	**6** (mol/L)	**7** (mol/L)
2.5	1.85E-01	5.65E-02	6.40E-04	2.28E-05
5	1.38E-01	9.24E-02	1.10E-03	1.69E-04
10	9.28E-02	1.35E-01	1.64E-03	4.97E-04
15	6.69E-02	1.53E-01	1.88E-03	9.35E-04
20	5.21E-02	1.67E-01	2.05E-03	1.09E-03
30	3.49E-02	1.82E-01	2.25E-03	1.65E-03
60	1.43E-02	2.03E-01	2.60E-03	2.25E-03
150	5.99E-03	2.09E-01	2.74E-03	2.73E-03

Validation set: T = 31.0°C; MeCN: 24 mL
Input as dispensed: 7.77 mmol thymine; 5.44 mmol **2**; 13.0 mmol TMSOTf; 7.77 mmol HMDS

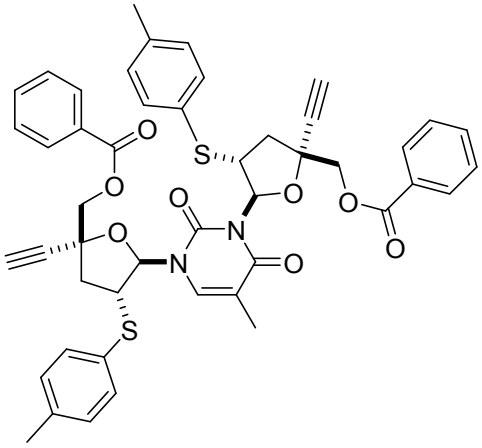
Time (min)	**2** (mol/L)	**4** (mol/L)	**6** (mol/L)	**7** (mol/L)
2.5	1.99E-01	3.72E-02	4.21E-04	0.00E+00
5	1.54E-01	6.44E-02	7.58E-04	0.00E+00
10	1.25E-01	1.04E-01	1.22E-03	1.35E-04
15	1.06E-01	1.29E-01	1.55E-03	2.03E-04
20	8.37E-02	1.46E-01	1.76E-03	3.05E-04
30	5.89E-02	1.69E-01	2.07E-03	6.33E-04
60	2.45E-02	1.94E-01	2.40E-03	1.04E-03
120	8.37E-03	2.07E-01	2.60E-03	1.47E-03



6

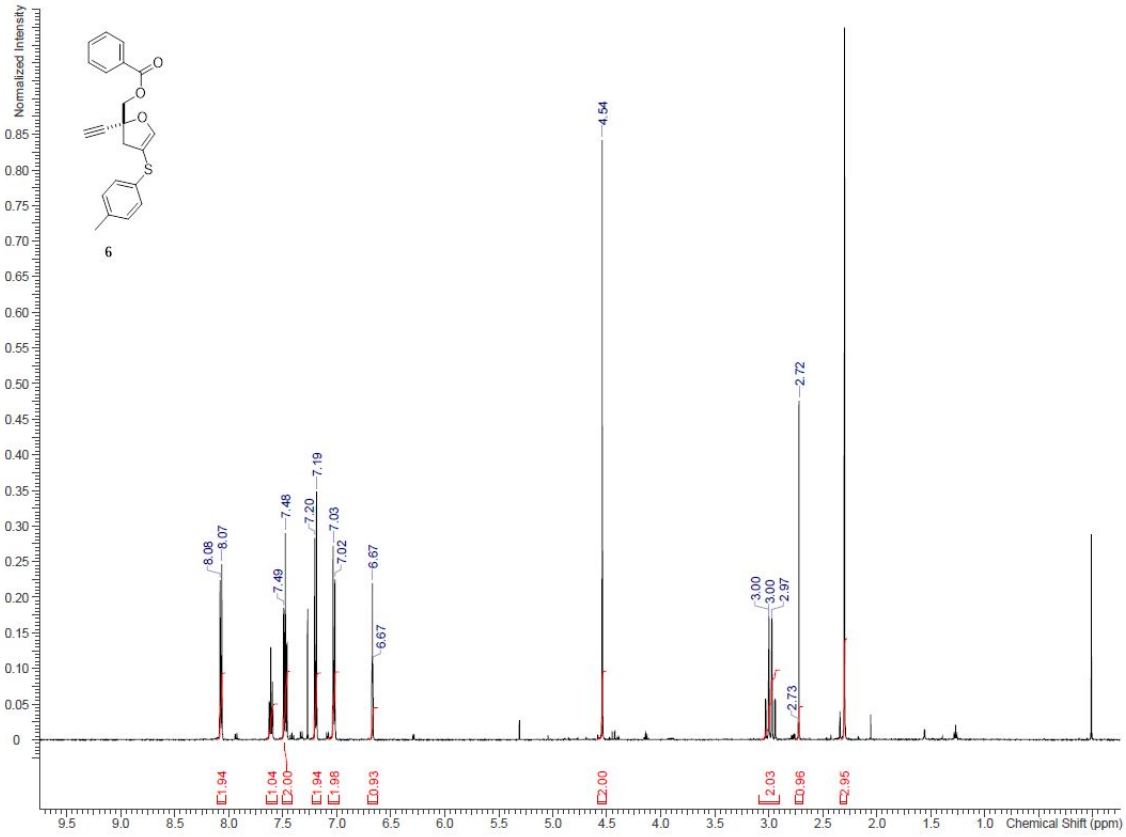
Preparation of (*R*)-(2-ethynyl-4-(p-tolylthio)-2,3-dihydrofuran-2-yl)methyl benzoate (6): In a 500 mL RBF, 16.0 g of **2** (33.9 mmol, 1.0 equiv) was dissolved in 250 mL acetonitrile and 12 mL of water and 4.2 mL of concentrated hydrochloric acid (36 wt%, 44.0 mmol, 1.3 equiv) was added. Aged the resulting biphasic mixture with stirring for 16 h. Added 100 mL of toluene and removed aqueous layer. Washed organic layer with 100 mL of 1 M potassium phosphate dibasic and 50 mL brine. Dried organic layer of Na_2SO_4, filtered and concentrated to a crude oil which was used directly in the next step.

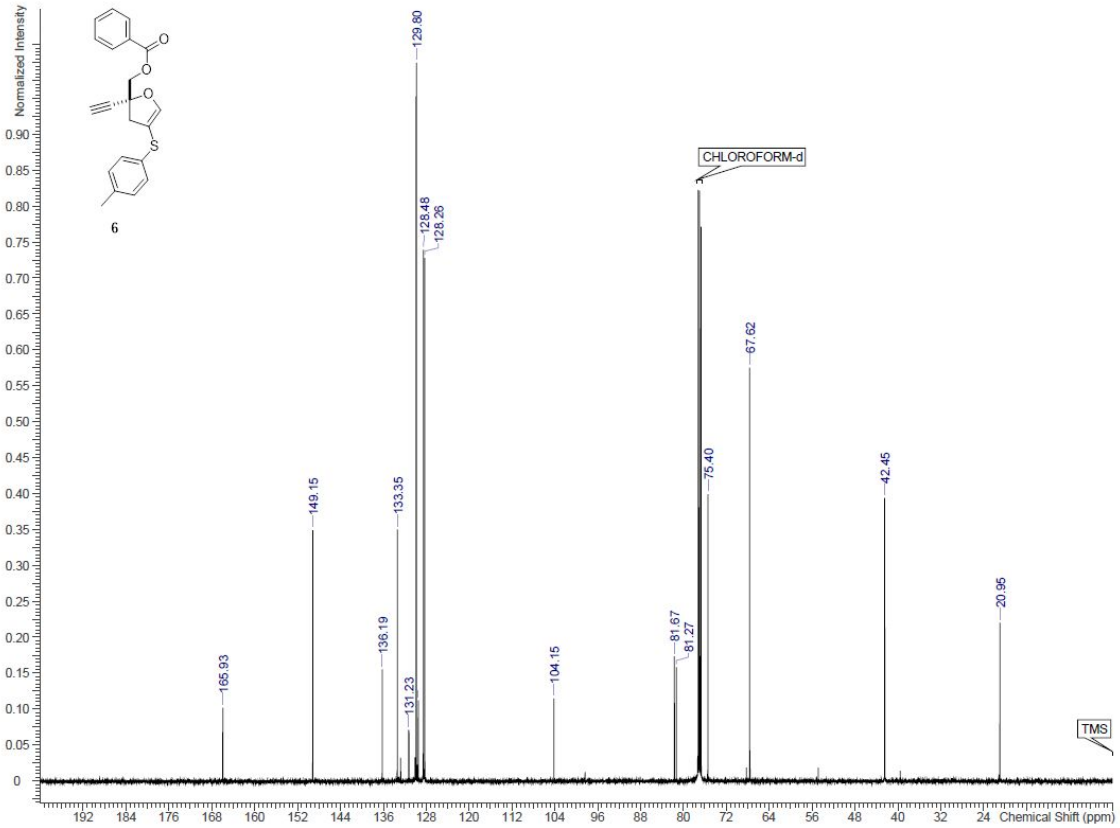
In a 250 mL RBF under nitrogen, 13.0 g of the crude lactol (35.3 mmol, 1.0 equiv) was dissolved in 130 mL of DCM for addition of 5.92 mL of methanesulfonyl chloride (42.4 mmol, 1.2 equiv) and 8.1 g of DIPEA (45.9 mmol, 1.3 equiv). Heated to reflux at 40 ^oC for 3 h. Cooled to room temperature and washed with 100 mL water. Dried organic layer over Na_2SO_4, filtered and concentrated. Dissolved in minimal DCM and loaded directly on an SiO_2 column for purification with hexane/EtOAc. After concentration, obtained 2.1 g of **6** (87 wt% QNMR, 17% yield) as a clear oil. ^1H NMR ($CDCl_3$, 500 MHz) δ 8.08 (m, 2H), 7.60 (m, 1H), 7.48 (m, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.03 (d, *J* = 8.0 Hz, 2H), 6.67 (m, 1H), 4.54 (s, 2H), 2.98 (dd, *J* = 13.8,.9 Hz, 2H), 2.72 (s, 1H), 2.30 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz) δ 165.9, 149.2, 136.2, 133.4, 131.2, 129.9, 129.8, 129.5, 128.5, 128.3, 104.2, 81.7, 81.3, 75.4, 67.6, 42.5, 21.0 ppm. HRMS (DCI) calculated $C_{21}H_{18}O_3S$ (M+): 350.0977, found: 350.0986.

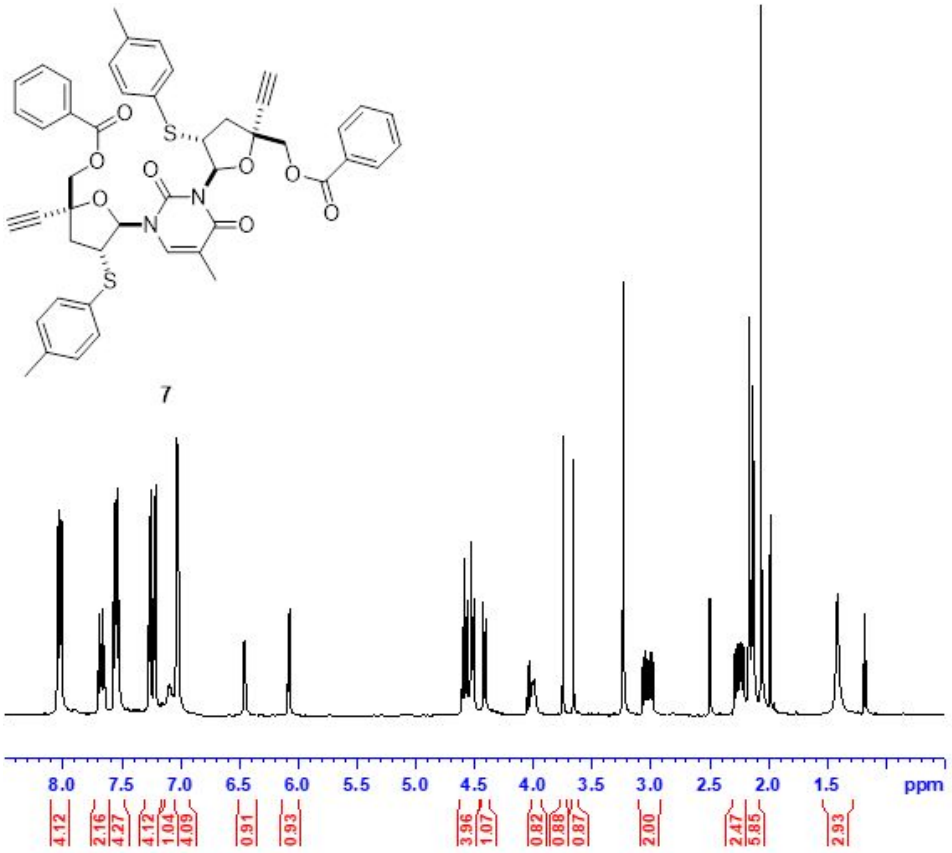


7

Preparation of ((2*R*,2'*R*,4*R*,4'*R*,5*R*,5'*R*)-(5-methyl-2,4-dioxopyrimidine-1,3(2*H*,4*H*)-diyl)bis(2-ethynyl-4-(*p*-tolylthio)tetrahydrofuran-5,2-diyl))bis(methylene) dibenzoate (7): In a 100 mL RBF under nitrogen 5.0 g of **4** (10.5 mmol, 1.0 equiv)) was dissolved in 50 mL acetonitrile for addition of 1.55 mL hexamethyldisilazane (7.35 mmol, 0.7 equiv) and 1.94 mL of trimethylsilyl trifluoromethanesulfonate (10.5 mmol, 1.0 equiv). Aged the resulting slurry for 1 h at RT then added 5.0 g of **2** (10.5 mmol, 1.0 equiv). Heated the resulting slurry for 3 h at 40 °C then allowed to cool to room temperature. Added 100 mL of 1 M potassium phosphate dibasic and extracted twice with 50 mL DCM. Dried combined organic layers over Na_2SO_4, filtered and concentrated. Dissolved in minimal DCM and loaded directly on an SiO_2 column for purification with hexane/EtOAc. After concentration, obtained 6.3 g of **7** (72% yield) as white crystalline solids. ^{1}H NMR (600 MHz, d_6-DMSO, 50°C) δ 8.04 (d, *J* = 7.7 Hz, 2H), 8.02 (d, *J* = 7.7 Hz, 2H), 7.69 (t, *J* = 7.4 Hz, 2H), 7.66 (t, *J* = 7.4 Hz, 1H), 7.56 (t, *J* = 7.7 Hz, 2H), 7.53 (t, *J* = 7.7 Hz, 2H), 7.26 (d, *J* = 7.9 Hz, 2H), 7.22 (d, *J* = 7.9 Hz, 1H), 7.09 (m, 1H), 7.02 (2xd, *J* = 7.9 Hz, 4H), 6.45 (d, *J* = 6.1 Hz, 1H), 6.08 (d, *J* = 7.9 Hz, 1H), 4.59 (d, *J* = 11.3 Hz, 1H), 4.57 (d, *J* = 11.3 Hz, 1H), 4.52 (m, 1H), 4.52 (d, *J* = 11.3 Hz, 1H), 4.41 (d, *J* = 11.3 Hz, 1H), 4.00 (m, 1H), 3.75 (s, 1H), 3.66 (s, 1H), 3.05 (dd, *J* = 13.2, 9.2 Hz, 1H), 3.00 (dd, *J* = 13.4, 9.0 Hz, 1H), 2.27 (dd, *J* = 13.4, 8.8 Hz, 1H), 2.23 (dd, *J* = 13.2, 5.8 Hz, 1H), 2.16 (s, 3H), 2.13 (br, 3H), 1.41 (s, 3H) ppm; ^{13}C NMR (151 MHz, d_6-DMSO, 50°C) δ 165.1, 165.0, 161.4, 149.7, 137.2, 134.2, 133.5, 133.3, 132.8, 131.7, 129.7, 129.4, 129.3, 129.2, 129.1, 129.0, 128.7, 128.5, 127.9, 109.6, 89.9, 88.7, 82.9, 82.4, 77.4, 77.1, 76.5, 75.1, 67.5, 67.2, 46.6, 44.6, 40.8, 40.0, 20.3, 20.2, 11.8 ppm. HRMS (ESI) calculated for protonated species $C_{47}H_{44}O_8N_2S_2$ (M+H): 827.2455, found: 827.2446.


Normalized Intensity
6
8.08
8.07
7.49
7.48
7.20
7.19
7.03
7.02
6.67
6.67
4.54
3.00
3.00
2.97
2.72
2.73
1.94
1.04
2.00
1.94
1.98
0.93
2.00
2.03
0.96
2.95
Chemical Shift (ppm)


Normalized Intensity
6
129.80
128.48
128.26
CHLOROFORM-d
67.62
75.40
149.15
133.35
42.45
136.19
20.95
81.67
81.27
165.93
131.23
104.15
TMS
Chemical Shift (ppm)


7
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
4.12
2.16
4.27
4.12
1.04
4.09
0.91
0.93
3.96
1.07
0.82
0.88
0.87
2.00
2.47
5.85
2.93

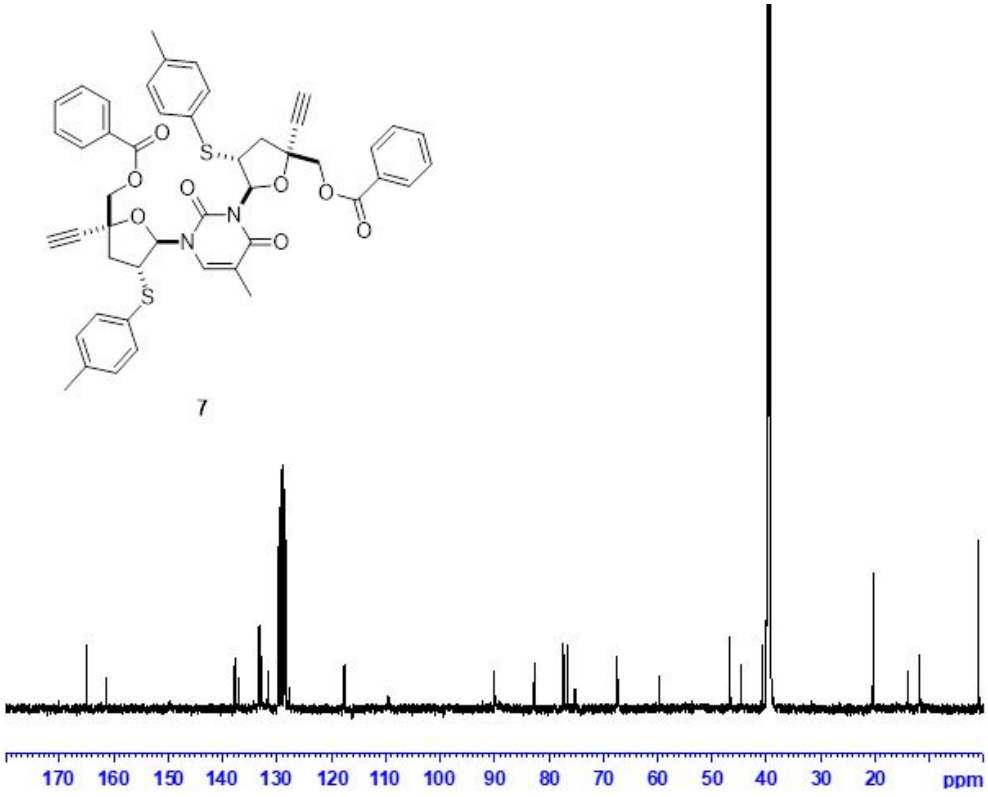
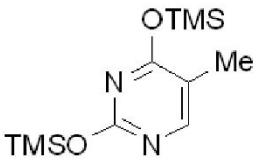
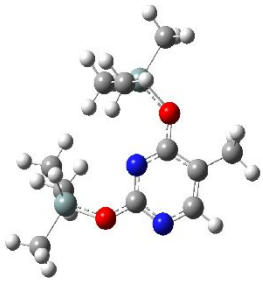

7
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

Table S5. Coordinates for Optimized Structures.

Compound **8** B3LYP/6-311+G(2d,p)

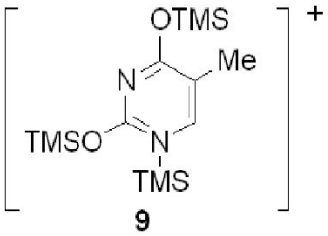


8

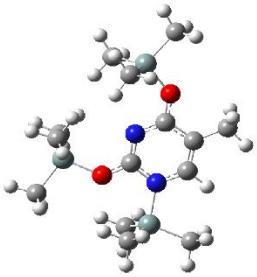


N	-0.045473	0.536471	-0.062023
C	-1.053716	1.408153	-0.207508
N	-0.946341	2.729725	-0.241004
C	0.292124	3.212749	-0.102620
C	1.422744	2.433728	0.065075
C	1.173889	1.050291	0.069141
C	2.802596	3.002161	0.220601
O	2.222174	0.231000	0.213766
Si	2.347879	-1.448673	-0.030451
O	-2.293827	0.930702	-0.344272
Si	-2.963679	-0.572067	0.048842
C	4.175057	-1.744083	0.244082
C	1.343398	-2.390837	1.235492
C	1.860077	-1.854340	-1.791028
C	-4.787566	-0.288330	-0.249999
C	-2.322655	-1.919259	-1.082984
C	-2.629192	-0.945529	1.853903
H	0.383298	4.295913	-0.128300
H	2.772865	4.092722	0.190104
H	3.255106	2.699066	1.168117
H	3.470075	2.656732	-0.572993
H	4.420416	-2.801699	0.112825
H	4.780364	-1.169720	-0.461109
H	4.472685	-1.455747	1.255185
H	1.551419	-3.462188	1.158437
H	0.273343	-2.240574	1.095075
H	1.601448	-2.075268	2.249652
H	2.502627	-1.327360	-2.500985
H	1.966248	-2.926546	-1.979526
H	0.826191	-1.575147	-1.997778
H	-5.367173	-1.184751	-0.012302
H	-5.162045	0.530560	0.368457
H	-4.978605	-0.031985	-1.294860
H	-2.882204	-2.845756	-0.923281
H	-1.266657	-2.125209	-0.908284
H	-2.444377	-1.634678	-2.131270
H	-3.064935	-0.174245	2.494038
H	-3.073672	-1.904112	2.136779
H	-1.559845	-0.994867	2.064873

Compound **9** B3LYP/6-311+G(2d,p)



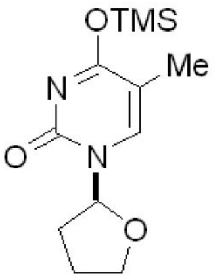
9

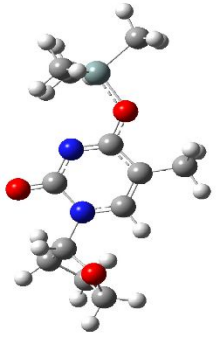


N	0.620311	-0.039739	-0.033741
C	-0.701044	-0.060865	0.007502
N	-1.439937	-1.206291	-0.008901
C	-0.751428	-2.387073	-0.093653
C	0.605642	-2.454705	-0.153388
C	1.281221	-1.198727	-0.106775
C	1.358502	-3.747197	-0.248327
O	2.581410	-1.220909	-0.141182
Si	3.834671	-0.024496	0.079959
O	-1.398773	1.041357	0.072794
Si	-0.914487	2.721367	-0.065553
C	5.361960	-1.048863	-0.198836
C	3.692733	0.585318	1.836914
C	-2.545916	3.586243	0.174465
C	0.289159	3.120969	1.297747
C	-0.234019	2.950966	-1.785072
H	-1.353551	-3.283089	-0.110058
H	0.675390	-4.596117	-0.273476
H	1.975538	-3.772895	-1.148735
H	2.031343	-3.870085	0.602738
H	6.258154	-0.436294	-0.068083
H	5.421713	-1.878608	0.508725
H	5.388116	-1.460899	-1.210151
H	3.816347	-0.235551	2.547207
H	4.480625	1.316031	2.040514

H	2.734472	1.067534	2.035534
H	-2.404513	4.668178	0.101735
H	-3.276850	3.301550	-0.585355
H	-2.973999	3.379689	1.157983
H	0.463113	4.200642	1.322065
H	1.250486	2.629079	1.153740
H	-0.105206	2.832236	2.274933
H	-0.985681	2.715459	-2.542110
H	0.060073	3.994379	-1.929692
H	0.643709	2.330204	-1.968731
Si	-3.319227	-1.171507	0.081273
C	-3.776599	-0.379811	1.704122
H	-3.496851	0.671655	1.748870
H	-4.860135	-0.445096	1.838988
H	-3.312571	-0.900000	2.545416
C	-3.928103	-0.286262	-1.440714
H	-5.018824	-0.357921	-1.481004
H	-3.662959	0.769922	-1.444225
H	-3.538467	-0.746519	-2.351784
C	-3.835671	-2.967357	0.050477
H	-4.928146	-2.989584	0.109315
H	-3.560865	-3.482565	-0.872570
H	-3.463854	-3.541457	0.902020
C	3.641706	1.311174	-1.205897
H	3.555944	0.886673	-2.209021
H	2.772757	1.942847	-1.022210
H	4.528732	1.951272	-1.197872

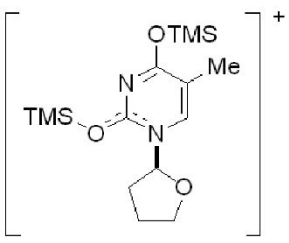
Analog for Compound **10** B3LYP/6-311+G(2d,p)

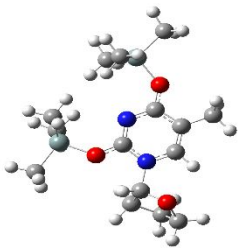




C	-4.813709	0.740559	0.199651
C	-4.308008	-0.080576	1.381541
C	-3.639406	-1.265269	0.675546
C	-3.062757	-0.616174	-0.587445
O	-3.886800	0.488628	-0.881924
N	-1.654455	-0.159411	-0.399097
C	-1.321979	1.151699	-0.309765
C	-0.034331	1.563003	-0.157397
C	0.925538	0.503264	-0.112088
N	0.631745	-0.765555	-0.221670
C	-0.665017	-1.174612	-0.383378
O	-1.008840	-2.341305	-0.504569
O	2.201642	0.857869	0.049133
C	0.363174	3.007055	-0.057264
Si	3.530046	-0.230104	0.145543
C	4.953492	0.963032	0.384127
C	3.341297	-1.348792	1.631885
C	3.711349	-1.175114	-1.456972
H	-5.809235	0.420455	-0.122328
H	-4.836026	1.816393	0.381278
H	-3.577368	0.486999	1.962747
H	-5.111389	-0.381291	2.054324
H	-4.383207	-2.007022	0.375834
H	-2.877013	-1.774330	1.259042
H	-3.042352	-1.297723	-1.435512
H	-2.147456	1.845130	-0.386457
H	-0.512544	3.653997	-0.133885
H	0.862715	3.219399	0.891286
H	1.061489	3.283794	-0.850820
H	5.900261	0.422374	0.469387
H	5.037752	1.652789	-0.459170
H	4.825120	1.556573	1.292584
H	2.516588	-2.048129	1.492913
H	3.154886	-0.769379	2.539884
H	4.259733	-1.922600	1.788091
H	3.737538	-0.496452	-2.313461
H	4.647536	-1.741462	-1.454472
H	2.885430	-1.873273	-1.595276

Analog for Compound **11** B3LYP/6-311+G(2d,p)





C	4.681301	-2.146138	-0.040884
C	4.357076	-1.425522	1.261444
C	3.766794	-0.103961	0.753001
C	3.062650	-0.525194	-0.542179
O	3.682814	-1.681282	-0.997021
N	1.578605	-0.823219	-0.323723
C	1.115153	-2.103094	-0.289797
C	-0.204799	-2.387767	-0.118187
C	-1.067367	-1.256258	-0.006193
N	-0.606844	-0.001532	-0.055464
C	0.688623	0.201080	-0.208144
O	1.211559	1.392659	-0.263084
O	-2.339328	-1.488305	0.142735
C	-0.739173	-3.787493	-0.075918
C	-3.645912	0.813596	1.432358
C	-3.886521	0.207659	-1.624660
C	-5.096438	-1.739307	0.463755
Si	-3.769904	-0.486965	0.102323
Si	0.519515	2.991091	-0.041353
C	-0.838581	3.239266	-1.290707
C	-0.042049	3.095382	1.732463
C	2.002872	4.058988	-0.388441
H	5.665436	-1.877888	-0.430030
H	4.605774	-3.231390	0.011254
H	3.622750	-1.985055	1.845385
H	5.237320	-1.279689	1.886085
H	4.560101	0.600053	0.494004
H	3.101069	0.388955	1.458022
H	3.074582	0.240291	-1.315189
H	1.867305	-2.863749	-0.434226
H	-1.466177	-3.950561	-0.874030
H	0.064153	-4.515335	-0.186996
H	-1.253603	-3.978970	0.867939
H	-3.414300	0.369341	2.403311
H	-2.887762	1.562459	1.204286
H	-4.606881	1.327012	1.529232
H	-3.027262	0.829272	-1.881223
H	-4.783540	0.826422	-1.717061
H	-3.962792	-0.592528	-2.364534
H	-4.966145	-2.186544	1.451772
H	-6.081374	-1.265128	0.442420
H	-5.099219	-2.542526	-0.276192
H	-0.498025	3.003598	-2.301743
H	-1.717727	2.633900	-1.071635
H	-1.144578	4.289503	-1.286295
H	-0.463540	4.085843	1.926640
H	0.793535	2.956444	2.422516
H	-0.809769	2.357502	1.969328
H	2.361773	3.927779	-1.411761
H	1.743507	5.113892	-0.264053
H	2.826370	3.840587	0.294995