Supporting Information

Efficient *N*-arylation and *N*-alkenylation of the five DNA/RNA nucleobases

*Mikkel F. Jacobsen, Martin M. Knudsen and Kurt V. Gothelf**

Center for Catalysis and Interdisciplinary Nanoscience Center (iNANO), Department of Chemistry,
University of Aarhus, Langelandsgade 140, 8000 Aarhus C, Denmark

kvg@chem.au.dk

Contents:

Experimental procedures and characterization for compounds 7a-g , 8a-g , 8i-l , 13a-g , 15a-g and 19a-e ...	2-16
Single crystal X-ray crystallographic analysis: ORTEP plots of 15f and 19b	17
Copies of ¹ H NMR and ¹³ C NMR spectra for compounds 7a , 7c , 8i , 8l , 13c , 15a , 19a , 20-24 and 26	18-43

General Experimental Methods. Unless otherwise stated, all reactions were carried out under nitrogen. Reactions were monitored by thin-layer chromatography (TLC) analysis on Merck® silica gel 60 F₂₅₄ TLC plates. Spots were visualized by exposure to ultraviolet (UV) light (254 nm), or by staining with a 5% solution of phosphormolybdenic acid (PMA) in ethanol or basic aqueous potassium permanganate (KMnO₄) and then heating. Flash chromatography was carried out using Merck® silica gel 60 (230-400 mesh). Acetonitrile (MeCN) and dichloromethane (CH₂Cl₂) were dried by distillation from CaH₂. *N,N*-Dimethylformamide (DMF) was dried over 3Å molecular sieves. All other solvents were of HPLC quality and used as such. All reagents were purchased at the highest commercial quality and used without further purification. NMR spectra were recorded at 400 MHz (¹H NMR) and at 100 MHz (¹³C NMR), and calibrated to the residual solvent peak. The following abbreviations are used for NMR data: s, singlet; d, doublet; q, quartet; t, triplet; m, multiplet; br, broad. Coupling constants are rounded to nearest 0.5 Hz. All compounds synthesized were determined to be >98% pure by ¹H NMR. Melting points are uncorrected.

Compounds **6**, ¹ **12**, ² **14**³ and **18**³ were prepared according to literature procedures.

3-(4-*Tert*-butylbenzyl)-5-methyl-1-phenylpyrimidine-2,4(1*H*,3*H*)-dione (7a).

The reaction was carried out as for **8h** (0.50 mmol of **1** used). Reaction time: 67 h; white solid; yield of **7a**: 100 mg, 57%. *R*_f = 0.60 (20:1 CH₂Cl₂:EtOAc); mp 141-142 °C (from CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃) δ 7.50 (d, *J* = 8.5 Hz, 2H), 7.44-7.47 (m, 2H), 7.36-7.41 (m, 1H), 7.30-7.34 (m, 4H), 7.13 (q, *J* = 1.0 Hz, 1H), 1.97 (d, *J* = 1.0 Hz, 3H), 1.29 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 163.8, 151.2, 150.5, 139.5, 138.7, 133.9, 129.6 (2C), 129.5 (2C), 128.6, 126.5 (2C), 125.3 (2C), 110.5, 44.4, 34.5, 31.4, 13.1 (3C); HRMS (ES) *m/e* calcd for C₂₂H₂₄N₂O₂Na ([M+Na]⁺) 371.1735, found 371.1732.

3-(4-*Tert*-butylbenzyl)-5-methyl-1-*p*-tolylpyrimidine-2,4(1*H*,3*H*)-dione (7d).

The reaction was carried out as for **8h** (0.40 mmol of **1** used). Reaction time: 45 h; yield of **7d**: 79.5 mg, 55%. *R*_f = 0.33 (40:1 CH₂Cl₂:EtOAc); mp 158-159 °C (from CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃) δ 7.50 (d, *J* = 8.50 Hz, 2H), 7.32 (d, *J* = 8.50 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 7.18 (d, *J* = 8.5 Hz, 2H), 7.10 (q, *J* = 1.0 Hz, 1H), 5.15 (s, 2H), 2.38 (s, 3H), 1.96 (d, *J* = 1.0 Hz, 3H), 1.29 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 163.8, 151.3,

150.5, 138.8, 138.6, 137.0, 134.0, 130.1 (2C), 129.5 (2C), 126.2 (2C), 125.3 (2C), 110.2, 44.4, 34.5, 31.4, 21.2, 13.1 (3C); HRMS (ES) m/e calcd for $C_{23}H_{26}N_2O_2Na$ ($[M+Na]^+$) 385.1892, found 385.1890.

3-(4-*Tert*-butylbenzyl)-1-(4-methoxyphenyl)-5-methylpyrimidine-2,4(1*H*,3*H*)-dione (7f).

The reaction was carried out as for **8h** (0.40 mmol of **1** used). Reaction time: 45 h; white solid; yield of **7f**: 46.1 mg, 31%. R_f = 0.21 (40:1 CH_2Cl_2 :EtOAc); mp 140-141 °C (from CH_2Cl_2); 1H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, J = 8.5 Hz, 2H), 7.32 (d, J = 8.5 Hz, 2H), 7.22 (d, J = 9.0 Hz, 2H), 7.10 (q, J = 1.0 Hz, 1H), 6.95 (d, J = 9.0 Hz, 2H), 5.15 (s, 2H), 3.83 (s, 3H), 1.96 (d, J = 1.0 Hz, 3H), 1.29 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.9, 159.5, 151.5, 150.5, 139.1, 134.0, 132.3, 129.5 (2C), 127.7 (2C), 125.3 (2C), 114.7 (2C), 110.2, 55.7, 44.5, 34.6, 31.4, 13.1 (3C); HRMS (ES) m/e calcd for $C_{23}H_{26}N_2O_3Na$ ($[M+Na]^+$) 401.1841, found 401.1849.

3-(4-*Tert*-butylbenzyl)-1-(4-chlorophenyl)-5-methylpyrimidine-2,4(1*H*,3*H*)-dione (8a).

The reaction was carried out as for **8h** (0.40 mmol of **1** used). Reaction time: 45 h; white solid; yield of **8a**: 121 mg, 79%. R_f = 0.43 (40:1 CH_2Cl_2 :EtOAc); mp 170-171 °C (from CH_2Cl_2); 1H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, J = 8.5 Hz, 2H), 7.42 (d, J = 9.0 Hz, 2H), 7.32 (d, J = 8.5 Hz, 2H), 7.26 (d, J = 9.0 Hz, 2H), 7.09 (q, J = 1.0 Hz, 1H), 5.14 (s, 2H), 1.97 (d, J = 1.0 Hz, 3H), 1.29 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.6, 151.0, 150.6, 138.1, 137.9, 134.4, 133.8, 129.6 (2C), 129.4 (2C), 127.9 (2C), 125.3 (2C), 110.9, 44.5, 34.5, 31.4, 13.1 (3C); HRMS (ES) m/e calcd for $C_{22}H_{23}ClN_2O_2Na$ ($[M+Na]^+$) 405.1346, found 405.1336.

***Tert*-butyl 5-methyl-2,6-dioxo-3-phenyl-2,3-dihydropyrimidine-1(6*H*)-carboxylate (7b).**

The reaction was carried out as for **8h** (0.40 mmol of **4** used). Reaction time: 48 h; white solid; yield of **7a**: 87 mg, 87%. $R_f = 0.2$ (CH_2Cl_2); mp 104-106 °C (from CH_2Cl_2); ^1H NMR (400 MHz, CDCl_3) δ 7.47-7.45 (m, 2H), 7.43-7.40 (m, 1H), 7.36-7.34 (m, 2H), 7.16 (d, $J = 1.0$ Hz, 1H), 1.97 (d, $J = 1.0$ Hz, 1H), 1.60 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 161.8, 148.7, 148.0, 140.1, 138.5, 129.8, 129.0, 126.5, 111.1, 87.0, 27.6, 12.5 (3C); HRMS (ES) m/e calcd for $\text{C}_{11}\text{H}_{10}\text{N}_2\text{O}_2\text{Na}$ ($[\text{M}-\text{Boc}+\text{H}+\text{Na}]^+$) 225.0640, found 225.0632.

***Tert*-butyl 3-(3-chlorophenyl)-5-methyl-2,6-dioxo-2,3-dihydropyrimidine-1(6*H*)-carboxylate (**8b**).**

The reaction was carried out as for **8h** (0.40 mmol of **4** used). Reaction time: 71 h; white solid; yield of **8b**: 96 mg, 71%. $R_f = 0.33$ (CH_2Cl_2); mp 231-232 °C (from CH_2Cl_2); ^1H NMR (400 MHz, CDCl_3) δ 7.41-7.38 (m, 3H), 7.27-7.25 (m, 2H), 7.13 (s, 1H), 1.97 (s, 3H), 1.60 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 161.6, 148.4, 147.8, 139.4, 139.4, 135.3, 130.7, 129.3, 127.0, 124.8, 111.6, 87.2, 27.6, 12.6 (3C); HRMS (ES) m/e calcd for $\text{C}_{11}\text{H}_9\text{ClN}_2\text{O}_2\text{Na}$ ($[\text{M}-\text{Boc}+\text{H}+\text{Na}]^+$) 259.0250, found 259.0255.

3-Benzoyl-5-methyl-1-phenylpyrimidine-2,4(1*H*,3*H*)-dione (7c**).**

The reaction was carried out as for **8h** (0.50 mmol of **6** used). Reaction time: 48 h; white solid; yield of **7c**: 141 mg, 92%. $R_f = 0.54$ (20:1 CH_2Cl_2 :EtOAc); mp 168-169 °C (from CH_2Cl_2); ^1H NMR (400 MHz, CDCl_3) δ 7.98 (dd, $J = 1.0, 8.5$ Hz, 2H), 7.65 (tt, $J = 1.0, 7.5$ Hz, 1H), 7.37-7.52 (m, 7H), 7.30 (q, $J = 1.0$ Hz, 1H), 2.01 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 168.9, 163.2, 149.3, 140.5, 138.3, 135.1, 131.7, 130.5 (2C), 129.6 (2C), 129.2 (2C), 128.9, 126.3 (2C), 111.3, 12.5; HRMS (ES) m/e calcd for $\text{C}_{18}\text{H}_{14}\text{N}_2\text{O}_3\text{Na}$ ($[\text{M}+\text{Na}]^+$) 329.0902, found 329.0916.

3-Benzoyl-5-methyl-1-*p*-tolylpyrimidine-2,4(1*H*,3*H*)-dione (7e).

The reaction was carried out as for **8h** (0.40 mmol of **6** used). Reaction time: 70 h; white solid; yield of **7e**: 112 mg, 87%. R_f = 0.39 (40:1 CH₂Cl₂:EtOAc); mp 156-157 °C (from CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃) δ 7.96-7.98 (m, 2H), 7.62-7.66 (m, 1H), 7.47-7.51 (m, 2H), 7.27 (q, J = 1.0 Hz, 1H), 2.38 (s, 3H), 2.00 (d, J = 1.0 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 169.0, 163.3, 149.3, 140.7, 139.0, 135.7, 135.0, 131.7, 130.5 (2C), 130.1 (2C), 129.2 (2C), 126.0 (2C), 111.0, 21.2, 12.4; HRMS (ES) m/e calcd for C₁₉H₁₆N₂O₃Na ([M+Na]⁺) 343.1059, found 343.1071.

3-Benzoyl-1-(4-methoxyphenyl)-5-methylpyrimidine-2,4(1*H*,3*H*)-dione (7g).

The reaction was carried out as for **8h** (0.40 mmol of **6** used). Reaction time: 67 h; white solid; yield of **7g**: 89.1 mg, 66%. R_f = 0.40 (20:1 CH₂Cl₂:EtOAc); mp 180-181 °C (from CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃) δ 7.97 (dd, J = 1.0, 8.0 Hz, 2H), 7.63 (tt, J = 1.0, 7.5 Hz, 1H), 7.49 (t, J = 8.0 Hz, 2H), 7.27 (d, J = 9.0 Hz, 2H), 7.25 (q, J = 1.0 Hz, 1H), 6.95 (d, J = 9.0 Hz, 2H), 3.81 (s, 3H), 1.98 (d, J = 1.0 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 169.0, 163.3, 159.6, 149.5, 140.9, 135.0, 131.6, 131.0, 130.5 (2C), 129.2 (2C), 127.6 (2C), 114.7 (2C), 110.9, 55.6, 12.4; HRMS (ES) m/e calcd for C₁₉H₁₆N₂O₄Na ([M+Na]⁺) 359.1008, found 359.1013.

3-Benzoyl-5-methyl-1-(2,4,5-trimethylphenyl)pyrimidine-2,4(1*H*,3*H*)-dione (8c).

The reaction was carried out as for **8h** (0.40 mmol of **6** used). Reaction time: 67 h; white solid; yield of **8c**: 93.7 mg, 67%. $R_f = 0.57$ (20:1 CH₂Cl₂:EtOAc); mp 198-199 °C (from CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃) δ 7.95 (dd, $J = 1.0, 8.5$ Hz, 2H), 7.62 (tt, $J = 1.0, 7.5$ Hz, 1H), 7.48 (tt, $J = 1.5, 8.0$ Hz, 2H), 7.11 (q, $J = 1.0$ Hz, 1H), 7.06 (s, 1H), 6.99 (s, 1H), 2.23 (s, 3H), 2.22 (s, 3H), 2.17 (s, 3H), 1.97 (d, $J = 1.0$ Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 168.9, 163.4, 149.0, 141.1, 138.4, 135.9, 134.9, 134.6, 132.5, 132.3, 131.7, 130.4 (2C), 129.1 (2C), 128.2, 110.5, 19.4, 19.3, 17.1, 12.4; HRMS (ES) m/e calcd for C₂₁H₂₀N₂O₃Na ([M+Na]⁺) 371.1372, found 371.1379.

3-Benzoyl-1-(4-fluoro-3-methylphenyl)-5-methylpyrimidine-2,4(1H,3H)-dione (8d).

The reaction was carried out as for **8h** (0.40 mmol of **6** used). Reaction time: 42 h; white solid; yield of **8d**: 121 mg, 89%. $R_f = 0.42$ (40:1 CH₂Cl₂:EtOAc); mp 155-156 °C (from CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃) δ 7.95-7.98 (m, 2H), 7.65 (tt, $J = 1.5, 7.5$ Hz, 1H), 7.48-7.52 (m, 2H), 7.25 (q, $J = 1.0$ Hz, 1H), 7.15-7.23 (m, 2H), 7.08 (t, $J = 9.0$ Hz, 1H), 2.30 (d, $J = 1.0$ Hz, 3H), 2.00 (d, $J = 1.0$ Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 168.9, 162.7 (d, $J = 102.5$ Hz), 159.7, 149.4, 140.5, 135.2, 133.8 (d, $J = 3.5$ Hz), 131.6, 130.6 (2C), 129.6 (d, $J = 6.0$ Hz), 129.3 (2C), 126.7 (d, $J = 19.0$ Hz), 125.5 (d, $J = 9.0$ Hz), 116.1 (d, $J = 24.0$ Hz), 111.3, 14.7 (d, $J = 3.5$ Hz), 12.5; HRMS (ES) m/e calcd for C₁₉H₁₅FN₂O₃Na ([M+Na]⁺) 361.0964, found 361.0959.

3-Benzoyl-5-methyl-1-(3-nitrophenyl)pyrimidine-2,4(1H,3H)-dione (8e).

The reaction was carried out as for **8h** (0.40 mmol of **6** used). Reaction time: 75 h; beige solid; yield of **8e**: 138 mg, 98%. $R_f = 0.55$ (10:1 CH₂Cl₂:EtOAc); mp 193-194 °C (from CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃) δ 8.26-8.30 (m, 2H), 7.96-7.99 (m, 2H), 7.80 (dq, $J = 1.0, 8.0$ Hz, 1H), 7.65-7.70 (m, 2H), 7.50-7.54 (m, 2H), 7.34 (q, $J = 1.0$ Hz, 1H), 2.04 (d, $J = 1.0$ Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 168.4, 162.8, 149.0, 148.8, 139.1, 139.0, 135.4, 132.6, 131.4, 130.6 (2C), 130.5, 129.3 (2C), 123.7, 121.6, 112.7, 12.7; HRMS (ES) m/e calcd for C₁₈H₁₃N₃O₅Na ([M+Na]⁺) 374.0753, found 374.0758.

3-Benzoyl-1-(3,5-dibromophenyl)-5-methylpyrimidine-2,4(1H,3H)-dione (8f).

The reaction was carried out as for **8h** (0.40 mmol of **6** used). Reaction time: 74 h; white solid; yield of **8f**: 140 mg, 75%. $R_f = 0.33$ (CH_2Cl_2); mp 173-174 °C (from CH_2Cl_2); ^1H NMR (400 MHz, CDCl_3) δ 7.95-7.97 (m, 2H), 7.71 (t, $J = 1.5$ Hz, 1H), 7.66 (tt, $J = 1.0, 7.5$ Hz, 1H), 7.53 (d, $J = 1.5$ Hz, 2H), 7.51 (t, $J = 8.0$ Hz, 2H), 7.24 (q, $J = 1.0$ Hz, 1H), 2.01 (d, $J = 1.0$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 168.4, 162.8, 148.8, 139.8, 139.1, 135.3, 134.5, 131.3, 130.5 (2C), 129.3 (2C), 128.4 (2C), 123.3, 112.2, 12.5; HRMS (ES) m/e calcd for $\text{C}_{18}\text{H}_{12}^{79}\text{Br}_2\text{N}_2\text{O}_3\text{Na}$ ($[\text{M}+\text{Na}]^+$) 486.9092, found 486.9100.

3-Benzoyl-1-(4-bromophenyl)-5-methylpyrimidine-2,4(1H,3H)-dione (8g).

The reaction was carried out as for **8h** (0.40 mmol of **6** used). Reaction time: 18 h; white solid; yield of **8g**: 152 mg, 98%. $R_f = 0.68$ (10:1 CH_2Cl_2 :EtOAc); mp 229-230 °C (from CH_2Cl_2); ^1H NMR (400 MHz, CDCl_3) δ 7.95-7.98 (m, 2H), 7.66 (tt, $J = 1.0, 7.5$ Hz, 1H), 7.58-7.61 (m, 2H), 7.50 (tt, $J = 1.5, 8.0$ Hz, 2H), 7.26-7.29 (m, 2H), 7.25 (q, $J = 1.0$ Hz, 1H), 2.01 (d, $J = 1.0$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 168.7, 163.0, 149.1, 139.8, 137.2, 135.2, 132.8 (2C), 131.5, 130.5 (2C), 129.2 (2C), 128.0 (2C), 122.8, 111.8, 12.5; HRMS (ES) m/e calcd for $\text{C}_{18}\text{H}_{13}^{79}\text{BrN}_2\text{O}_3\text{Na}$ ($[\text{M}+\text{Na}]^+$) 407.0007, found 406.9999.

(E)-3-Benzoyl-5-methyl-1-styrylpyrimidine-2,4(1H,3H)-dione (8i).

The reaction was carried out as for **8h** (0.40 mmol of **6** used). Reaction time: 68 h; white solid; yield of **8i**: 129 mg, 97%. $R_f = 0.29$ (80:1 CH_2Cl_2 :EtOAc); mp 188-189 °C (from CH_2Cl_2); ^1H NMR (400 MHz, CDCl_3) δ 7.94-7.97 (m, 2H), 7.65 (tt, $J = 1.0, 7.5$ Hz, 1H), 7.56 (d, $J = 15.0$ Hz, 1H), 7.55 (q, $J = 1.0$ Hz, 1H), 7.47-7.51 (m, 2H),

7.25-7.40 (m, 5H), 6.48 (d, $J = 15.0$ Hz, 1H), 2.04 (d, $J = 1.0$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 168.5, 162.5, 148.5, 135.4, 135.3, 134.3, 131.4, 130.6 (2C), 129.3 (2C), 129.0 (2C), 128.3, 126.4 (2C), 123.2, 119.1, 112.2, 12.8; HRMS (ES) m/e calcd for $\text{C}_{20}\text{H}_{16}\text{N}_2\text{O}_3\text{Na}$ ($[\text{M}+\text{Na}]^+$) 355.1059, found 355.1049.

(*E*)-3-Benzoyl-5-methyl-1-(3-phenylprop-1-enyl)pyrimidine-2,4(1*H*,3*H*)-dione (8j).

The reaction was carried out as for **8h** (0.40 mmol of **6** used). Reaction time: 93 h; white solid; yield of **8j**: 136 mg, 94%. $R_f = 0.65$ (20:1 CH_2Cl_2 :EtOAc); mp 153-154 °C (from CH_2Cl_2); ^1H NMR (400 MHz, CDCl_3) δ 7.91-7.94 (m, 2H), 7.64 (tt, $J = 1.0$, 7.5 Hz, 1H), 7.46-7.50 (m, 2H), 7.37 (q, $J = 1.0$ Hz, 1H), 7.29-7.34 (m, 2H), 7.20-7.25 (m, 3H), 6.96 (dt, $J = 1.5$, 14.5 Hz, 1H), 5.82 (dt, $J = 7.0$, 14.5 Hz, 1H), 3.47 (d, $J = 7.0$ Hz, 2H), 1.96 (d, $J = 1.0$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 168.6, 162.6, 148.4, 138.8, 136.0, 135.2, 131.4, 130.5 (2C), 129.2 (2C), 128.7 (2C), 128.5 (2C), 126.7, 124.5, 119.4, 111.6, 36.2, 12.6; HRMS (ES) m/e calcd for $\text{C}_{21}\text{H}_{18}\text{N}_2\text{O}_3\text{Na}$ ($[\text{M}+\text{Na}]^+$) 369.1215, found 369.1216.

3-Benzoyl-1-phenylpyrimidine-2,4(1*H*,3*H*)-dione (8k).

The reaction was carried out as for **8h** (0.40 mmol of **9** used). Reaction time: 24 h; white solid; yield of **8k**: 103 mg, 88%. $R_f = 0.43$ (20:1 CH_2Cl_2 :EtOAc); mp 157-158 °C (from CH_2Cl_2); ^1H NMR (400 MHz, CDCl_3) δ 7.97-7.99 (m, 2H), 7.63-7.67 (m, 1H), 7.35-7.52 (m, 8H), 5.91 (d, $J = 8.0$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 168.7, 162.4, 149.2, 144.5, 138.0, 135.2, 131.4, 130.5 (2C), 129.6 (2C), 129.2 (2C), 129.1, 126.2 (2C), 102.6; HRMS (ES) m/e calcd for $\text{C}_{17}\text{H}_{12}\text{N}_2\text{O}_3\text{Na}$ ($[\text{M}+\text{Na}]^+$) 315.0746, found 315.0750.

(*E*)-3-Benzoyl-1-styrylpyrimidine-2,4(1*H*,3*H*)-dione (8l).

The reaction was carried out as for **8h** (0.40 mmol of **9** used). Reaction time: 44 h; white solid; yield of **8l**: 116 mg, 91%. $R_f = 0.41$ (40:1 CH₂Cl₂:EtOAc); mp 210-211 °C (from CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃) δ 7.96-7.99 (m, 2H), 7.72 (d, $J = 8.0$ Hz, 1H), 7.67 (tt, $J = 1.5, 7.5$ Hz, 1H), 7.56 (d, $J = 15.0$ Hz, 1H), 7.50-7.54 (m, 2H), 7.28-7.42 (m, 5H), 6.62 (d, $J = 15.0$ Hz, 1H), 5.98 (d, $J = 8.0$ Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 168.2, 161.7, 148.4, 139.6, 135.4, 133.9, 131.3, 130.6 (2C), 129.3 (2C), 129.1 (2C), 128.6, 126.6 (2C), 123.3, 120.2, 103.5; HRMS (ES) m/e calcd for C₁₉H₁₄N₂O₃Na ([M+Na]⁺) 341.0902, found 341.0905.

4-(Allylthio)-1-phenylpyrimidin-2(1H)-one (13a).

The reaction was carried out as for **8h** (0.30 mmol of **12** used). Reaction time: 20 h; white solid; yield of **13a**: 57 mg, 78%. $R_f = 0.20$ (9:1 CH₂Cl₂:EtOAc); mp 117-119 °C (from CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃) δ 7.51-7.37 (m, 6H), 6.27 (d, $J = 7.0$ Hz, 1H), 6.00-5.93 (m, 1H), 5.34 (d, $J = 17.0$ Hz, 1H), 5.18 (d, $J = 10.0$ Hz, 1H), 3.95 (d, $J = 7.0$ Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 177.7, 153.9, 144.4, 140.4, 132.5, 129.7, 128.9, 126.3, 118.9, 103.7, 32.7; HRMS (ES) m/e calcd for C₁₃H₁₂N₂SONa ([M+Na]⁺) 267.0568, found 267.0561.

4-(Allylthio)-1-*p*-tolylpyrimidin-2(1H)-one (13b).

The reaction was carried out as for **8h** (0.40 mmol of **12** used). Reaction time: 24 h; white solid; yield of **13b**: 90 mg, 87 %. $R_f = 0.20$ (9:1 CH₂Cl₂:EtOAc); mp 121-122 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.38 (d, $J = 7.0$ Hz, 1H), 7.29-8.24 (m, 4H), 6.25 (d, $J = 7.0$ Hz, 1H), 6.01-5.91 (m, 1H), 5.34 (dd, $J = 1.0, 17.0$ Hz, 1H), 5.17 (dd, $J = 1.0, 10.0$ Hz, 1H), 3.94 (d, $J = 7.0$ Hz, 2H), 2.39 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 177.5, 154.1, 144.6, 139.0, 137.9, 132.6, 130.2, 126.0, 118.9, 103.6, 32.7, 21.3; HRMS (ES) m/e calcd for C₁₄H₁₄N₂SONa ([M+Na]⁺) 281.0725, found 281.0711.

4-(Allylthio)-1-(4-methoxyphenyl)pyrimidin-2(1H)-one (13c).

The reaction was carried out as for **8h** (0.40 mmol of **12** used). Reaction time: 25 h; white solid; yield of **13c**: 68 mg, 62%. R_f = 0.30 (9:1 CH₂Cl₂:EtOAc); mp 116-117 °C (from CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃) δ 7.38 (d, J = 7.0 Hz, 1H), 7.28 (d, J = 7.0 Hz, 2H), 6.97 (d, J = 7.0 Hz, 2H), 6.24 (d, J = 7.0 Hz, 1H), 6.00-5.90 (m, 1H), 5.33 (dd, J = 1.0, 17.0 Hz, 1H), 5.17 (d, J = 1.0, 10.0 Hz, 1H), 3.93 (d, J = 1.0 Hz, 2H), 3.83 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 177.4, 159.7, 154.2, 144.7, 133.2, 132.6, 127.4, 118.9, 114.8, 103.6, 55.8, 32.7; HRMS (ES) m/e calcd for C₁₄H₁₄N₂SO₂Na ([M+Na]⁺) 297.0674, found 297.0689.

4-(Allylthio)-1-(4-bromophenyl)pyrimidin-2(1H)-one (13d).

The reaction was carried out as for **8h** (0.40 mmol of **12** used). Reaction time: 40 h; white solid; yield of **13d**: 118 mg, 87%. R_f = 0.30 (9:1 CH₂Cl₂:EtOAc); mp 155-156 °C (from CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃) δ 7.60 (d, J = 7.0 Hz, 2H), 7.36 (d, J = 7.0 Hz, 1H), 7.28 (d, J = 7.0 Hz, 2H), 6.28 (d, J = 7.0 Hz, 1H), 6.00-5.92 (m, 1H), 5.34 (dd, J = 1.0, 16.5, 1H), 5.18 (dd, J = 1.0, 10.0 Hz, 1H), 3.93 (d, J = 7.0 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 178.1, 153.6, 143.8, 139.3, 132.9, 132.3, 128.0, 122.8, 119.1, 104.1, 32.8; HRMS (ES) m/e calcd for C₁₃H₁₁⁷⁹BrN₂SONa ([M+Na]⁺) 344.9673, found 344.9689.

4-(Allylthio)-1-(4-iodophenyl)pyrimidin-2(1H)-one (13e).

The reaction was carried out as for **8h** (0.89 mmol of **12** used). Reaction time: 44 h; white solid; yield of **13e**: 281 mg, 85%. $R_f = 0.30$ (9:1 CH₂Cl₂:EtOAc); mp 164-165 °C (from CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃) δ 7.81 (d, $J = 8.5$ Hz, 2H), 7.35 (d, $J = 7.0$ Hz, 1H), 7.14 (d, $J = 8.5$ Hz, 2H), 6.28 (d, $J = 7.0$ Hz, 1H), 6.00-5.90 (m, 1H), 5.34 (dd, $J = 1.0, 17.0$ Hz, 1H), 5.18 (d, $J = 10.0$ Hz, 1H), 3.93 (d, $J = 7.0$ Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 178.1, 153.6, 143.7, 140.1, 138.9, 132.3, 128.1, 119.1, 104.1, 94.4, 32.8; HRMS (ES) m/e calcd for C₁₃H₁₁IN₂SONa ([M+Na]⁺) 392.9534, found 392.9529.

4-(Allylthio)-1-(4-fluoro-3-methylphenyl)pyrimidin-2(1H)-one (13f).

The reaction was carried out as for **8h** (0.40 mmol of **12** used). Reaction time: 48 h; white solid; yield of **13f**: 101 mg, 93%. $R_f = 0.30$ (9:1 CH₂Cl₂:EtOAc); mp 150-151 °C (from CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃) δ 7.37 (d, $J = 7.0$ Hz, 1H), 7.22-7.06 (m, 3H), 6.26 (d, $J = 7.0$ Hz, 1H), 5.98-5.92 (m, 1H), 5.33 (dd, $J = 1.0, 17.0$ Hz, 1H), 5.17 (d, $J = 10.0$ Hz, 1H), 3.92 (d, $J = 7.0$ Hz, 2H), 2.30 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 177.8, 161.1 (d, $J = 47.5$ Hz), 154.0, 144.4, 136.0 (d, $J = 3.5$ Hz), 132.4, 129.5 (d, $J = 6.0$ Hz), 126.6 (d, $J = 19.0$ Hz), 125.4 (d, $J = 9.0$ Hz), 119.0, 116.1 (d, $J = 24.0$), 103.7, 32.7, 14.9 (d, $J = 3.5$ Hz); HRMS (ES) m/e calcd for C₁₄H₁₃FN₂SONa ([M+Na]⁺) 299.0630, found 299.0622.

(E)-4-(Allylthio)-1-(3-phenylprop-1-enyl)pyrimidin-2(1H)-one (13g).

The reaction was carried out as for **8h** (0.40 mmol of **12** used). Reaction time: 44 h; white solid; yield of **13g**: 116 mg, 83 %. $R_f = 0.40$ (9:1 CH₂Cl₂:EtOAc); mp 67-68 °C (from CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃) δ 7.49 (d, $J = 7.0$ Hz, 1H), 7.33-7.30 (m, 2H), 7.25-7.21 (m, 3H), 6.19 (d, $J = 7.0$, 1H), 5.90-5.58 (m, 2H), 5.32 (dq, $J = 1.5, 17.0$ Hz, 1H), 5.16 (dq, $J = 1.5, 10.0$ Hz, 1H), 3.90 (dt, $J = 1.5, 7.0$ Hz, 2H), 3.53 (d, $J = 7.0$ Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 177.3, 153.0, 139.9, 139.0, 132.3, 128.9, 128.7, 127.5, 126.8, 121.9, 119.0, 104.2, 36.4, 32.7; HRMS (ES) m/e calcd for C₁₆H₁₆N₂SONa ([M+Na]⁺) 307.0881, found 307.0896.

Di-*tert*-butyl 9-phenyl-9*H*-purin-6-yliminodicarbonate (15a).

The reaction was carried out as for **8h**, except Et₃N and DMF was employed (0.40 mmol of **14** used). Reaction time: 90 h; white solid; yield of **15a**: 152 mg, 93%. *R*_f = 0.60 (10:1 CH₂Cl₂:EtOAc); mp 129-130 °C (from CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃) δ 8.94 (s, 1H), 8.38 (s, 1H), 7.72-7.75 (m, 2H), 7.58-7.63 (m, 2H), 7.50 (tt, *J* = 1.0, 7.5 Hz, 1H), 1.50 (s, 18H); ¹³C NMR (100 MHz, CDCl₃) δ 152.9 (2C), 152.7, 150.8, 150.5, 143.7, 134.2, 130.0 (2C), 129.3, 128.6, 123.5 (2C), 83.9 (2C), 27.8 (6C); HRMS (ES) *m/e* calcd for C₂₁H₂₅N₅O₄Na ([M+Na]⁺) 434.1804, found 434.1810.

Di-*tert*-butyl 9-*p*-tolyl-9*H*-purin-6-yliminodicarbonate (15b).

The reaction was carried out as for **8h**, except Et₃N and DMF was employed (0.40 mmol of **14** used). Reaction time: 46 h; white solid; yield of **15b**: 116.6 mg, 69%. *R*_f = 0.57 (10:1 CH₂Cl₂:EtOAc); mp 161-162 °C (from CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃) δ 8.93 (s, 1H), 8.33 (s, 1H), 7.57-7.60 (m, 2H), 7.39-7.41 (m, 2H), 2.46 (s, 3H), 1.49 (s, 18H); ¹³C NMR (100 MHz, CDCl₃) δ 153.1, 152.7 (2C), 150.8, 150.6, 143.9, 138.9, 131.7, 130.6 (2C), 129.3, 123.6 (2C), 83.9 (2C), 27.9 (6C), 21.2; HRMS (ES) *m/e* calcd for C₂₂H₂₇N₅O₄Na ([M+Na]⁺) 448.1961, found 448.1961.

Di-*tert*-butyl 9-(4-methoxyphenyl)-9*H*-purin-6-yliminodicarbonate (15c).

The reaction was carried out as for **8h**, except Et₃N and DMF was employed (0.40 mmol of **14** used). Reaction time: 74 h; white solid; yield of **15c**: 136 mg, 77%. *R*_f = 0.45 (10:1 CH₂Cl₂:EtOAc); mp 170-171 °C (from

CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃) δ 8.92 (s, 1H), 8.29 (s, 1H), 8.57-8.61 (m, 2H), 7.08-7.12 (m, 2H), 3.89 (s, 3H), 1.50 (s, 18H); ¹³C NMR (100 MHz, CDCl₃) δ 159.8, 153.3, 152.8 (2C), 150.8, 150.6, 144.1, 129.2, 127.0, 125.3 (2C), 115.2 (2C), 84.0 (2C), 55.7, 27.9 (6C); HRMS (ES) *m/e* calcd for C₂₂H₂₇N₅O₅Na ([M+Na]⁺) 464.1910, found 464.1907.

Di-*tert*-butyl 9-(2,4,5-trimethylphenyl)-9*H*-purin-6-yliminodicarbonate (15d**).**

The reaction was carried out as for **8h**, except Et₃N and DMF was employed (0.40 mmol of **14** used). Reaction time: 67 h; white solid; yield of **15d**: 85.1 mg, 47%. *R*_f = 0.30 (10:1 CH₂Cl₂:EtOAc); mp 141-142 °C (from CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃) δ 8.86 (s, 1H), 8.12 (s, 1H), 7.20 (s, 1H), 7.09 (s, 1H), 2.32 (s, 3H), 2.30 (s, 3H), 2.03 (s, 3H), 1.49 (s, 18H); ¹³C NMR (100 MHz, CDCl₃) δ 154.0, 152.9 (2C), 150.8, 150.6, 145.1, 139.1, 135.9, 132.8, 132.3, 130.1, 128.5, 128.3, 83.9 (2C), 27.9 (6C), 19.6, 19.4, 17.3; HRMS (ES) *m/e* calcd for C₂₄H₃₁N₅O₄Na ([M+Na]⁺) 476.2274, found 476.2274.

Di-*tert*-butyl 9-(4-bromophenyl)-9*H*-purin-6-yliminodicarbonate (15e**).**

The reaction was carried out as for **8h**, except Et₃N and DMF was employed (0.40 mmol of **14** used). Reaction time: 74 h; white solid; yield of **15e**: 168 mg, 77%. *R*_f = 0.69 (10:1 CH₂Cl₂:EtOAc); mp 158-159 °C (from CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃) δ 8.93 (s, 1H), 8.35 (s, 1H), 7.72-7.75 (m, 2H), 7.63-7.67 (m, 2H), 1.50 (s, 18H); ¹³C NMR (100 MHz, CDCl₃) δ 152.9 (2C), 151.0, 150.6, 143.2, 133.2 (2C), 132.2, 129.3, 124.9 (2C), 122.4, 117.3, 84.1 (2C), 27.9 (6C); HRMS (ES) *m/e* calcd for C₂₁H₂₄⁷⁹BrN₅O₄Na ([M+Na]⁺) 512.0909, found 512.0903.

Di-tert-butyl 9-(4-iodophenyl)-9H-purin-6-yliminodicarbonate (15f).

The reaction was carried out as for **8h**, except Et₃N and DMF was employed (0.40 mmol of **14** used). Reaction time: 114 h; white solid; yield of **15f**: 166 mg, 77%. *R*_f = 0.50 (10:1 CH₂Cl₂:EtOAc); mp 167-168 °C (from CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃) δ 8.93 (s, 1H), 8.34 (s, 1H), 7.92-7.95 (m, 2H), 7.51-7.54 (m, 2H), 1.50 (s, 18H); ¹³C NMR (100 MHz, CDCl₃) δ 153.0, 152.8 (2C), 151.0, 150.6, 143.1, 139.2 (2C), 134.0, 129.4, 125.1 (2C), 93.7, 84.1 (2C), 27.9 (6C); HRMS (ES) *m/e* calcd for C₂₁H₂₅IN₅O₄ (MH⁺) 538.0951, found 538.0956.

Di-tert-butyl 9-(3-phenylprop-1-enyl)-9H-purin-6-yliminodicarbonate (15g).

The reaction was carried out as for **8h**, except Et₃N and DMF was employed (0.40 mmol of **14** used). Reaction time: 42 h; clear oil; yield of **15g**: 153 mg, 85%. *R*_f = 0.49 (10:1 CH₂Cl₂:EtOAc); ¹H NMR (400 MHz, CDCl₃) δ 8.89 (s, 1H), 8.22 (s, 1H), 7.25-7.37 (m, 5H), 7.08 (dt, *J* = 1.5, 14.5 Hz, 1H), 6.69 (dt, *J* = 7.0, 14.5 Hz, 1H), 3.62 (d, *J* = 7.0 Hz, 2H), 1.44 (s, 18H); ¹³C NMR (100 MHz, CDCl₃) δ 152.5 (2C), 152.2, 150.5, 150.3, 142.4, 138.5, 129.2, 128.8 (2C), 128.6 (2C), 126.8, 122.4, 120.9, 83.8 (2C), 36.4, 27.8 (6C); HRMS (ES) *m/e* calcd for C₂₄H₃₀N₅O₄ (MH⁺) 452.2298, found 452.3201.

Di-tert-butyl 6-chloro-9-phenyl-9H-purin-2-yliminodicarbonate (19a).

The reaction was carried out as for **8h** (0.245 mmol of **18** used). Reaction time: 44 h; white solid; yield of **19a**: 88.9 mg, 81%. *R*_f = 0.50 (10:1 CH₂Cl₂:EtOAc); mp 179-180 °C (from CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃) δ 8.45 (s, 1H), 7.69-7.72 (m, 2H), 7.57-7.61 (m, 2H), 7.51 (tt, *J* = 1.0, 7.5 Hz, 1H), 1.45 (s, 18H); ¹³C NMR (100

MHz, CDCl₃) δ 152.6 (2C), 151.9, 150.6, 145.0, 133.9, 130.0 (2C), 130.0, 129.0, 129.0 (2C), 123.3, 83.8 (2C), 27.9 (6C); HRMS (ES) m/e calcd for C₂₁H₂₄ClN₅O₄Na ([M+Na]⁺) 468.1415, found 468.1425.

Di-*tert*-butyl 6-chloro-9-(4-fluoro-3-methylphenyl)-9H-purin-2-yliminodicarbonate (19b).

The reaction was carried out as for **8h** (0.40 mmol of **18** used). Reaction time: 42 h; white solid; yield of **19b**: 113.3 mg, 59%. R_f = 0.48 (10:1 CH₂Cl₂:EtOAc); mp 171-172 °C (from CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃) δ 8.37 (s, 1H), 7.52 (dd, J = 2.0, 6.5 Hz, 1H), 7.45-7.49 (m, 1H), 7.21 (t, J = 9.0 Hz, 1H), 2.39 (d, J = 2.0 Hz, 3H), 1.46 (s, 18H); ¹³C NMR (100 MHz, CDCl₃) δ 161.1 (d, J = 248.5 Hz), 152.7 (2C), 152.3 (d, J = 4.0 Hz), 151.9, 150.7, 144.9, 130.4 (d, J = 4.5 Hz), 129.5 (d, J = 3.0 Hz), 127.3 (d, J = 19.0 Hz), 126.7 (d, J = 5.5 Hz), 122.6 (d, J = 8.5 Hz), 116.6 (d, J = 24.5 Hz), 83.8 (2C), 28.0 (6C), 14.9 (d, J = 3.5 Hz); HRMS (ES) m/e calcd for C₂₂H₂₅ClFN₅O₄Na ([M+Na]⁺) 500.1477, found 500.1493.

Di-*tert*-butyl 6-chloro-9-(2,4,5-trimethylphenyl)-9H-purin-2-yliminodicarbonate (19c).

The reaction was carried out as for **8h** (0.40 mmol of **18** used). Reaction time: 42 h; white solid; yield of **19c**: 81.8 mg, 42%. R_f = 0.54 (10:1 CH₂Cl₂:EtOAc); mp 162-163 °C (from CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃) δ 8.18 (s, 1H), 7.19 (s, 1H), 7.07 (s, 1H), 2.32 (s, 3H), 2.29 (s, 3H), 2.06 (s, 3H), 1.40 (s, 18H); ¹³C NMR (100 MHz, CDCl₃) δ 153.1, 152.4 (2C), 151.7, 150.4, 146.5, 139.3, 135.9, 132.8, 132.0, 129.9, 129.7, 128.1, 83.6 (2C), 28.0 (6C), 19.6, 19.3, 17.5; HRMS (ES) m/e calcd for C₂₄H₃₀ClN₅O₄Na ([M+Na]⁺) 510.1884, found 510.1919.

Di-tert-butyl 6-chloro-9-(4-bromophenyl)-9H-purin-2-yliminodicarbonate (19d).

The reaction was carried out as for **8h**, except Et₃N and DMF was employed (0.40 mmol of **18** used). Reaction time: 40 h; white solid; yield of **19d**: 143.9 mg, 69%. *R*_f = 0.50 (10:1 CH₂Cl₂:EtOAc); mp 183-184 °C (from CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃) δ 8.42 (s, 1H), 7.70-7.74 (m, 2H), 7.61-7.65 (m, 2H), 1.46 (s, 18H); ¹³C NMR (100 MHz, CDCl₃) δ 152.8 (2C), 152.1, 152.0, 150.7, 144.2, 133.3 (2C), 132.9, 130.6, 124.7 (2C), 122.8, 83.9 (2C), 28.0 (6C); HRMS (ES) *m/e* calcd for C₂₁H₂₃BrClN₅O₄Na ([M+Na]⁺) 546.0520, found 546.0533.

Di-tert-butyl 6-chloro-9-(3-phenylprop-1-enyl)-9H-purin-2-yliminodicarbonate (19e).

The reaction was carried out as for **8h**, except Et₃N and DMF was employed (0.40 mmol of **18** used). Reaction time: 40 h; clear oil; yield of **19e**: 142.9 mg, 74%. *R*_f = 0.54 (10:1 CH₂Cl₂:EtOAc); (from CH₂Cl₂); ¹H NMR (400 MHz, CDCl₃) δ 8.27 (s, 1H), 7.32-7.36 (m, 2H), 7.25-7.28 (m, 3H), 7.00 (dt, *J* = 1.5, 14.5 Hz, 1H), 6.68 (dt, *J* = 7.0, 14.5 Hz, 1H), 3.60 (d, *J* = 7.0 Hz, 2H), 1.45 (s, 18H); ¹³C NMR (100 MHz, CDCl₃) δ 152.4 (2C), 151.5, 150.6, 149.9, 143.6, 138.2, 130.3, 128.9 (2C), 128.7 (2C), 126.9, 123.5, 120.6, 83.9 (2C), 36.4, 27.9 (6C); HRMS (ES) *m/e* calcd for C₂₄H₂₈ClN₅O₄Na ([M+Na]⁺) 508.1728, found 508.1713.

References

- (1) Frieden, M.; Giraud, M.; Reese, C. B.; Song, Q. *J. Chem. Soc., Perkin Trans 1* **1998**, 2827-2832.
- (2) Mizutani, M.; Sanemitsu, Y.; Tamaru, Y.; Yoshida, Z.-I. *Tetrahedron* **1985**, 41, 5289-5294.
- (3) Dey, S.; Garner, P. *J. Org. Chem.* **2000**, 65, 7697-7699.

Single crystal X-ray crystallographic analysis of **15f** and **19b**:

Thermal ellipsoid plot of **15f** (ORTEP, 50% probability level)

Hydrogen atoms are omitted for clarity.

Thermal ellipsoid plot of **19b** (ORTEP, 50% probability level)

Hydrogen atoms are omitted for clarity.

^1H NMR Spectra (400 MHz) of **7a** in CDCl_3

^{13}C NMR Spectra (100 MHz) of **7a** in CDCl_3

^1H NMR Spectra (400 MHz) of **7c** in CDCl_3

^{13}C NMR Spectra (100 MHz) of **7c** in CDCl_3

¹H NMR Spectra (400 MHz) of **8i** in CDCl₃

^{13}C NMR Spectra (100 MHz) of **8i** in CDCl_3

^1H NMR Spectra (400 MHz) of **8I** in CDCl_3

^{13}C NMR Spectra (100 MHz) of **81** in CDCl_3

¹H NMR Spectra (400 MHz) of **13c** in CDCl₃

^{13}C NMR Spectra (100 MHz) of **13c** in CDCl_3

^1H NMR Spectra (400 MHz) of **15a** in CDCl_3

^{13}C NMR Spectra (100 MHz) of **15a** in CDCl_3

¹H NMR Spectra (400 MHz) of **19a** in CDCl₃

^{13}C NMR Spectra (100 MHz) of **19a** in CDCl_3

^1H NMR Spectra (400 MHz) of **20** in CDCl_3

^{13}C NMR Spectra (100 MHz) of **20** in CDCl_3

¹H NMR Spectra (400 MHz) of **21** in CDCl₃

^{13}C NMR Spectra (100 MHz) of **21** in CDCl_3

¹H NMR Spectra (400 MHz) of **22** in *d*⁶-DMSO

^{13}C NMR Spectra (100 MHz) of **22** in d^6 -DMSO

^1H NMR Spectra (400 MHz) of **23** in d^6 -DMSO

^{13}C NMR Spectra (100 MHz) of **23** in d^6 -DMSO

^1H NMR Spectra (400 MHz) of **24** in d^6 -DMSO

^{13}C NMR Spectra (100 MHz) of **24** in d^6 -DMSO

^1H NMR Spectra (400 MHz) of **26** in d^6 -DMSO

^{13}C NMR Spectra (100 MHz) of **26** in d^6 -DMSO