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Supporting Information

for

Suzuki-Miyaura and Sonogashira Coupling of 6-Chloropurines and Ribosides in Water

Jan Pschierer and Herbert Plenio*

Anorganische Chemie im Zintl-Institut, TU Darmstadt, Petersenstrasse 18, 64287 Darmstadt, Germany

plenio@tu-darmstadt.de

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Experimental Section

All chemicals were purchased as reagent grade from commercial suppliers and used without further purification, unless otherwise noted. Used solvents (water, *n*-butanol; all technical grade) were deaerated via freeze and thaw technique (3X). For crosscoupling reactions under anhydrous conditions, *n*-butanol (technical grade, dried over molecular sieves, 4 Å) was used. Potassium carbonate, used in cross coupling reactions, was technical grade. All “phosphines” mentioned in this publication were used in the form of their air stable phosphonium salts and deprotonated *in situ* during the catalyst preparation. All experiments were carried out under an argon atmosphere, unless otherwise noted. Proton (^1H NMR), carbon (^{13}C NMR), and phosphorus (^{31}P NMR) nuclear magnetic resonance spectra were recorded on Bruker DRX 500 at 500 MHz, 125.75 and 202.46, respectively, at 293 K. The chemical shifts are given in parts per million (ppm) on the delta scale (δ) and are referenced to tetramethylsilane (0 ppm), ^1H NMR, and 65% aq. H_3PO_4 . (0 ppm), ^{31}P Abbreviations for NMR data: s) singlet; d) doublet; t) triplet; q) quartet; qi) quintet; dd) doublet of doublets; dt) doublet of triplets; dq) doublet of quartets; tt) triplet of triplets; m) multiplet. Melting points were recorded on an uncorrected Laboratory Devices Mel-Temp instrument. Mass spectra were recorded on a Finnigan MAT 95 magnetic sector spectrometer. Thin layer chromatography (TLC) was performed using Fluka silica gel 60 F 254 (0.2 mm) on aluminum plates. Silica gel columns for chromatography were prepared with E. Merck silica gel 60 (0.063-0.20 mesh ASTM).

Suzuki-Miyaura-Coupling of chlorpurines with $\text{Pd}/\text{cataCXium}^{\text{®}}$ *F sulf*

Preparation of the catalyst stock solution. $[\text{Na}_2\text{PdCl}_4]$ (14.7 mg, 0.05 mmol), phosphine ligand (0.1 mmol) and K_2CO_3 (56 mg, 0.4 mmol) were placed in a Schlenk tube under argon. Degassed water (5.0 mL) was added and the mixture was stirred at 45 °C for 3 h until the clear solution turned off white). This stock solution had a Pd concentration of 0.01 mol L^{-1} .

General procedure for cross coupling reaction. Boronic acid (1.5 mmol), chloropurine (1.0 mmol) and K_2CO_3 (345 mg, 2.5 mmol) were placed in a 25 mL Schlenk tube and evacuated and backfilled with Ar thrice. Degassed water (1.5 mL) and degassed *n*-butanol (4.5 mL) were then added together with the appropriate volume of catalyst stock solution (e.g., 1 mL of the solution prepared above was added to obtain a catalyst loading of 1 mol %).

The reaction mixture was stirred for 16 h at 100 °C and then cooled to room temperature. The combined organic layers were dried with brine and $MgSO_4$. Conversion was determined by product isolation: The organic layer was concentrated in vacuo and the residue was purified by column chromatography ($CH_2Cl_2/MeOH/NEt_3 = 5/ 1/ 1$ as eluent) to afford the pure corresponding cross coupling product.

For analytical approach, the aqueous layer is extracted with methyl *tert*.-butyl ether (5.0 mL) twice.

Procedure in pure water. Procedure as the same as mentioned above, only *n*-Butanol is omitted and 5.0 ml of water are used. Reaction mixture is extracted with *n*-Butanol twice.

Sonogashira-Coupling of chlorpurines with $Pd/cataCXium^{\text{®}} F sulf$

Preparation of the catalyst stock solution. $[Na_2PdCl_4]$ (14.7 mg, 0.05 mmol), phosphine ligand (0.1 mmol) and K_2CO_3 (56 mg, 0.4 mmol) were placed in a Schlenk tube under argon. Degassed water (5.0 mL) was added and the mixture was stirred at 45 °C for 3 h until the clear solution turned off white). This stock solution had a Pd concentration of 0.01 mol L^{-1} .

General procedure for cross coupling reaction. Chloropurine (1.0 mmol) and K_2CO_3 (184 mg, 1.33 mmol) were placed in a 25 mL Schlenk tube and evacuated and backfilled with Ar thrice. Degassed water (1.5 mL) and degassed *n*-butanol (4.5 mL) was then added together with the acetylene (1.13 mmol) and the appropriate volume of catalyst stock solution (e.g., 1 mL of the solution prepared above was added to obtain a catalyst loading of 1 mol %).

The reaction mixture was stirred for 16 h at 95 °C and then cooled to room temperature. The combined organic layers were dried with brine and MgSO₄. Conversion was determined by product isolation: The organic layer was concentrated in vacuo and the residue was purified by column chromatography (Cyclohexane/EtOAc/NEt₃ = 9/ 1/ 1 as eluent) to afford the pure corresponding cross coupling product.

For analytical approach, the aqueous layer is extracted with methyl *tert.*-butyl ether (5.0 mL) twice.

Procedure in pure water. Procedure as the same as mentioned above, only *n*-Butanol is omitted and 5.0 ml of water are used. Reaction mixture is extracted with *n*-Butanol twice.

Analytical data of the purines

6-*p*-tolyl-purine (table 1, entry 1). ¹H NMR (500 MHz, DMSO-*d*₆) δ 8.85 (s, 1H, NH), 8.55 (s, 1H, NH), 7.33 (d, ³*J* = 7.4 Hz, 2H, ar), 7.06 (d, ³*J* = 8.1, 2H, ar), 2.33 (s, 3H, CH₃). ¹³C {¹H} NMR (125.8 MHz DMSO-*d*₆) δ 153.16, 151.42, 145.01, 141.06, 132.79, 129.82, 127.63, 124.68, 121.02, 20.78. HRMS is in accord with previously published data.^[1] Melting Point 283 – 285 °C.

6-Naphtyl-purine (table 1 , entry 2). ¹H NMR (500 MHz, DMSO-*d*₆) δ 9.06 (s, 1H, purine-2), 8.59 (s, 1H, purine-8), 8.13-7.93 (m, 4H, ar), 7.71-7.48 (m, 3H, ar). ¹³C {¹H} NMR (125.8 MHz DMSO-*d*₆) δ 154.35, 151.61, 154.90, 133.42, 132.76, 130.46, 129.94, 129.2, 128.27, 126.56, 126.10, 125.67, 125.17. HRMS (m/z): calcd for C₁₅H₁₀N₄: 245.0828; found: 245.08377. Melting Point 286 – 288 °C.

6-*p*-tolyl-2-amino-purine (table 1, entry 3). ¹H NMR (500 MHz, DMSO-*d*₆) δ 12.72 (bs, 1H, NH), 8.62 (d, ³*J* = 7.94 Hz, 2H, ar), 8.11 (s, 1H, purine-H), 7.41 (d, ³*J* = 7.91 Hz, 2H, ar), 6.38 (s, 2H, NH₂), 2.39 (s, 3H, CH₃). ¹³C {¹H} NMR (125.8 MHz DMSO-*d*₆) δ 160.05, 155.28, 152.89, 140.37, 139.99, 133.38, 128.98, 128.81, 127.97, 21.03. HRMS (m/z): calcd for C₁₂H₁₁N₅: 225.1016; found: 225.09982. Melting Point 260 – 262 °C.

6-Naphtyl-2-amino-purine (table 1, entry 4). ^1H NMR (500 MHz, DMSO- d_6) δ 8.19-7.98 (m, 2H, ar), 8.01 (s, 1H, purine-H), 7.85 (d, $^3J = 7.83$ Hz, 2H, ar), 7.7-7.45 (m, 3H, ar), 6.38 (s, 2H, NH_2). ^{13}C $\{^1\text{H}\}$ NMR (125.8 MHz DMSO- d_6) δ 160.05, 155.92, 142.02, 133.8, 133.28, 130.57, 129.22, 128.44, 128.06, 127.68, 126.11, 125.82, 125.02, 124.73. HRMS (m/z): calcd for $\text{C}_{15}\text{H}_{11}\text{N}_5$: 260.0937; found: 260.09472. Melting Point 270 – 272 $^\circ\text{C}$.

6-(3-bromophenyl)-2-amino-purine (table 1, entry 5). ^1H NMR (500 MHz, DMSO- d_6) δ 8.16(s, 1H, ar), 8.02 (s, 1H, purine-8), 7.87 (dd, $^3J = 8.0$, $J = 4.9$ Hz, 1H, ar), 7.63 (d, 1H, $^3J = 7.83$ Hz, ar), 7.45 (d, 1H, $^3J = 7.81$ Hz, ar), 6.36 (s, 2H, NH_2). ^{13}C $\{^1\text{H}\}$ NMR (125.8 MHz DMSO- d_6) δ 162.37, 156.12, 145.01, 137.01, 135.98, 134.00, 131.62, 130.43, 129.12, 129.05, 122.43. HRMS (m/z): calcd for $\text{C}_{11}\text{H}_8\text{BrN}_5$: 289.0012; found: 289.00143. Melting Point 249 – 250 $^\circ\text{C}$.

6-(ferrocenyl)-purine (table 1, entry 6). ^1H NMR (500 MHz, DMSO- d_6) δ 8.24(s, 1H, purine-2), 7.51(s, 1H, purine-8), 4.24 (s, sH, fc), 4.14 (s, 2H, fc), 4.135 (s, 5H, fc). ^{13}C $\{^1\text{H}\}$ NMR (125.8 MHz DMSO- d_6) δ 155.45, 135.84, 149.24, 144.49, 134.91, 75.09, 74.22, 70.62. HRMS (m/z): calcd for $\text{C}_{15}\text{H}_{13}\text{FeN}_4$: 319.0584; found: 319.05941. Melting Point 250 – 252 $^\circ\text{C}$.

6-(3-thiophenyl)-2-amino-purine (table 1, entry 7). ^1H NMR (500 MHz, DMSO- d_6) δ 8.55(s, 1H, ar), 7.93 (d, $^3J = 7.45$ Hz, 1H, ar), 7.83 (s, 1H, purine-8), 7.27 (d, 1H, $^3J = 7.8$ Hz, ar), 5.89 (s, 2H, NH_2). ^{13}C $\{^1\text{H}\}$ NMR (125.8 MHz DMSO- d_6) δ 159.2, 156.75, 150.04, 146.54, 145.00, 125.25, 121.02, 120.75, 118.10. HRMS (m/z): calcd for $\text{C}_9\text{H}_7\text{N}_5\text{S}$: 217.0424; found: 217.04179. Melting Point 287 – 290 $^\circ\text{C}$.

6-(3-furanyl)-2-chloro-purine (table 1, entry 8). ^1H NMR (500 MHz, DMSO- d_6) δ 8.91 (d, $^3J = 8.5$ Hz, 1H, ar), 8.82 (d, $^3J = 7.96$ Hz, 1H, ar), 8.57 (s, 1H, purine-8), 8.45(s, 1H, ar). ^{13}C $\{^1\text{H}\}$ NMR (125.8 MHz DMSO- d_6) δ 155.04, 152.23, 147.25, 147.05, 146.48, 142.56, 130.18, 114.37, 101.15. HRMS (m/z): calcd for $\text{C}_9\text{H}_5\text{ClN}_4\text{O}$: 220.0148; found: 220.01517. Melting Point 284 – 286 $^\circ\text{C}$.

6-(*p*-Tolyl)-2-chloro-purine (table 1, entry 9). ^1H NMR (500 MHz, DMSO- d_6) δ 8.37 (d, $^3J = 8.3$ Hz, 2H, ar), 8.08 (s, 1H, purine-8), 7.18 (d, $^3J = 7.9$ Hz, 2H, ar), 2.55 (s, 3H, CH_3). ^{13}C { ^1H } NMR (125.8 MHz DMSO- d_6) δ 160.29, 145.94, 144.87, 140.05, 135.11, 134.39, 130.05, 125.21, 124.67, 15.87. HRMS (m/z): calcd for $\text{C}_{12}\text{H}_9\text{ClN}_4$: 244.0573; found: 244.05427. Melting Point 268 – 271 °C.

2,6-di-(*p*-Tolyl)-purine (table 1, entry 10). ^1H NMR (500 MHz, DMSO- d_6) δ 13.53 (bs, NH, 1H), 8.86 (s, 1H, H-8), 8.69 (d, $^3J = 7.8$ Hz, 2H, ar), 8.63 (d, $^3J = 7.9$ Hz, 2H, ar), 7.34 (d, $^3J = 8.9$ Hz, 2H, ar), 7.06 (d, $^3J = 7.7$ Hz, 2H, ar), 2.42 (s, 3H, CH_3), 2.34 (s, 3H, CH_3). ^{13}C { ^1H } NMR (125.8 MHz DMSO- d_6) δ 161.05, 158.12, 145.01, 140.12, 138.85, 138.34, 135.08, 131.47, 128.86, 128.10, 127.09, 126.24, 20.14, 18.97. HRMS (m/z): calcd for $\text{C}_{19}\text{H}_{16}\text{N}_4$: 300.1439; found: 300.14499. Melting Point 287 – 289 °C.

6-Naphtyl-2-chloro-purine (table 1, entry 11). ^1H NMR (500 MHz, DMSO- d_6) δ 8.6(s, 1H, purine-8), 8.13-7.8 (m, 4H, ar), 7.72-7.48 (m, 3H, ar). ^{13}C { ^1H } NMR (125.8 MHz DMSO- d_6) δ 157.04, 146.08, 145.06, 143.76, 138.73, 135.10, 132.74, 131.05, 128.79, 128.36, 125.94, 125.57, 125.04, 124.36, 123.43. HRMS (m/z): calcd for $\text{C}_{15}\text{H}_9\text{ClN}_4$: 279.0434; found: 279.04366. Melting Point 275 – 277 °C.

6-(ferrocenyl)-2-chloro-purine (table 1, entry 12). ^1H NMR (500 MHz, DMSO- d_6) δ 8.07(s, 1H, purine-8), 4.34 (s, 2H, fc), 4.26 (s, 2H, fc), 4.12 (s, 5H, fc). ^{13}C { ^1H } NMR (125.8 MHz DMSO- d_6) δ 166.23, 158.49, 146.27, 144.58, 132.54, 73.03, 71.17, 67.24. HRMS (m/z): calcd for $\text{C}_{15}\text{H}_{11}\text{ClFeN}_4$: 338.0041; found: 338.00511. Melting Point 257 – 260 °C.

6-*p*-Tolyl- β -D-ribofuranosyl-purine (table 2, entry 1). ^1H NMR (500 MHz, DMSO- d_6) δ 8.89(s, 1H, purine-H), 8.72(d, 2H, $^3J = 8.4$ Hz, ar), 7.48(s, 1H, purine-H), 7.35(d, 2H, $^3J = 7.9$ Hz), 6.13(s, 1H), 4.61(s, 1H), 4.32-4.07(m, 4H), 3.74-3.58(m, 2H). ^{13}C { ^1H } NMR (125.8 MHz DMSO- d_6) δ 153.43, 151.29, 155.73, 141.96, 136.31, 129.16, 128.76, 127.91, 126.26, 124.95, 87.62, 85.86, 73.96, 70.14, 63.84, 21.46. HRMS (m/z): calcd for $\text{C}_{17}\text{H}_{18}\text{N}_4\text{O}_4$ 342.1328; found: 342.13351, highly viscous oil.

6-Naphtyl – β -D-ribofuranosyl-purine (table 2, entry 2). ^1H NMR (500 MHz, DMSO- d_6) δ 9.09(s, 1H, purine-H), 8.22(d, 3J = 8.1 Hz, 1H, ar), 8.07(d, 3J = 7.6 Hz, 1H, ar), 7.89 (s, 1H, purine-H), 7.76-7.51(m, 5H, ar), 6.17(s, 1H), 4.63(d, 3J = 9.1 Hz, 1H), 4.08(s, 1H), 3.76-3.11(m, 6H). ^{13}C { ^1H } NMR (125.8 MHz DMSO- d_6) δ 156.86, 152.17, 144.92, 143.11, 139.02, 138.76, 131.68, 130.62, 129.96, 128.91, 126.17, 125.83, 125.16, 124.90, 87.63, 85.14, 74.87, 70.04, 64.17. HRMS (m/z): calcd for $\text{C}_{20}\text{H}_{18}\text{N}_4\text{O}_4$ 378.1328; found 378.13286, highly viscous oil.

6-(3-thiophenyl)- β -D-ribofuranosyl-purine (table 2, entry 3). ^1H NMR (500 MHz, DMSO- d_6) δ 8.91(s, 1H, purine-H), 8.67(s, 1H, purine-H), 8.36(d, 3J = 6.4 Hz, 1H, ar), 8.02 (s, 1H, ar), 7.74(d, 3J = 9.5 Hz, 1H, ar), 6.17(dd, 2J = 3.53 Hz, J = 38.2 Hz, 1H, 4.87(d, J = 21.6 Hz, 1H), 4.31-3.91(m, 3H), 3.61-3.42(m, 2H). ^{13}C { ^1H } NMR (125.8 MHz DMSO- d_6) δ 158.17, 157.46, 155.63, 152.29, 150.69, 150.04, 146.23, 129.76, 114.62, 96.78, 94.83, 83.07, 82.98, 68.92. HRMS (m/z): calcd for $\text{C}_{14}\text{H}_{14}\text{N}_4\text{O}_4\text{S}$ 334.0723; found 334.07179, highly viscous oil.

6-(3-furanyl)- β -D-ribofuranosyl-purine (table 2, entry 4). ^1H NMR (500 MHz, DMSO- d_6) δ 9.79 (s, 1H, purine-H), 8.81 (s, 1H, purine-H), 7.86 (s, 1H, ar), 7.41 (d, 3J = 9.63 Hz, 1H, ar), 7.04 (s, 1H, ar), 6.23 (d, J = 23.7 Hz, 1H), 4.93 (d, J = 17.1 Hz, 1H), 4.71 (s, 1H), 4.48-4.45 (m, 1H), 4.15 (d, J = 19.3 Hz, 3H), 3.67-3.41 (m, 2H). ^{13}C { ^1H } NMR (125.8 MHz DMSO- d_6) δ 151.81, 150.87, 148.57, 146.09, 144.58, 144.18, 129.73, 122.87, 108.91, 90.72, 87.81, 77.01, 76.49, 62.11. HRMS (m/z): calcd for $\text{C}_{14}\text{H}_{14}\text{N}_4\text{O}_5$ 318.1073; found 318.10761, highly viscous oil.

6-(ferrocenyl)- β -D-ribofuranosyl-purine (table 2, entry 5). ^1H NMR (500 MHz, DMSO- d_6) δ 8.84 (s, 1H, purine-H), 7.54 (s, 1H, purine-H), 6.32 (s, 1H), 4.61 (s, 1H), 4.32-4.21 (m, 3H), 4.24 (s, 2H, fc), 4.13 (s, 2H, fc), 4.03 (s, 5H, fc), 3.71-3.53 (m, 2H). ^{13}C { ^1H } NMR (125.8 MHz DMSO- d_6) δ 159.21, 151.96, 148.76, 140.22, 137.31, 88.71, 84.93, 73.26, 72.13, 71.47, 70.89, 67.69, 61.84. HRMS (m/z): calcd for $\text{C}_{20}\text{H}_{22}\text{FeN}_4\text{O}_4$ 452.1068; found 452.10282, highly viscous oil.

6-(Hex-1-ynyl) -purine (table 3, entry 1). ^1H NMR (500 MHz, DMSO- d_6) δ 8.32 (s, 1H), 8.05 (s, 1H), 1.91-1.75 (m, 6H, alkyl), 1.37-1.29 (m, 3H, CH_3). ^{13}C { ^1H } NMR (125.8 MHz DMSO- d_6) δ 157.07, 146.62, 144.03, 132.90, 88.41, 77.96, 33.85, 33.34, 25.51, 24.77. HRMS (m/z): calcd for $\text{C}_{11}\text{H}_{12}\text{N}_4$: 211.3867; found: 211.36952. Melting Point 199 – 202 $^\circ\text{C}$.

6-(Phenylethynyl) -purine (table 3, entry 2). ^1H NMR (500 MHz, DMSO- d_6) δ 8.86 (s, 1H), 8.60 (s, 1H), 7.29-7.27 (m, 5H). ^{13}C { ^1H } NMR (125.8 MHz DMSO- d_6) δ 155.55, 152.31, 150.91, 135.36, 134.40, 130.53, 128.63, 128.06, 124.41, 96.58, 93.31. HRMS (m/z): calcd for $\text{C}_{13}\text{H}_8\text{N}_4$: 220.0719; found: 220.07102. Melting Point 224 – 227 $^\circ\text{C}$.

6-(2,4,6-Trimethyl-phenylethynyl) -purine (table 3, entry 3). ^1H NMR (500 MHz, DMSO- d_6) δ 8.44 (s, 1H), 8.26 (s, 1H), 6.93 (s, 2H), 2.41 (s, 9H). ^{13}C { ^1H } NMR (125.8 MHz DMSO- d_6) δ 154.53, 148.43, 140.29, 139.72, 138.04, 138.01, 136.57, 136.47, 134.87, 129.76, 125.39, 88.25, 86.97, 21.18, 20.02. HRMS (m/z): calcd for $\text{C}_{16}\text{H}_{14}\text{N}_4$: 262.1269; found: 262.12761. Melting Point 218 – 220 $^\circ\text{C}$.

6-(4-Methoxy-phenylethynyl) –purine (table 3, entry 4) ^1H NMR (500 MHz, DMSO- d_6) δ 8.63 (s, 1H), 8.50 (s, 1H), 7.46, (d, 3J = 8.67 Hz, 2H), 7.07 (d, 3J = 8.16 Hz, 2H), 3.80 (s, 3H). ^{13}C { ^1H } NMR (125.8 MHz DMSO- d_6) δ 160.12, 159.97, 154.68, 150.17, 134.27, 133.56, 128.18, 115.07, 114.86, 83.86, 79.50, 55.34. HRMS (m/z): calcd for $\text{C}_{14}\text{H}_{10}\text{N}_4\text{O}$: 250.0825, found: 250.08265, highly viscous oil.

6-(Ferrocenylethynyl) –purine (table 3, entry 5) ^1H NMR (500 MHz, DMSO- d_6) δ 8.55 (s, 1H), 7.33 (s, 1H), 4.54 (s, 2H), 4.34-4.21 (m, 7H). ^{13}C { ^1H } NMR (125.8 MHz DMSO- d_6) δ 161.25, 156.84, 152.03, 138.01, 132.30, 82.73, 77.21, 71.54, 70.08, 69.01. HRMS (m/z): calcd for $\text{C}_{17}\text{H}_{12}\text{FeN}_4$: 328.0428; found: 328.04584, highly viscous oil.

6-(Hex-1-ynyl) - β -D-ribofuranosyl-purine (table 4, entry 1). ^1H NMR (500 MHz, DMSO- d_6) δ 8.60 (s, 1H), 7.85 (s, 1H), 5.84 (d, J = 21.6 Hz, 1H), 4.02-4.01 (m, 2H), 3.83-3.57 (m, 3H), 3.43 (s, 2H), 1.74 (s, 2H), 1.42 (s, 2H), 0.97 (m, 3H). ^{13}C { ^1H } NMR (125.8 MHz DMSO- d_6) δ 155.61, 151.45, 148.07, 145.96, 132.53, 89.68, 86.59, 82.92, 78.24, 74.02, 72.10, 63.36, 25.81, 18.23, 12.90, 7.41. HRMS (m/z): calcd for $\text{C}_{16}\text{H}_{20}\text{N}_4\text{O}_4$: 332.1548, found: 323.15501, highly viscous oil.

6-(Phenylethynyl) - β -D-ribofuranosyl-purine (table 4, entry 2). ^1H NMR (500 MHz, DMSO- d_6) δ 8.71 (s, 1H), 8.15 (s, 1H), 7.34-7.32 (m, 5H), 5.94 (s, 1H), 4.52 (s, 1H), 4.19-4.10 (m, 5H), 3.94-3.83 (m, 2H). ^{13}C { ^1H } NMR (125.8 MHz DMSO- d_6) δ 156.91, 152.96, 148.11, 145.87, 132.55, 129.36, 128.31, 126.12, 97.61, 94.35, 89.55, 86.96, 74.35, 72.74, 63.11. HRMS (m/z): calcd for $\text{C}_{18}\text{H}_{16}\text{N}_4\text{O}_4$: 352.1268, found: 352.12702, highly viscous oil.

6-(4-Methoxy-phenylethynyl) - β -D-ribofuranosyl-purine (table 4, entry 3). ^1H NMR (500 MHz, DMSO- d_6) δ 8.61 (s, 1H), 8.56 (s, 1H), 7.47 (d, 3J = 7.3 Hz, 2H), 7.04 (d, 3J = 7.6 Hz, 2H), 5.86 (s, 1H), 4.39 (s, 1H), 4.16-3.91 (m, 4H), 3.82 (s, 3H), 3.65-3.47 (m, 2H). ^{13}C { ^1H } NMR (125.8 MHz DMSO- d_6) δ 160.05, 155.90, 151.26, 148.03, 145.55, 138.36, 132.65, 116.72, 115.91, 97.01, 92.71, 89.81, 87.69, 73.49, 72.11, 62.35, 54.41. HRMS (m/z): calcd for $\text{C}_{19}\text{H}_{18}\text{N}_4\text{O}_5$: 382.1347, found: 382.13491, highly viscous oil.

6-(Ferrocenylethynyl)- β -D-ribofuranosyl-purine (table 4, entry 4). ^1H NMR (500 MHz, DMSO- d_6) δ 8.94 (s, 1H), 8.82 (s, 1H), 6.06 (d, J = 5.24 Hz, 1H), 5.55 (d, J = 5.66 Hz, 1H), 5.23 (d, J = 5.11 Hz, 1H), 5.09 (t, J = 5.47 Hz, 1H), 4.60 (q, J = 5.21 Hz, 1H), 4.13 (s, 2H), 4.11 (s, 5H), 4.05 (s, 2H), 4.01 (q, J = 3.95 Hz, 1H), 3.66 (m, 2H). ^{13}C { ^1H } NMR (125.8 MHz DMSO- d_6) δ 152.09, 151.97, 149.65, 146.12, 131.73, 88.53, 86.06, 83.02, 76.02, 74.31, 70.41, 69.47, 69.01, 61.35. HRMS (m/z): calcd for $\text{C}_{22}\text{H}_{20}\text{FeN}_4\text{O}_4$: 460.0861; found: 460.08416, highly viscous oil.

[1] C.A. Fleckenstein, H. Plenio, *Chem. Eur. J.* **2008**, *14*, 4267.

6-p-Tolyl-purine
 ^1H NMR (500 MHz, DMSO)

6-p-Tolyl-purine
 ^{13}C NMR (125 MHz, DMSO)

6-Naphtyl-purine
¹H NMR (500 MHz, DMSO)

6-Naphtyl-purine
 ^{13}C NMR (125 MHz, DMSO)

6-Naphtyl-purine

MS

Massenspektrometrie Hochauflösung			
Auftraggeber:	Pschierer	Summenformel	Abweichung (mmu)
Probe:	JP P53	C15 H9 N4	1
Aufnahme Nr.:	65204	C17 H11 N1 O1	-0.3
Gemessene Masse:	245.08377		Ber. Masse
Zulässige Abweichung:	5 (mmu)		245.0826
			245.0841

6-p-Tolyl-2-amino-purine
 ^1H NMR (500 MHz, DMSO)

6-p-Tolyl-2-amino-purine
 ^{13}C NMR (125 MHz, DMSO)

6-p-Tolyl-2-amino-purine

MS

Massenspektrometrie Hochauflösung

Auftraggeber: Pschierer

Probe: JP P54

Aufnahme Nr.: 65205

Gemessene Masse: 225.09982

Zulässige Abweichung: 5 (mmu)

Summenformel	Abweichung (mmu)	Ber. Masse
C9 H13 N4 O3	1	225.0988
C11 H15 N1 O4	-0.3	225.1001
C12 H11 N5	-1.8	225.1016
C14 H13 N2 O1	-3	225.1028

6-Naphtyl-2-amino-purine
 ^1H NMR (500 MHz, DMSO)

6-Naphtyl-2-amino-purine
 ^{13}C NMR (125 MHz, DMSO)

6-Naphtyl-2-amino-purine

MS

Massenspektrometrie Hochauflösung			
Auftraggeber:	Pschierer	Summenformel	Abweichung (mmu)
Probe:	JP P55	C15 H10 N5	1
Aufnahme Nr.:	85192	C17 H12 N2 O1	-0.3
Gemessene Masse:	260.09472		Ber. Masse
Zulässige Abweichung:	5 (mmu)		260.0937
			260.095

6-(3-bromophenyl)-2-amino-purine

^1H NMR (500 MHz, DMSO)

6-(3-bromophenyl)-2-amino-purine

^{13}C NMR (125 MHz, DMSO)

6-(3-bromophenyl)-2-amino-purine

MS

Massenspektrometrie Hochauflösung

Auftraggeber: Pschierer

Probe: JP P56

Aufnahme Nr.: 65206

Gemessene Masse: 298.00143

Zulässige Abweichung: 5 (mmu)

Summenformel	Abweichung (mmu)	Ber. Masse
C ₁₁ H ₈ BrN ₅	0.2	298.0012

6-(ferrocenyl)-purine
 ^1H NMR (500 MHz, DMSO)

6-(ferrocenyl)-purine
 ^{13}C NMR (125 MHz, DMSO)

6-(ferrocenyl)-purine

MS

Massenspektrometrie Hochauflösung

Auftraggeber: Pschierer

Probe: JP P44

Aufnahme Nr.: 85100

Gemessene Masse: 319.05941

Zulässige Abweichung: 5 (mmu)

Summenformel	Abweichung (mmu)	Ber. Masse
C ₁₅ H ₁₃ Fe ₁ N ₄	1	319.0584

6-(3-thiophenyl)-2-amino-purine

^1H NMR (500 MHz, DMSO)

6-(3-thiophenyl)-2-amino-purine

^{13}C NMR (125 MHz, DMSO)

6-(3-thiophenyl)-2-amino-purine

MS

Massenspektrometrie Hochauflösung

Auftraggeber: Pschierer

Probe: JP P59

Aufnahme Nr.: 65184

Gemessene Masse: 217.04179

Zulässige Abweichung: 5 (mmu)

Summenformel	Abweichung (mmu)	Ber. Masse
C9 H7 N5 S1	-0.6	217.0424
C11 H9 N2 O1 S1	-1.8	217.0436
C12 H3 N5	2.8	217.039
C14 H5 N2 O1	1.6	217.0402

6-(3-furanyl)-2-chloro-purine

^1H NMR (500 MHz, DMSO)

6-(3-furanyl)-2-chloro-purine

^{13}C NMR (125 MHz, DMSO)

6-(3-furanyl)-2-chloro-purine

MS

Massenspektrometrie Hochauflösung

Auftraggeber: Pschierer

Probe: JP P63

Aufnahme Nr.: 85226

Gemessene Masse: 220.01517

Zulässige Abweichung: 5 (mmu)

Summenformel	Abweichung (mmu)	Ber. Masse
C8 H7 N3 O4 Cl1	3.1	220.0121
C7 H2 N5 O4	4.5	220.0107
C8 H9 O5 Cl1	1.9	220.0133
* C9 H5 N4 O1 Cl1	0.4	220.0148 *
C9 H4 N2 O5	3.2	220.012
C11 H7 N1 O2 Cl1	-0.9	220.0161
C12 H2 N3 O2	0.5	220.0147
C14 H4 O3	-0.8	220.016
C17 H2 N1	-3.5	220.0187

6-(p-Tolyl)-2-chloro-purine

^1H NMR (500 MHz, DMSO)

6-(p-Tolyl)-2-chloro-purine

^{13}C NMR (125 MHz, DMSO)

6-(p-Tolyl)-2-chloro-purine

MS

Massenspektrometrie Hochauflösung

Auftraggeber: Pschierer

Probe: JP P60

Aufnahme Nr.: 65229

Gemessene Masse: 244.05427

Zulässige Abweichung: 5 (mmu)

Summenformel	Abweichung (mmu)	Ber. Masse
C12 H9 N4 Cl1	-3.1	244.0573

2,6-di-(p-Tolyl)-purine
 ^1H NMR (500 MHz, DMSO)

2,6-di-(p-Tolyl)-purine
 ^{13}C NMR (125 MHz, DMSO)

2,6-di-(p-Tolyl)-purine

MS

Massenspektrometrie Hochauflösung

Auftraggeber: Pschierer

Probe: JP P52

Aufnahme Nr.: 65002

Gemessene Masse: 300.14499

Zulässige Abweichung: 5 (mmu)

Summenformel	Abweichung (mmu)	Ber. Masse
C ₁₉ H ₁₆ N ₄	1	300.1439

6-Naphtyl-2-chloro-purine
 ^1H NMR (500 MHz, DMSO)

6-Naphtyl-2-chloro-purine
 ^{13}C NMR (125 MHz, DMSO)

6-Naphtyl-2-chloro-purine

MS

Massenspektrometrie Hochauflösung			
Auftraggeber:	Pschierer	Summenformel	Abweichung (mmu)
Probe:	JP P61	C15 H8 N4 Cl1	0.3
Aufnahme Nr.:	65219	C16 H3 N8	1.6
Gemessene Masse:	279.04366		
Zulässige Abweichung:	5 (mmu)		

6-(ferrocenyl)-2-chloro-purine

^1H NMR (500 MHz, DMSO)

6-(ferrocenyl)-2-chloro-purine

^{13}C NMR (125 MHz, DMSO)

6-(ferrocenyl)-2-chloro-purine

MS

Massenspektrometrie Hochauflösung

Auftraggeber: Pschierer

Probe: JP P44

Aufnahme Nr.: 65133

Gemessene Masse: 338.00511

Zulässige Abweichung: 5 (mmu)

Summenformel	Abweichung (mmu)	Ber. Masse
C ₁₅ H ₁₁ Fe ₁ N ₄	1	338.0041

6-*p*-Tolyl- β -D-ribofuranosyl-purine

^1H NMR (500 MHz, DMSO)

6-*p*-Tolyl- β -D-ribofuranosyl-purine

^{13}C NMR (125 MHz, DMSO)

6-*p*-Tolyl- β -D-ribofuranosyl-purine

MS

**Massenspektrometrie
Hochauflösung**

Auftraggeber:	Pschierer	Summenformel	Abweichung (mmu)	Ber. Masse
Probe:	JP I-18	C17 H18 N4 O4	0.7	342.1328
Aufnahme Nr.:	65636			
Gemessene Masse:	342.13351			
Zulässige Abweichung:	5 (mmu)			

6-Naphtyl – β -D-ribofuranosyl-purine

^1H NMR (500 MHz, DMSO)

6-Naphtyl – β -D-ribofuranosyl-purine

^{13}C NMR (125 MHz, DMSO)

6-Naphtyl – β -D-ribofuranosyl-purine

MS

**Massenspektrometrie
Hochauflösung**

Auftraggeber:	Pschierer	Summenformel	Abweichung (mmu)	Ber. Masse
Probe:	JP I-6	C ₂₀ H ₁₈ N ₄ O ₄	0.1	378.1328
Aufnahme Nr.:	65838			

Gemessene Masse: 378.13286

Zulässige Abweichung: 5 (mmu)

6-(3-thiophenyl)- β -D-ribofuranosyl-purine

^1H NMR (500 MHz, DMSO)

6-(3-thiophenyl)- β -D-ribofuranosyl-purine

^{13}C NMR (125 MHz, DMSO)

6-(3-thiophenyl)- β -D-ribofuranosyl-purine

MS

**Massenspektrometrie
Hochauflösung**

Auftraggeber: Pschierer

Probe: JP I-7

Aufnahme Nr.: 65639

Gemessene Masse: 334.07179

Zulässige Abweichung: 5 (mmu)

Summenformel	Abweichung (mmu)	Ber. Masse
C ₁₄ H ₁₄ N ₄ O ₄ S ₁	-0.6	334.0723

6-(3-furanyl)- β -D-ribofuranosyl-purine

^1H NMR (500 MHz, DMSO)

6-(3-furanyl)- β -D-ribofuranosyl-purine

^{13}C NMR (125 MHz, DMSO)

6-(3-furanyl)- β -D-ribofuranosyl-purine

MS

**Massenspektrometrie
Hochauflösung**

Auftraggeber:	Pschierer	Summenformel	Abweichung (mmu)	Ber. Masse
Probe:	JP I-11	C14 H14 N4 O5	0.3	318.1073
Aufnahme Nr.:	65686			

Gemessene Masse: 318.10761

Zulässige Abweichung: 5 (mmu)

6-(ferrocenyl)- β -D-ribofuranosyl-purine

^1H NMR (500 MHz, DMSO)

6-(ferrocenyl)- β -D-ribofuranosyl-purine

^{13}C NMR (125 MHz, DMSO)

6-(ferrocenyl)- β -D-ribofuranosyl-purine

MS

Massenspektrometrie Hochauflösung

Auftraggeber: Pschierer

Probe: JP I-10

Aufnahme Nr.: 65884

Gemessene Masse: 452.10282

Zulässige Abweichung: 5 (mmu)

Summenformel	Abweichung (mmu)	Ber. Masse
C ₂₀ H ₂₂ FeN ₄ O ₄	-4	452.1068

6-(Hex-1-ynyl) -purine
¹H NMR (500 MHz, DMSO)

6-(Hex-1-ynyl) -purine
¹³C NMR (125 MHz, DMSO)

6-(Hex-1-ynyl) -purine

MS

Massenspektrometrie Hochauflösung

Auftraggeber: Pschierer

Probe: JP I-16

Aufnahme Nr.: 85052

Gemessene Masse: 211.36952

Zulässige Abweichung: 5 (mmu)

Summenformel	Abweichung (mmu)	Ber. Masse
C ₁₁ H ₁₂ N ₄	3	211.3665

6-(Phenylethynyl) –purine
¹H NMR (500 MHz, DMSO)

6-(Phenylethynyl) –purine
¹³C NMR (125 MHz, DMSO)

6-(Phenylethynyl) –purine

MS

Massenspektrometrie Hochauflösung

Auftraggeber: Pschierer

Probe: JP I-18

Aufnahme Nr.: 65226

Gemessene Masse: 262.12761

Zulässige Abweichung: 5 (mmu)

Summenformel	Abweichung (mmu)	Ber. Masse
C ₁₆ H ₁₄ N ₄	0.8	262.1268

6-(2,4,6-Trimethyl-phenylethynyl) -purine

^1H NMR (500 MHz, DMSO)

6-(2,4,6-Trimethyl-phenylethynyl) -purine

¹³C NMR (125 MHz, DMSO)

6-(2,4,6-Trimethyl-phenylethynyl) -purine

MS

**Massenspektrometrie
Hochauflösung**

Auftraggeber:

Probe:

Aufnahme Nr.:

Gemessene Masse: 250.08265

Zulässige Abweichung: 5 (mmu)

Summenformel	Abweichung (mmu)	Ber. Masse
C ₁₄ H ₁₀ N ₄ O ₁	0.1	250.0825

6-(4-Methoxy-phenylethynyl) –purine

^1H NMR (500 MHz, DMSO)

6-(4-Methoxy-phenylethynyl) –purine

^{13}C NMR (125 MHz, DMSO)

6-(4-Methoxy-phenylethynyl) –purine

MS

**Massenspektrometrie
Hochauflösung**

Auftraggeber:	Pschierer	Summenformel	Abweichung (mmu)	Ber. Masse
Probe:	JP I-20	C ₁₄ H ₁₀ N ₄ O ₁	0.1	250.0825
Aufnahme Nr.:	65688			
Gemessene Masse:	250.08265			
Zulässige Abweichung:	5 (mmu)			

6-(Ferrocenylethynyl) –purine

^1H NMR (500 MHz, DMSO)

6-(Ferrocenylethynyl) –purine

^{13}C NMR (125 MHz, DMSO)

6-(Ferrocenylethynyl) –purine

MS

Massenspektrometrie Hochauflösung

Auftraggeber: Pschierer

Probe: JP I-13

Aufnahme Nr.: 65696

Gemessene Masse: 328.04584

Zulässige Abweichung: 5 (mmu)

Summenformel	Abweichung (mmu)	Ber. Masse
C ₁₇ H ₁₂ Fe ₁ N ₄	3	328.0428

6-(Hex-1-ynyl) - β -D-ribofuranosyl-purine

^1H NMR (500 MHz, DMSO)

6-(Hex-1-ynyl) - β -D-ribofuranosyl-purine

^{13}C NMR (125 MHz, DMSO)

6-(Hex-1-ynyl) - β -D-ribofuranosyl-purine

MS

**Massenspektrometrie
Hochauflösung**

Auftraggeber:	Pschierer	Summenformel	Abweichung (mmu)	Ber. Masse
Probe:	JP I-21	C ₁₆ H ₂₀ N ₄ O ₄	0.2	332.1548
Aufnahme Nr.:	65651			
Gemessene Masse:	332.15501			
Zulässige Abweichung:	5 (mmu)			

6-(Phenylethynyl) - β -D-ribofuranosyl-purine

^1H NMR (500 MHz, DMSO)

6-(Phenylethynyl) - β -D-ribofuranosyl-purine

^{13}C NMR (125 MHz, DMSO)

6-(Phenylethynyl) - β -D-ribofuranosyl-purine

MS

**Massenspektrometrie
Hochauflösung**

Auftraggeber:	Pschierer	Summenformel	Abweichung (mmu)	Ber. Masse
Probe:	JP I-33	C ₁₈ H ₁₆ N ₄ O ₄	0.2	352.1268
Aufnahme Nr.:	66642			
Gemessene Masse:	352.12702			
Zulässige Abweichung:	5 (mmu)			

6-(4-Methoxy-phenylethynyl) - β -D-ribofuranosyl-purine

^1H NMR (500 MHz, DMSO)

6-(4-Methoxy-phenylethynyl) - β -D-ribofuranosyl-purine

^{13}C NMR (125 MHz, DMSO)

6-(4-Methoxy-phenylethynyl) - β -D-ribofuranosyl-purine

MS

**Massenspektrometrie
Hochauflösung**

Auftraggeber:	Pschierer	Summenformel	Abweichung (mmu)	Ber. Masse
Probe:	JP I-22	C ₁₉ H ₁₈ N ₄ O ₅	0.2	382.1347
Aufnahme Nr.:	65686			
Gemessene Masse:	382.13491			
Zulässige Abweichung:	5 (mmu)			

6-(Ferrocenylethynyl)- β -D-ribofuranosyl-purine

^1H NMR (500 MHz, DMSO)

6-(Ferrocenylethynyl)- β -D-ribofuranosyl-purine

^{13}C NMR (125 MHz, DMSO)

6-(Ferrocenylethynyl)- β -D-ribofuranosyl-purine

MS

**Massenspektrometrie
Hochauflösung**

Auftraggeber: Pschierer

Probe: JP I-25

Aufnahme Nr.: 65884

Gemessene Masse: 460.08416

Zulässige Abweichung: 5 (mmu)

Summenformel	Abweichung (mmu)	Ber. Masse
C ₂₂ H ₂₀ Fe ₁ N ₄ O ₄	-2	460.0861