

Supplementary Information for

***Efficient approach to novel 1 α -triazolyl-5 α -androstane derivatives
as potent antiproliferative agents***

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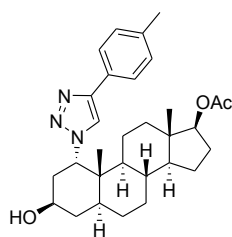
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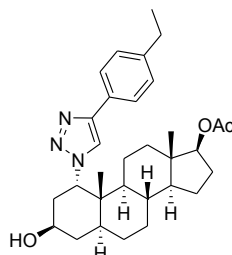
S2-S9

β -Acetoxy-1 α -[4'-(4''-tolyl)-1'H-1',2',3'-triazol-1'-yl]-5 α -androstan-3 β -ol (**7b**)



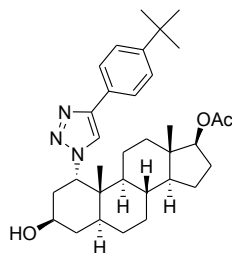
Alkyne: 4-tolylacetylene (**6b**, 0.09 mL) as described in the **General procedure 4.4**. After purification with CH₂Cl₂/EtOAc (90:10) as eluent, **7b** was obtained as a white solid (362 mg, 93%), mp 274-275 °C, *R*_f = 0.41 (ss E); ¹H NMR (500 MHz, CDCl₃): δ_{H} = 0.20 (m, 1H), 0.75 (s, 3H, 18-H₃), 0.81-0.88 (m, 3H), 1.05 (s, 3H, 19-H₃), 1.18-1.26 (m, 2H), 1.36-1.44 (m, 4H), 1.50-1.79 (m, 6H), 1.98 (s, 3H, Ac-CH₃), 2.04 (m, 2H), 2.36 (m, 2H), 2.38 (s, 3H, 4''-CH₃), 4.00 (bs, 1H, 3-H), 4.42 (t, 1H, *J* = 8.3 Hz, 17-H), 4.55 (d, 1H, *J* = 4.9 Hz, 1-H), 5.29 (d, 1H, *J* = 10.2 Hz, 3-OH), 7.23 (d, 2H, *J* = 7.7 Hz, 3''-H and 5''-H), 7.69 (d, 2H, *J* = 7.7 Hz, 2''-H and 6''-H), 7.85 (s, 1H, 5'-H); ¹³C NMR (125 MHz, CDCl₃): δ_{C} = 12.4 (C-18), 13.3 (C-19), 21.1 (Ac-CH₃), 21.2 (4''-CH₃), 21.3 (CH₂), 23.3 (CH₂), 27.4 (CH₂), 28.6 (CH₂), 30.3 (CH₂), 32.8 (CH), 33.2 (CH₂), 35.8 (CH), 36.2 (CH₂), 36.3 (CH₂), 40.4 (C-10), 42.6 (C-13), 47.5 (CH), 50.5 (CH), 63.7 and 64.0 (C-1 and C-3), 82.4 (C-17), 122.0 (C-5'), 125.6 (2C, C-2'' and C-6''), 127.3 (C-1''), 129.6 (2C, C-3'' and C-5''), 138.2 (C-4''), 146.7 (C-4'), 170.9 (Ac-CO); ESI-MS: 492 [M+H]⁺; Anal. Calcd for C₃₀H₄₁N₃O₃ C, 73.29; H, 8.41; N, 8.55. Found: C, 73.43; H, 8.28; N, 8.62.

17 β -Acetoxy-1 α -[4'-(4''-ethylphenyl)-1'H-1',2',3'-triazol-1'-yl]-5 α -androstan-3 β -ol (**7c**)



Alkyne: 4-ethylphenylacetylene (**6c**, 0.12 mL) as described in the **General procedure 4.4**. After purification with CH₂Cl₂/EtOAc (80:20) as eluent, **7c** was obtained as a white solid (372 mg, 92%), mp 253-255 °C, *R*_f = 0.27 (ss D); ¹H NMR (500 MHz, CDCl₃): δ_{H} = 0.19 (m, 1H), 0.75 (s, 3H, 18-H₃), 0.80-0.89 (m, 3H), 1.05 (s, 3H, 19-H₃), 1.20 (m, 2H), 1.26 (t, 3H, *J* = 7.6 Hz, 4''-CH₂CH₃), 1.36-1.43 (m, 4H), 1.51-1.80 (m, 6H), 1.98 (s, 3H, Ac-CH₃), 2.04 (m, 2H), 2.37 (m, 2H), 2.67 (q, 2H, *J* = 7.6 Hz, 4''-CH₂CH₃), 4.00 (bs, 1H, 3-H), 4.42 (t, 1H, *J* = 8.4 Hz, 17-H), 4.55 (d, 1H, *J* = 5.4 Hz, 1-H), 5.30 (d, 1H, *J* = 10.3 Hz, 3-OH), 7.26 (d, 2H, *J* = 7.7 Hz, 3''-H and 5''-H), 7.71 (d, 2H, *J* = 7.7 Hz, 2''-H and 6''-H), 7.89 (s, 1H, 5'-H); ¹³C NMR (125 MHz, CDCl₃): δ_{C} = 12.4 (C-18), 13.3 (C-19), 15.5 (4''-CH₂CH₃), 21.0 (Ac-CH₃), 21.3 (CH₂), 23.3 (CH₂), 27.4 (CH₂), 28.6 (2C, 2 × CH₂), 30.3 (CH₂), 32.8 (CH), 33.1 (CH₂), 35.8 (CH), 36.3 (2C, 2 × CH₂), 40.4 (C-10), 42.6 (C-13), 47.5 (CH), 50.5 (CH), 63.7 and 64.0 (C-1 and C-3), 82.4 (C-17), 122.0 (C-5'), 125.7 (2C, C-2'' and C-6''), 127.6 (C-1''), 128.4 (2C, C-3'' and C-5''), 144.6 (C-4''), 146.7 (C-4'), 170.9 (Ac-CO); ESI-MS: 506 [M+H]⁺; Anal. Calcd for C₃₁H₄₃N₃O₃ C, 73.63; H, 8.57; N, 8.31. Found: C, 73.51; H, 8.75; N, 8.46.

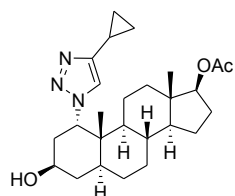
17 β -Acetoxy-1 α -[4'-(4''-tert-butylphenyl)-1'H-1',2',3'-triazol-1'-yl]-5 α -androstan-3 β -ol (**7d**)



Alkyne: 4-tert-butylphenylacetylene (**6d**, 0.16 mL) as described in the **General procedure 4.4**. After purification with CH₂Cl₂/EtOAc (80:20) as eluent, **7d** was obtained as a white solid (397 mg, 93%), mp 271-273 °C, *R*_f = 0.29 (ss E); ¹H NMR (500 MHz, CDCl₃): δ_{H} = 0.19 (m, 1H), 0.75 (s, 3H, 18-H₃), 0.79-0.89 (m, 3H), 1.05 (s, 3H, 19-H₃), 1.20 (m, 2H), 1.34 (s, 9H, 4''-tBu-CH₃), 1.36-1.43 (m, 4H), 1.51-1.79 (m, 6H), 1.98 (s, 3H, Ac-CH₃), 2.04 (m, 2H), 2.37 (m, 2H), 4.00 (bs, 1H, 3-H), 4.43 (t, 1H, *J* = 8.4 Hz, 17-H), 4.56 (d, 1H, *J* = 5.4 Hz, 1-H), 5.32 (d, 1H, *J* = 10.3 Hz, 3-OH), 7.45 (d, 2H, *J* = 7.9 Hz, 3''-H and 5''-H), 7.73 (d, 2H, *J* = 7.9

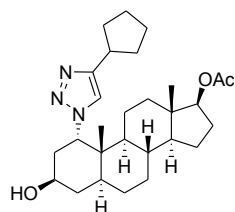
H_z, 2''-H and 6''-H), 7.87 (s, 1H, 5'-H); ¹³C NMR (125 MHz, CDCl₃): δ_C = 12.4 (C-18), 13.3 (C-19), 21.1 (Ac-CH₃), 21.3 (CH₂), 23.3 (CH₂), 27.4 (CH₂), 28.6 (CH₂), 30.4 (CH₂), 31.3 (3C, 4''-*t*Bu-CH₃), 32.8 (CH), 33.2 (CH₂), 34.7 (4''-*t*Bu-C), 35.8 (CH), 36.3 (2C, 2 × CH₂), 40.4 (C-10), 42.6 (C-13), 47.5 (CH), 50.5 (CH), 63.7 and 63.9 (C-1 and C-3), 82.4 (C-17), 122.1 (C-5'), 125.5 (2C) and 125.8 (2C): (C-2'', C-3'', C-5'' and C-6''), 127.3 (C-1''), 146.6 (C-4'), 151.4 (C-4''), 170.9 (Ac-CO); ESI-MS: 534 [M+H]⁺; Anal. Calcd for C₃₃H₄₇N₃O₃ C, 74.26; H, 8.88; N, 7.87. Found: C, 74.45; H, 8.81; N, 7.99.

17β-Acetoxy-1α-[4'-cyclopropyl-1'H-1',2',3'-triazol-1'-yl]-5α-androstan-3β-ol (7e)



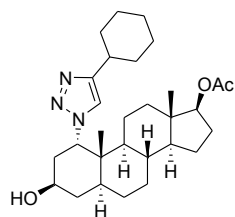
Alkyne: cyclopropylacetylene (**6e**, 0.07 mL) as described in the **General procedure 4.4**. After purification with CH₂Cl₂/EtOAc (80:20) as eluent, **7e** was obtained as a white solid (338 mg, 96%), mp 237-239 °C, *R*_f = 0.29 (ss E); ¹H NMR (500 MHz, CDCl₃): δ_H = 0.01 (m, 1H), 0.75 (s, 3H, 18-H₃), 0.77-0.90 (m, 5H), 0.96 (m, 2H), 1.01 (s, 3H, 19-H₃), 1.14-1.27 (m, 2H), 1.31-1.47 (m, 5H), 1.54 (m, 2H), 1.62-1.75 (m, 3H), 1.90-1.97 (m, 2H), 2.00 (s, 3H, Ac-CH₃), 2.06 (m, 1H), 2.33 (m, 2H), 3.94 (bs, 1H, 3-H), 4.38 (d, 1H, *J* = 5.3 Hz, 1-H), 4.50 (t, 1H, *J* = 8.5 Hz, 17-H), 5.54 (d, 1H, *J* = 10.9 Hz, 3-OH), 7.28 (s, 1H, 5'-H); ¹³C NMR (125 MHz, CDCl₃): δ_C = 6.5 (C-1''), 7.7 and 8.2 (C-2'' and C-3''), 12.4 (C-18), 13.3 (C-19), 21.1 (Ac-CH₃), 21.3 (CH₂), 23.2 (CH₂), 27.3 (CH₂), 28.6 (CH₂), 30.3 (CH₂), 32.7 (CH), 33.0 (CH₂), 35.8 (CH), 36.4 (2C, 2 × CH₂), 40.4 (C-10), 42.7 (C-13), 47.4 (CH), 50.6 (CH), 63.4 and 63.9 (C-1 and C-3), 82.4 (C-17), 122.7 (C-5'), 149.0 (C-4'), 171.0 (Ac-CO); ESI-MS: 442 [M+H]⁺; Anal. Calcd for C₂₆H₃₉N₃O₃ C, 70.71; H, 8.90; N, 9.52. Found: C, 70.81; H, 8.71; N, 9.66.

17β-Acetoxy-1α-[4'-cyclopentyl-1'H-1',2',3'-triazol-1'-yl]-5α-androstan-3β-ol (7f)



Alkyne: cyclopentylacetylene (**6f**, 0.10 mL) as described in the **General procedure 4.4**. After purification with CH₂Cl₂/EtOAc (80:20) as eluent, **7f** was obtained as a white solid (349 mg, 93%), mp 265-267 °C, *R*_f = 0.30 (ss D); ¹H NMR (500 MHz, CDCl₃): δ_H = 0.04 (m, 1H), 0.75 (s, 3H, 18-H₃), 0.79-0.86 (m, 3H), 1.02 (s, 3H, 19-H₃), 1.15-1.46 (m, 8H), 1.51-1.77 (m, 11H), 2.00 (s, 3H, Ac-CH₃), 2.09 (m, 3H), 2.34 (m, 2H), 3.17 (m, 1H), 3.95 (m, 1H, 3-H), 4.40 (d, 1H, *J* = 5.6 Hz, 1-H), 4.46 (t, 1H, *J* = 8.5 Hz, 17-H), 5.70 (d, 1H, *J* = 11.2 Hz, 3-OH), 7.29 (s, 1H, 5'-H); ¹³C NMR (125 MHz, CDCl₃): δ_C = 12.4 (C-18), 13.3 (C-19), 21.1 (Ac-CH₃), 21.4 (CH₂), 23.3 (CH₂), 25.1 (CH₂), 27.4 (CH₂), 28.6 (CH₂), 30.3 (CH₂), 32.7 (CH), 33.0 (CH₂), 33.2 (CH₂), 33.3 (CH₂), 35.8 (CH), 36.4 (3C, 3 × CH₂), 36.5 (CH), 40.4 (C-10), 42.6 (C-13), 47.5 (CH), 50.7 (CH), 63.4 and 63.9 (C-1 and C-3), 82.5 (C-17), 122.8 (C-5'), 151.5 (C-4'), 171.1 (Ac-CO); ESI-MS: 470 [M+H]⁺; Anal. Calcd for C₂₈H₄₃N₃O₃ C, 71.61; H, 9.23; N, 8.95. Found: C, 71.72; H, 9.36; N, 8.87.

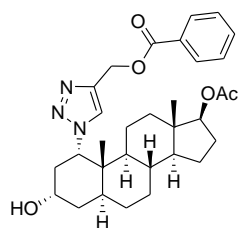
17β-Acetoxy-1α-[4'-cyclohexyl-1'H-1',2',3'-triazol-1'-yl]-5α-androstan-3β-ol (7g)



Alkyne: cyclohexylacetylene (**6g**, 0.11 mL) as described in the **General procedure 4.4**. After purification with CH₂Cl₂/EtOAc (80:20) as eluent, **7g** was obtained as a white solid (375 mg, 97%), mp 243-245 °C, *R*_f = 0.28 (ss D); ¹H NMR (500 MHz, CDCl₃): δ_H = 0.04 (m, 1H), 0.76 (s, 3H, 18-H₃), 0.79-0.86 (m, 3H), 1.02 (s, 3H, 19-H₃), 1.15-1.45 (m, 13H), 1.51-1.79 (m, 8H), 2.00 (s, 3H, Ac-

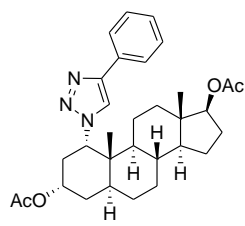
CH₃), 2.04 (m, 3H), 2.35 (m, 2H), 2.75 (m, 1H), 3.95 (m, 1H, 3-H), 4.40 (d, 1H, *J* = 5.5 Hz, 1-H), 4.46 (t, 1H, *J* = 8.5 Hz, 17-H), 5.71 (d, 1H, *J* = 11.2 Hz, 3-OH), 7.27 (s, 1H, 5'-H); ¹³C NMR (125 MHz, CDCl₃): δ_C = 12.4 (C-18), 13.3 (C-19), 21.1 (Ac-CH₃), 21.4 (CH₂), 25.9 (CH₂), 26.0 (CH₂), 27.4 (CH₂), 28.6 (CH₂), 30.3 (CH₂), 32.7 (CH), 33.0 (2C, 2 × CH₂), 33.1 (CH₂), 33.3 (CH₂), 35.0 (CH), 35.8 (CH), 36.4 (3C, 3 × CH₂), 40.5 (C-10), 42.6 (C-13), 47.5 (CH), 50.7 (CH), 63.5 and 63.9 (C-1 and C-3), 82.5 (C-17), 122.5 (C-5'), 152.4 (C-4'), 171.1 (Ac-CO); ESI-MS: 484 [M+H]⁺; Anal. Calcd for C₂₉H₄₅N₃O₃ C, 72.01; H, 9.38; N, 8.69. Found: C, 71.89; H, 9.47; N, 8.84.

17β-Acetoxy-1α-[4'-(*O*-benzoyl)hydroxymethyl-1'*H*-1',2',3'-triazol-1'-yl]-5α-androstan-3α-ol (8h)



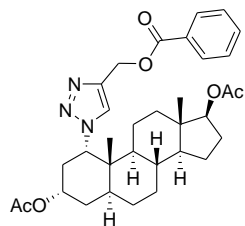
Substrate: **5**, alkyne: benzoic acid propargyl ester (**6h**, 0.13 mL) as described in the **General procedure 4.6**. After purification with CH₂Cl₂/EtOAc (80:20) as eluent, **8h** was obtained as a white solid (351 mg, 83%), mp 226-228 °C, *R*_f = 0.26 (ss F); ¹H NMR (500 MHz, CDCl₃): δ_H = 0.15 (m, 1H), 0.71 (s, 3H, 18-H₃), 0.76 (m, 3H), 1.08 (s, 3H, 19-H₃), 1.14-1.36 (m, 6H), 1.45-1.55 (m, 4H), 1.85 (m, 1H), 1.99 (s, 3H, Ac-CH₃), 2.03 (m, 3H), 2.35 (m, 1H), 2.53 (m, 1H), 4.44 (m, 1H, 17-H), 4.53 (m, 1H, 3-H), 4.61 (bs, 1H, 1-H), 5.44 (s, 2H, *O*-CH₂), 7.41 (t, 2H, *J* = 7.3 Hz, 3''-H and 5''-H), 7.53 (t, 1H, *J* = 7.2 Hz, 4''-H), 7.67 (s, 1H, 5'-H), 8.01 (d, 2H, *J* = 7.2 Hz, 2''-H and 6''-H); ¹³C NMR (125 MHz, CDCl₃): δ_C = 12.3 (C-18), 13.8 (C-19), 21.1 (Ac-CH₃), 21.2 (CH₂), 23.3 (CH₂), 27.4 (CH₂), 28.7 (CH₂), 30.5 (CH₂), 35.6 (CH), 36.3 (2C, 2 × CH₂), 37.6 (CH₂), 37.9 (CH), 40.1 (C-10), 42.5 (C-13), 47.5 (CH), 50.3 (CH), 57.9 (*O*-CH₂), 65.6 (2C, C-1 and C-3), 82.5 (C-17), 126.1 (C-5'), 128.4 (2C, C-3'' and C-5''), 129.7 (2C, C-2'' and C-6''), 133.2 (C-4''), 141.3 (2C, C-1'' and C-4'), 166.4 (C=O), 170.8 (Ac-CO); ESI-MS: 536 [M+H]⁺; Anal. Calcd for C₃₁H₄₁N₃O₅ C, 69.51; H, 7.71; N, 7.84. Found: C, 69.68; H, 7.87; N, 8.03.

3α,17β-Diacetoxy-1α-[4'-phenyl-1'*H*-1',2',3'-triazol-1'-yl]-5α-androstane (10a)



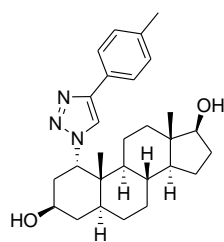
Substrate: **9**, alkyne: phenylacetylene (**6a**, 0.08 mL) as described in the **General procedure 4.6**. After purification with CH₂Cl₂/EtOAc (90:10) as eluent, **10a** was obtained as a white solid (112 mg, 30%), mp 158-160 °C, *R*_f = 0.32 (ss B); ¹H NMR (500 MHz, CDCl₃): δ_H = 0.36 (m, 1H), 0.75 (s, 3H, 18-H₃), 0.79-0.91 (m, 3H), 1.14 (s, 3H, 19-H₃), 1.19-1.31 (m, 2H), 1.35-1.46 (m, 5H), 1.49-1.63 (m, 4H), 1.97 (s, 3H, Ac-CH₃), 1.99 (s, 3H, Ac-CH₃), 2.02-2.20 (m, 4H), 2.41 (m, 1H), 4.43 (t, 1H, *J* = 8.6 Hz, 17-H), 4.77 (bs, 1H, 1-H), 5.52 (m, 1H, 3-H), 7.33 (t, 1H, *J* = 7.6 Hz, 4''-H), 7.42 (t, 2H, *J* = 7.6 Hz, 3''-H and 5''-H), 7.77 (s, 1H, 5'-H), 7.83 (d, 2H, *J* = 7.6 Hz, 2''-H and 6''-H); ¹³C NMR (125 MHz, CDCl₃): δ_C = 12.3 (C-18), 13.9 (C-19), 21.0 (Ac-CH₃), 21.1 (CH₂), 21.2 (Ac-CH₃), 23.3 (CH₂), 27.4 (CH₂), 28.6 (CH₂), 30.4 (CH₂), 32.7 (CH₂), 33.4 (CH₂), 35.7 (CH), 36.3 (CH₂), 37.7 (CH), 40.1 (C-10), 42.6 (C-13), 47.4 (CH), 50.3 (CH), 64.9 and 69.2 (C-1 and C-3), 82.4 (C-17), 120.8 (C-5'), 125.7 (2C, C-2'' and C-6''), 128.1 (C-4''), 128.8 (2C, C-3'' and C-5''), 130.5 (C-1''), 146.5 (C-4'), 170.0 and 170.9 (2 × Ac-CO); ESI-MS: 520 [M+H]⁺; Anal. Calcd for C₃₁H₄₁N₃O₄ C, 71.65; H, 7.95; N, 8.09. Found: C, 71.83; H, 7.79; N, 8.36.

3 α ,17 β -Diacetoxy-1 α -[4'-(*O*-benzoyl)hydroxymethyl-1'*H*-1'2'3'-triazol-1'-yl]-5 α -androstane (10h)



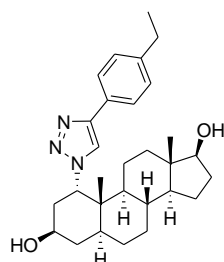
Substrate: **9**, alkyne: benzoic acid propargyl ester (**6h**, 0.12 mL) as described in the **General procedure 4.6**. After purification with CH₂Cl₂/EtOAc (90:10) as eluent, **10h** was obtained as a white solid (357 mg, 86%), mp 261-263 °C, *R*_f = 0.38 (ss C); ¹H NMR (500 MHz, CDCl₃): δ_H = 0.12 (m, 1H), 0.71 (s, 3H, 18-H₃), 0.75 (m, 3H), 1.09 (s, 3H, 19-H₃), 1.13-1.56 (m, 11H), 1.97 (s, 3H, Ac-CH₃), 1.99 (s, 3H, Ac-CH₃), 2.01-2.14 (m, 4H), 2.37 (m, 1H), 4.28 (t, 1H, *J* = 8.5 Hz, 17-H), 4.67 (bs, 1H, 1-H), 5.42-5.52 (m, 3H, *O*-CH₂ and 3-H), 7.41 (t, 2H, *J* = 7.4 Hz, 3''-H and 5''-H), 7.53 (t, 1H, *J* = 7.4 Hz, 4''-H), 7.71 (s, 1H, 5'-H), 8.02 (d, 2H, *J* = 7.4 Hz, 2''-H and 6''-H); ¹³C NMR (125 MHz, CDCl₃): δ_C = 12.3 (C-18), 13.8 (C-19), 21.0 (CH₂), 21.1 (Ac-CH₃), 21.2 (Ac-CH₃), 23.3 (CH₂), 27.4 (CH₂), 28.5 (CH₂), 30.3 (CH₂), 32.6 (CH₂), 33.4 (CH₂), 35.6 (CH), 36.2 (CH₂), 37.5 (CH₂), 40.1 (C-10), 42.4 (C-13), 47.4 (CH), 50.3 (CH), 58.0 (*O*-CH₂), 64.9 and 69.1 (C-1 and C-3), 82.4 (C-17), 125.8 (C-5'), 128.4 (2C, C-3'' and C-5''), 129.7 (2C, C-2'' and C-6''), 133.1 (C-4''), 141.5 (2C, C-1'' and C-4'), 166.4 (C=O), 170.0 and 170.8 (2 × Ac-CO); ESI-MS: 578 [M+H]⁺; Anal. Calcd for C₃₃H₄₃N₃O₆ C, 68.61; H, 7.50; N, 7.27. Found: C, 68.73; H, 7.65; N, 7.58.

1 α -[4'-(4''-Tolyl)-1'*H*-1',2',3'-triazol-1'-yl]-5 α -androstane-3 β ,17 β -diol (11b)



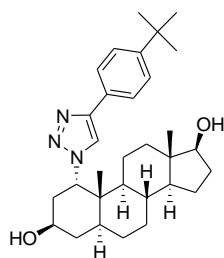
Substrate: **7b** (0.24 mmol) was used for the synthesis as described in the **General procedure 4.7**. Compound **11b** was obtained as a white solid (101 mg, 94%), mp 161-163 °C, *R*_f = 0.28 (ss F); ¹H NMR (500 MHz, CDCl₃): δ_H = 0.17 (m, 1H), 0.72 (s, 3H, 18-H₃), 0.75-0.83 (m, 3H), 1.07 (s, 3H, 19-H₃), 1.14-1.60 (m, 12H), 1.95 (m, 1H), 2.06 (m, 1H), 2.38 (m, 2H), 2.39 (s, 3H, 4''-CH₃), 3.46 (m, 1H, 17-H), 4.02 (m, 1H, 3-H), 4.56 (d, 1H, *J* = 5.5 Hz, 1-H), 5.25 (d, 1H, *J* = 10.5 Hz, 3-OH), 7.25 (d, 2H, *J* = 7.9 Hz, 3''-H and 5''-H), 7.71 (d, 2H, *J* = 7.9 Hz, 2''-H and 6''-H), 7.86 (s, 1H, 5'-H); ESI-MS: 450 [M+H]⁺; Anal. Calcd for C₂₈H₃₉N₃O₂ C, 74.80; H, 8.74; N, 9.35. Found: C, 74.96; H, 8.92; N, 9.22.

1 α -[4'-(4''-Ethylphenyl)-1'*H*-1',2',3'-triazol-1'-yl]-5 α -androstane-3 β ,17 β -diol (11c)



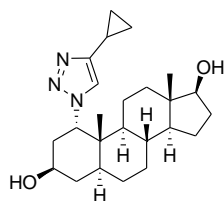
Substrate: **7c** (0.24 mmol) was used for the synthesis as described in the **General procedure 4.7**. Compound **11c** was obtained as a white solid (104 mg, 93%), mp 154-157 °C, *R*_f = 0.34 (ss F); ¹H NMR (500 MHz, CDCl₃): δ_H = 0.17 (m, 1H), 0.72 (s, 3H, 18-H₃), 0.75-0.84 (m, 3H), 1.07 (s, 3H, 19-H₃), 1.14-1.22 (m, 2H), 1.27 (t, 3H, *J* = 7.6 Hz, 4''-CH₂CH₃), 1.34-1.58 (m, 7H), 1.69-1.81 (m, 3H), 1.95 (m, 1H), 2.06 (m, 1H), 2.39 (m, 2H), 2.68 (q, 2H, *J* = 7.6 Hz, 4''-CH₂CH₃), 3.47 (m, 1H, 17-H), 4.02 (m, 1H, 3-H), 4.57 (d, 1H, *J* = 5.4 Hz, 1-H), 5.24 (d, 1H, *J* = 10.5 Hz, 3-OH), 7.27 (d, 2H, *J* = 8.0 Hz, 3''-H and 5''-H), 7.73 (d, 2H, *J* = 8.0 Hz, 2''-H and 6''-H), 7.87 (s, 1H, 5'-H); ESI-MS: 464 [M+H]⁺; Anal. Calcd for C₂₉H₄₁N₃O₂ C, 75.12; H, 8.91; N, 9.06. Found: C, 75.24; H, 9.06; N, 9.28.

1 α -[4'-(4''-*tert*-Butylphenyl)-1'*H*-1',2',3'-triazol-1'-yl]-5 α -androstane-3 β ,17 β -diol (11d)



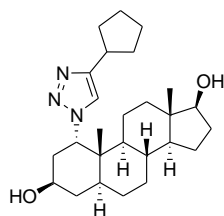
Substrate: **7d** (0.22 mmol) was used for the synthesis as described in the **General procedure 4.7**. Compound **11d** was obtained as a white solid (103 mg, 95%), mp 170-172 °C, $R_f = 0.38$ (ss F); $^1\text{H NMR}$ (500 MHz, CDCl_3): $\delta_{\text{H}} = 0.16$ (m, 1H), 0.72 (s, 3H, 18- H_3), 0.75-0.84 (m, 3H), 1.07 (s, 3H, 19- H_3), 1.14-1.28 (m, 2H), 1.35 (s, 9H, 4''-*t*Bu- CH_3), 1.38-1.57 (m, 7H), 1.69-1.81 (m, 3H), 1.96 (m, 1H), 2.07 (m, 1H), 2.39 (m, 2H), 3.47 (m, 1H, 17-H), 4.02 (m, 1H, 3-H), 4.57 (d, 1H, $J = 5.4$ Hz, 1-H), 5.25 (d, 1H, $J = 10.5$ Hz, 3-OH), 7.47 (d, 2H, $J = 8.1$ Hz, 3''-H and 5''-H), 7.76 (d, 2H, $J = 8.1$ Hz, 2''-H and 6''-H), 7.88 (s, 1H, 5'-H); ESI-MS: 492 $[\text{M}+\text{H}]^+$; Anal. Calcd for $\text{C}_{31}\text{H}_{45}\text{N}_3\text{O}_2$ C, 75.72; H, 9.22; N, 8.55. Found: C, 75.59; H, 9.04; N, 8.77.

1 α -[4'-Cyclopropyl-1'*H*-1',2',3'-triazol-1'-yl]-5 α -androstane-3 β ,17 β -diol (11e)



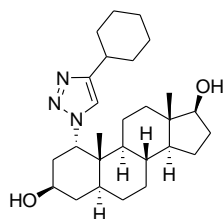
Substrate: **7e** (0.27 mmol) was used for the synthesis as described in the **General procedure 4.7**. Compound **11e** was obtained as a white solid (101 mg, 94%), mp 257-260 °C, $R_f = 0.22$ (ss H); $^1\text{H NMR}$ (500 MHz, CDCl_3): $\delta_{\text{H}} = 0.07$ (m, 1H), 0.72 (s, 3H, 18- H_3), 0.74-0.88 (m, 4H), 0.97 (m, 2H), 1.03 (s, 3H, 19- H_3), 1.15-1.24 (m, 2H), 1.32-1.44 (m, 6H), 1.47-1.59 (m, 2H), 1.66-1.78 (m, 3H), 1.93-2.03 (m, 3H), 2.35 (m, 2H), 3.54 (m, 1H, 17-H), 3.96 (m, 1H, 3-H), 4.40 (d, 1H, $J = 5.8$ Hz, 1-H), 5.50 (d, 1H, $J = 11.1$ Hz, 3-OH), 7.29 (s, 1H, 5'-H); ESI-MS: 400 $[\text{M}+\text{H}]^+$; Anal. Calcd for $\text{C}_{24}\text{H}_{37}\text{N}_3\text{O}_2$ C, 72.14; H, 9.33; N, 10.52. Found: C, 72.33; H, 9.15; N, 10.69.

1 α -[4'-Cyclopentyl-1'*H*-1',2',3'-triazol-1'-yl]-5 α -androstane-3 β ,17 β -diol (11f)



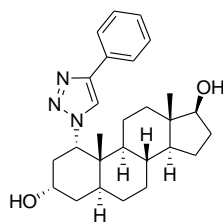
Substrate: **7f** (0.26 mmol) was used for the synthesis as described in the **General procedure 4.7**. Compound **11f** was obtained as a white solid (102 mg, 92%), mp 255-256 °C, $R_f = 0.24$ (ss G); $^1\text{H NMR}$ (500 MHz, CDCl_3): $\delta_{\text{H}} = 0.02$ (m, 1H), 0.68 (m, 1H), 0.72 (s, 3H, 18- H_3), 0.75-0.84 (m, 2H), 1.03 (s, 3H, 19- H_3), 1.15-1.45 (m, 9H), 1.47-1.77 (m, 9H), 2.00 (m, 2H), 2.10 (m, 2H), 2.35 (m, 2H), 3.19 (m, 1H), 3.51 (m, 1H, 17-H), 3.97 (m, 1H, 3-H), 4.41 (d, 1H, $J = 5.2$ Hz, 1-H), 5.72 (d, 1H, $J = 11.3$ Hz, 3-OH), 7.31 (s, 1H, 5'-H); ESI-MS: 428 $[\text{M}+\text{H}]^+$; Anal. Calcd for $\text{C}_{26}\text{H}_{41}\text{N}_3\text{O}_2$ C, 73.03; H, 9.66; N, 9.83. Found: C, 73.21; H, 9.82; N, 9.62.

1 α -[4'-Cyclohexyl-1'*H*-1',2',3'-triazol-1'-yl]-5 α -androstane-3 β ,17 β -diol (11g)



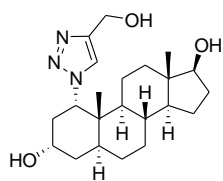
Substrate: **7g** (0.25 mmol) was used for the synthesis as described in the **General procedure 4.7**. Compound **11g** was obtained as a white solid (105 mg, 95%), mp 244-246 °C, $R_f = 0.31$ (ss G); $^1\text{H NMR}$ (500 MHz, CDCl_3): $\delta_{\text{H}} = 0.01$ (m, 1H), 0.68 (m, 1H), 0.72 (s, 3H, 18- H_3), 0.74-0.84 (m, 2H), 1.03 (s, 3H, 19- H_3), 1.16-1.58 (m, 14H), 1.66-1.81 (m, 6H), 1.94-2.03 (m, 4H), 2.35 (m, 2H), 2.78 (m, 1H), 3.51 (m, 1H, 17-H), 3.96 (m, 1H, 3-H), 4.41 (d, 1H, $J = 5.2$ Hz, 1-H), 5.73 (d, 1H, $J = 11.3$ Hz, 3-OH), 7.29 (s, 1H, 5'-H); ESI-MS: 442 $[\text{M}+\text{H}]^+$; Anal. Calcd for $\text{C}_{27}\text{H}_{43}\text{N}_3\text{O}_2$ C, 73.43; H, 9.81; N, 9.51. Found: C, 73.64; H, 9.67; N, 9.32.

4.7.8. 1 α -[4'-Phenyl-1'H-1',2',3'-triazol-1'-yl]-5 α -androstane-3 α ,17 β -diol (12a)



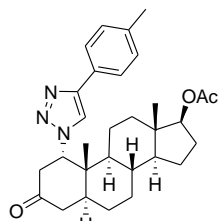
Substrate: **8a** (0.25 mmol) was used for the synthesis as described in the **General procedure 4.7**. Compound **12a** was obtained as a white solid (104 mg, 95%), mp 265-267 °C, R_f = 0.38 (ss G); $^1\text{H NMR}$ (500 MHz, MeOD): δ_{H} = 0.26 (m, 1H), 0.62 (m, 1H), 0.70 (s, 3H, 18-H₃), 0.76 (m, 2H), 1.14 (s, 3H, 19-H₃), 1.18 (m, 1H), 1.27-1.54 (m, 8H), 1.60 (m, 2H), 1.69 (m, 1H), 1.79-1.89 (m, 2H), 1.96 (m, 1H), 2.07 (m, 1H), 2.44 (m, 1H), 3.37 (t, 1H, J = 8.6 Hz, 17-H), 4.40 (m, 1H, 3-H), 4.59 (m, 2H, 1-H and OH), 7.33 (t, 1H, J = 7.4 Hz, 4''-H), 7.43 (t, 2H, J = 7.4 Hz, 3''-H and 5''-H), 7.82 (d, 2H, J = 7.4 Hz, 2''-H and 6''-H), 8.39 (s, 1H, 5'-H); ESI-MS: 436 [M+H]⁺; Anal. Calcd for C₂₇H₃₇N₃O₂ C, 74.45; H, 8.56; N, 9.65. Found: C, 74.62; H, 8.73; N, 9.92.

1 α -[4'-(*O*-Benzoyl)hydroxymethyl-1'H-1',2',3'-triazol-1'-yl]-5 α -androstane-3 α ,17 β -diol (12i)



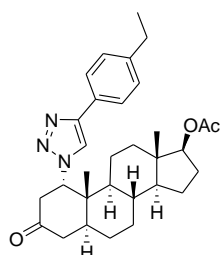
Substrate: **8h** (0.22 mmol) was used for the synthesis as described in the **General procedure 4.7**. Compound **12h** was obtained as a white solid (74 mg, 85%), mp 267-269 °C; $^1\text{H NMR}$ (500 MHz, MeOD): δ_{H} = 0.21 (m, 1H), 0.69 (s, 3H, 18-H₃), 0.70 (m, 3H), 1.12 (s, 3H, 19-H₃), 1.17 (m, 1H), 1.27-1.88 (m, 14H), 2.03 (m, 1H), 2.35 (m, 1H), 3.41 (m, 1H, 17-H), 4.30 (m, 1H, 3-H), 4.56 (bs, 1H, 1-H), 4.66 (s, 2H, *O*-CH₂), 7.96 (s, 1H, 5'-H); $^{13}\text{C NMR}$ (125 MHz, MeOD): δ_{C} = 11.9 (C-18), 14.3 (C-19), 22.3 (CH₂), 24.2 (CH₂), 30.0 (CH₂), 30.6 (CH₂), 32.1 (CH₂), 37.3 (CH), 37.6 (2C, 2 × CH₂), 38.5 (CH₂), 39.6 (CH), 41.3 (C-10), 44.2 (C-13), 49.4 (CH), 52.3 (CH), 56.5 (*O*-CH₂), 66.6 and 66.8 (C-1 and C-3), 82.3 (C-17), 126.0 (C-5'), 147.7 (C-4'); ESI-MS: 390 [M+H]⁺; Anal. Calcd for C₂₂H₃₅N₃O₃ C, 67.83; H, 9.06; N, 10.79. Found: C, 67.94; H, 9.19; N, 10.71.

17 β -Acetoxy-1 α -[4'-(4''-tolyl)-1'H-1',2',3'-triazol-1'-yl]-5 α -androstane-3-one (13b)



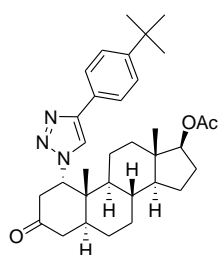
Following **General procedure 4.8.**, CH₂Cl₂/EtOAc (95:5) was used as eluent, yielding **2** (35 mg, 26%) and **13b** as a white solid (139 mg, 69%), mp 213-215 °C, R_f = 0.35 (ss C); $^1\text{H NMR}$ (500 MHz, CDCl₃): δ_{H} = 0.38 (m, 1H), 0.70 (m, 1H), 0.81 (s, 3H, 18-H₃), 0.87-0.96 (m, 1H), 1.10 (m, 1H), 1.24 (s, 3H, 19-H₃), 1.30 (m, 3H), 1.42-1.59 (m, 5H), 1.78 (m, 1H), 1.91 (m, 1H), 2.01 (s, 3H, Ac-CH₃), 2.07 (m, 1H), 2.16 (m, 1H), 2.30 (m, 1H), 2.37 (s, 3H, 4''-CH₃), 2.48 (m, 1H), 2.66 (m, 1H), 2.95 (m, 1H), 4.51 (t, 1H, J = 8.2 Hz, 17-H), 5.00 (d, 1H, J = 5.0 Hz, 1-H), 7.22 (d, 2H, J = 7.7 Hz, 3''-H and 5''-H), 7.58 (s, 1H, 5'-H), 7.69 (d, 2H, J = 7.7 Hz, 2''-H and 6''-H); $^{13}\text{C NMR}$ (125 MHz, CDCl₃): δ_{C} = 12.3 (C-18), 13.7 (C-19), 21.1 (Ac-CH₃), 21.1 (CH₂), 21.2 (4''-CH₃), 23.3 (CH₂), 27.4 (CH₂), 28.3 (CH₂), 30.0 (CH₂), 35.5 (CH), 36.4 (CH₂), 38.1 (CH), 40.0 (C-10), 42.7 (C-13), 43.0 (CH₂), 43.9 (CH₂), 47.4 (CH), 50.3 (CH), 64.5 (C-1), 82.3 (C-17), 119.5 (C-5'), 125.6 (2C, C-2'' and C-6''), 127.4 (C-1''), 129.5 (2C, C-3'' and C-5''), 138.1 (C-4''), 147.0 (C-4'), 170.9 (Ac-CO), 206.6 (C-3); ESI-MS: 490 [M+H]⁺; Anal. Calcd for C₃₀H₃₉N₃O₃ C, 73.59; H, 8.03; N, 8.58. Found: C, 73.72; H, 8.20; N, 8.48.

17 β -Acetoxy-1 α -[4'-(4''-ethylphenyl)-1'H-1',2',3'-triazol-1'-yl]-5 α -androstan-3-one (13c)



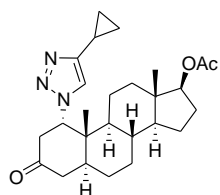
Following **General procedure 4.8.**, CH₂Cl₂/EtOAc (95:5) was used as eluent, yielding **2** (37 mg, 28%) and **13c** as a white solid (135 mg, 68%), mp 188-191 °C, *R*_f = 0.62 (ss C); ¹H NMR (500 MHz, CDCl₃): δ_H = 0.38 (m, 1H), 0.70 (m, 1H), 0.81 (s, 3H, 18-H₃), 0.91 (m, 1H), 1.10 (m, 1H), 1.24 (t, 3H, *J* = 7.5 Hz, 4''-CH₂CH₃), 1.25 (s, 3H, 19-H₃), 1.30 (m, 3H), 1.42-1.60 (m, 6H), 1.78 (m, 1H), 1.93 (m, 1H), 2.02 (s, 3H, Ac-CH₃), 2.07 (m, 1H), 2.16 (m, 1H), 2.32 (m, 1H), 2.51 (m, 1H), 2.67 (q, 2H, *J* = 7.5 Hz, 4''-CH₂CH₃), 2.95 (m, 1H), 4.52 (t, 1H, *J* = 8.3 Hz, 17-H), 5.00 (d, 1H, *J* = 5.0 Hz, 1-H), 7.25 (d, 2H, *J* = 7.7 Hz, 3''-H and 5''-H), 7.59 (s, 1H, 5'-H), 7.72 (d, 2H, *J* = 7.7 Hz, 2''-H and 6''-H); ¹³C NMR (125 MHz, CDCl₃): δ_C = 12.3 (C-18), 13.7 (C-19), 15.5 (4''-CH₂CH₃), 21.1 (Ac-CH₃), 21.1 (CH₂), 23.3 (CH₂), 27.4 (CH₂), 28.3 (CH₂), 28.7 (CH₂), 30.0 (CH₂), 35.6 (CH), 36.4 (CH₂), 38.1 (CH), 40.0 (C-10), 42.7 (C-13), 43.0 (CH₂), 43.9 (CH₂), 47.4 (CH), 50.3 (CH), 64.5 (C-1), 82.3 (C-17), 119.5 (C-5'), 125.7 (2C, C-2'' and C-6''), 127.6 (C-1''), 128.4 (2C, C-3'' and C-5''), 144.5 (C-4''), 147.1 (C-4'), 170.9 (Ac-CO), 206.6 (C-3); ESI-MS: 504 [M+H]⁺; Anal. Calcd for C₃₁H₄₁N₃O₃ C, 73.92; H, 8.20; N, 8.34. Found: C, 73.77; H, 8.31; N, 8.58.

17 β -Acetoxy-1 α -[4'-(4''-tert-butylphenyl)-1'H-1',2',3'-triazol-1'-yl]-5 α -androstan-3-one (13d)



Following **General procedure 4.8.**, CH₂Cl₂/EtOAc (95:5) was used as eluent, yielding **2** (23 mg, 19%) and **13d** as a white solid (149 mg, 75%), mp 213-216 °C, *R*_f = 0.64 (ss C); ¹H NMR (500 MHz, CDCl₃): δ_H = 0.37 (m, 1H), 0.70 (m, 1H), 0.81 (s, 3H, 18-H₃), 0.91 (m, 1H), 1.10 (m, 1H), 1.25 (s, 3H, 19-H₃), 1.30 (m, 3H), 1.34 (s, 9H, 4''-*t*Bu-CH₃), 1.42-1.60 (m, 6H), 1.78 (m, 1H), 1.93 (m, 1H), 2.02 (s, 3H, Ac-CH₃), 2.07 (m, 1H), 2.16 (m, 1H), 2.32 (m, 1H), 2.51 (m, 1H), 2.95 (m, 1H), 4.52 (t, 1H, *J* = 8.4 Hz, 17-H), 5.00 (d, 1H, *J* = 5.0 Hz, 1-H), 7.44 (d, 2H, *J* = 8.2 Hz, 3''-H and 5''-H), 7.61 (s, 1H, 5'-H), 7.74 (d, 2H, *J* = 8.2 Hz, 2''-H and 6''-H); ¹³C NMR (125 MHz, CDCl₃): δ_C = 12.3 (C-18), 13.7 (C-19), 21.0 (Ac-CH₃), 21.1 (CH₂), 23.3 (CH₂), 27.4 (CH₂), 28.3 (CH₂), 30.0 (CH₂), 31.2 (3C, 4''-*t*Bu-CH₃), 34.7 (4''-*t*Bu-C), 35.6 (CH), 36.4 (CH₂), 38.1 (CH), 40.4 (C-10), 42.7 (C-13), 43.0 (CH₂), 43.9 (CH₂), 47.5 (CH), 50.3 (CH), 64.5 (C-1), 82.3 (C-17), 119.5 (C-5'), 125.4 (2C) and 125.8 (2C): (C-2'', C-3'', C-5'' and C-6''), 127.4 (C-1''), 147.0 (C-4'), 151.4 (C-4''), 171.0 (Ac-CO), 206.5 (C-3); ESI-MS: 532 [M+H]⁺; Anal. Calcd for C₃₃H₄₅N₃O₃ C, 74.54; H, 8.53; N, 7.90. Found: C, 74.70; H, 8.36; N, 8.03.

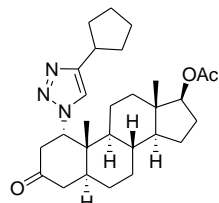
17 β -Acetoxy-1 α -[4'-cyclopropyl-1'H-1',2',3'-triazol-1'-yl]-5 α -androstan-3-one (13e)



Following **General procedure 4.8.**, CH₂Cl₂/EtOAc (80:20) was used as eluent, yielding **2** (34 mg, 24%) and **13e** as a white solid (141 mg, 71%), mp 176-179 °C, *R*_f = 0.47 (ss E); ¹H NMR (500 MHz, CDCl₃): δ_H = 0.30 (m, 1H), 0.72 (m, 1H), 0.80 (s, 3H, 18-H₃), 0.82-0.89 (m, 2H), 0.90-0.97 (m, 3H), 1.08 (m, 1H), 1.20 (s, 3H, 19-H₃), 1.23-1.33 (m, 2H), 1.39-1.60 (m, 6H), 1.73 (m, 1H), 1.83-1.93 (m, 2H), 2.02 (s, 3H, Ac-CH₃), 2.05-2.16 (m, 2H), 2.28 (dd, 1H, *J* = 16.6 Hz, *J* = 13.0 Hz), 2.45 (m, 1H), 2.58 (d, 1H, *J* = 16.8 Hz), 2.89 (dd, 1H, *J* = 16.8 Hz, *J* = 6.1 Hz), 4.55 (t, 1H, *J* = 8.3 Hz, 17-H), 4.88 (d, 1H, *J* = 5.0 Hz, 1-H), 7.11 (s, 1H, 5'-H); ¹³C NMR (125

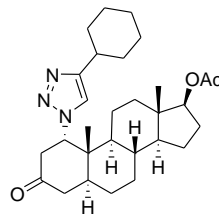
MHz, CDCl₃): δ_C = 6.6 (C-1''), 7.8 and 8.0 (C-2'' and C-3''), 12.3 (C-18), 13.7 (C-19), 21.0 (CH₂), 21.1 (Ac-CH₃), 23.3 (CH₂), 27.4 (CH₂), 28.3 (CH₂), 30.0 (CH₂), 35.5 (CH), 36.4 (CH₂), 38.1 (CH), 39.9 (C-10), 42.7 (C-13), 43.1 (CH₂), 43.9 (CH₂), 47.4 (CH), 50.4 (CH), 64.3 (C-1), 82.3 (C-17), 120.2 (C-5'), 149.2 (C-4'), 171.0 (Ac-CO), 206.7 (C-3); ESI-MS: 440 [M+H]⁺; Anal. Calcd for C₂₆H₃₇N₃O₃ C, 71.04; H, 8.48; N, 9.56. Found: C, 71.31; H, 8.32; N, 9.74.

17 β -Acetoxy-1 α -[4'-cyclopentyl-1'H-1',2',3'-triazol-1'-yl]-5 α -androstan-3-one (13f)



Following **General procedure 4.8.**, CH₂Cl₂/EtOAc (95:5) was used as eluent, yielding **2** (34 mg, 24%) and **13f** as a white solid (147 mg, 73%), mp 194-196 °C, *R_f* = 0.53 (ss E); ¹H NMR (500 MHz, CDCl₃): δ_H = 0.27 (m, 1H), 0.71 (m, 1H), 0.80 (s, 3H, 18-H₃), 0.90 (m, 1H), 1.03 (m, 1H), 1.21 (s, 3H, 19-H₃), 1.27 (m, 3H), 1.40-1.84 (m, 13H), 2.02 (s, 3H, Ac-CH₃), 2.07-2.18 (m, 4H), 2.28 (dd, 1H, *J* = 16.5 Hz, *J* = 13.0 Hz), 2.45 (m, 1H), 2.60 (d, 1H, *J* = 16.8 Hz), 2.89 (dd, 1H, *J* = 16.8 Hz, *J* = 6.0 Hz), 3.14 (m, 1H), 4.53 (t, 1H, *J* = 8.4 Hz, 17-H), 4.88 (d, 1H, *J* = 5.4 Hz, 1-H), 7.12 (s, 1H, 5'-H); ¹³C NMR (125 MHz, CDCl₃): δ_C = 12.4 (C-18), 13.7 (C-19), 21.0 (CH₂), 21.1 (Ac-CH₃), 23.3 (CH₂), 25.1 (CH₂), 27.4 (CH₂), 28.2 (CH₂), 30.1 (CH₂), 33.1 (CH₂), 33.3 (CH₂), 35.5 (CH), 36.4 (2C, 2 × CH₂), 36.6 (CH), 38.0 (CH), 39.9 (C-10), 42.7 (C-13), 43.0 (CH₂), 43.9 (CH₂), 47.5 (CH), 50.5 (CH), 64.2 (C-1), 82.4 (C-17), 120.1 (C-5'), 151.8 (C-4'), 171.0 (Ac-CO), 206.7 (C-3); ESI-MS: 468 [M+H]⁺; Anal. Calcd for C₂₈H₄₁N₃O₃ C, 71.91; H, 8.84; N, 8.99. Found: C, 72.04; H, 9.05; N, 9.25.

17 β -Acetoxy-1 α -[4'-cyclohexyl-1'H-1',2',3'-triazol-1'-yl]-5 α -androstan-3-one (13g)



Following **General procedure 4.8.**, CH₂Cl₂/EtOAc (80:20) was used as eluent, yielding **2** (34 mg, 24%) and **13g** as a white solid (142 mg, 72%), mp 202-204 °C, *R_f* = 0.42 (ss D); ¹H NMR (500 MHz, CDCl₃): δ_H = 0.25 (m, 1H), 0.70 (m, 1H), 0.80 (s, 3H, 18-H₃), 0.90 (m, 1H), 1.21 (s, 3H, 19-H₃), 1.25-1.60 (m, 14H), 1.69-1.84 (m, 5H), 2.02 (s, 3H, Ac-CH₃), 2.08-2.18 (m, 4H), 2.28 (dd, 1H, *J* = 16.5 Hz, *J* = 12.9 Hz), 2.46 (m, 1H), 2.62 (d, 1H, *J* = 16.8 Hz), 2.73 (m, 1H), 2.89 (dd, 1H, *J* = 16.8 Hz, *J* = 6.0 Hz), 4.53 (t, 1H, *J* = 8.2 Hz, 17-H), 4.88 (d, 1H, *J* = 5.2 Hz, 1-H), 7.10 (s, 1H, 5'-H); ¹³C NMR (125 MHz, CDCl₃): δ_C = 12.4 (C-18), 13.7 (C-19), 21.1 (CH₂), 21.2 (Ac-CH₃), 23.3 (CH₂), 26.0 (3C, 3 × CH₂), 27.4 (CH₂), 28.3 (CH₂), 30.1 (CH₂), 32.9 (2C, 2 × CH₂), 35.1 (CH), 35.5 (CH), 36.5 (CH₂), 38.0 (CH), 40.0 (C-10), 42.7 (C-13), 43.0 (CH₂), 43.9 (CH₂), 47.5 (CH), 50.5 (CH), 64.2 (C-1), 82.4 (C-17), 119.8 (C-5'), 152.8 (C-4'), 171.1 (Ac-CO), 206.7 (C-3); ESI-MS: 482 [M+H]⁺; Anal. Calcd for C₂₉H₄₃N₃O₃ C, 72.31; H, 9.00; N, 8.72. Found: C, 72.47; H, 9.19; N, 8.55.