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*Synthesis of methyl 2-acetamido-2-deoxy-1-seleno-\(\beta\)-D-gluco- and galactopyranosides: Selenium metabolites in human urine*

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NMR assignments for compounds 2, 3, 3a, 7 and 8.

* Tetra-O-acetyl-2-acetamido-2-deoxy-\(\beta\)-D-hexosamines (2, 7) *

**Compound 2:** \(^1H\)-NMR (600 MHz, DMSO) \(\delta\) 7.81 (1H, d, NH, J 9.2 Hz), 5.67 (1H, d, H-1, J 8.8 Hz), 5.28 (1H, s, H-4), 5.09 (1H, d, H-3, J 12 Hz), 4.20 (1H, t, H-5, J 6.5 Hz), 4.09 (1H, q, H-2, J 9.2 Hz), 4.05-4.00 (2H, m, H-6), 2.12, 2.03, 1.99, 1.91 (12H, s, Me of OAc), 1.78 (3H, s, Me of NHAc). \(^13C\)-NMR(150 MHz, DMSO) \(\delta\) 169.8-168.8 (CO), 92.5 (C\(_1\)), 70.9 (C\(_3\)), 70.0 (C\(_3\)), 66.5 (C\(_4\)), 61.3 (C\(_6\)), 48.3 (C\(_2\)), 22.6 (Me of NHAc), 20.4-20.3 (Me of OAc).

**Compound 7:** \(^1H\)-NMR(500 MHz, DMSO) \(\delta\) 7.97 (1H, d, NH, J 9.5 Hz), 5.71 (1H, d, H-1, J 8.8 Hz), 5.17 (1H, t, H-3, J 9.8 Hz), 4.88 (1H, t, H-4, J 9.6 Hz), 4.18 (1H, AB part of an ABX dd, H-6, J 12.9, 4.9 Hz), 3.99-3.90 (3H, m, H-2, H-5, H-6), 2.04, 2.00, 1.97, 1.92 (12H, s, Me of OAc), 1.76 (3H, s, Me of NHAc). \(^13C\)-NMR (125 MHz, DMSO) \(\delta\) 170.3-169.1 (CO), 91.9 (C\(_1\)), 72.4 (C\(_3\)), 71.7 (C\(_3\)), 68.3 (C\(_4\)), 61.7 (C\(_6\)), 52.2 (C\(_2\)), 22.8 (Me of NHAc), 20.7-20.5 (Me of OAc).
Tri-O-acetyl-2-acetamido-2-deoxy-1-chloro-α-D-hexosamines (3, 8)

**Compound 3**: $^1$H-NMR (400 MHz, CDCl$_3$) δ 6.29 (1H, d, H-1, J 4.1 Hz), 5.86 (1H, d, NH, J 8.8 Hz), 5.47 (1H, d, H-4, J 2.8 Hz), 5.29 (1H, dd, H-3, J 11.1, 2.8 Hz), 4.82-4.77 (1H, m, H-2), 4.52 (1H, t, H-5, J 6.5 Hz), 4.22 (1H, AB part of an ABX dd, H-6, J 11.1, 6.5 Hz), 4.10 (1H, AB part of an ABX dd, H-6, J 11.1, 6.5 Hz), 2.17, 2.06, 2.03, 2.01 (12H, s, Me). $^{13}$C-NMR(100 MHz, CDCl$_3$) δ 170.8-170 (CO), 94.9 (C$_1$), 69.9 (C$_5$), 67.3 (C$_3$), 66.5 (C$_4$), 61.1 (C$_6$), 49.2 (C$_2$), 23.1 (Me of NHAc), 20.7-20.6 (Me of OAc). **Compound 8**: $^1$H-NMR(500 MHz, CDCl$_3$) δ 6.17 (1H, d, H-1, J 3.6 Hz), 5.82 (1H, d, NH, J 9 Hz), 5.30 (1H, t, H-3, J 9.7 Hz), 5.19 (1H, t, H-4, J 9.8 Hz), 4.53-4.49 (1H, m, H-2), 4.29-4.27 (2H, m, H-5, H-6), 4.11 (1H, AB part of an ABX d, H-6, J 10.6 Hz), 2.09, 2.03 (9H, s, Me of OAc), 1.96 (3H, s, Me of NHAc). $^{13}$C-NMR(125 MHz, DMSO) δ 171.5-169.1 (CO), 93.6 (C$_1$), 70.9 (C$_3$), 70.1 (C$_3$), 66.9 (C$_4$), 61.1 (C$_6$), 53.5 (C$_2$), 23.1 (Me of NHAc), 20.7-20.5 (Me of OAc).

Tetra-O-acetyl-2-amino-2-deoxy-α-D-galactopyranose hydrochloride (3a)

**Compound 3a**: $^1$H-NMR (400 MHz, DMSO) δ 8.71 (3H, broad s, NH$_3^+$), 6.27 (1H, d, H-1, J 3.6 Hz), 5.37 (1H, d, H-4, J 3.2 Hz), 5.22 (1H, dd, H-3, J 11.2, 3.2 Hz), 4.38 (1H, t, H-5, J 6 Hz), 4.02 (2H, d, H-6, J 6.8 Hz), 3.75 (1H, broad d, H-2, J 11.2 Hz), 2.16, 2.11, 2.00, 1.96 (12H, s, Me).