Supporting information

Three-component Biginelli Cyclocondensation Reaction Using C-glycosylated Substrates. Preparation of a Collection of Dihydropyrimidinone glycoconjugates and the Synthesis of C-Glycosylated Monastrol Analogues

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- Crystallographic Information File (CIF) of compound (*R*)-17b.
- ORTEP plot of (*R*)-17b drawn at 40% probability level.

52

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Refinement of F2 against ALL reflections. The weighted R-factor wR and
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on F, with F set to zero for negative F2. The threshold expression of
F2 > 2sigma(F2) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F2 are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
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O2 O 0.47775(19) -0.02345(10) 0.27828(6) 0.0372(4) Uani 1 1 d . . .

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O3 O 0.58161(19) 0.04233(11) 0.21561(6) 0.0341(4) Uani 1 1 d . . .
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N1 N 0.4410(2) 0.29696(14) 0.25325(7) 0.0287(5) Uani 1 1 d . . .
H1N H 0.469(3) 0.351(2) 0.2414(11) 0.057(9) Uiso 1 1 d . . .
N2 N 0.3205(3) 0.23593(14) 0.31727(8) 0.0364(5) Uani 1 1 d . . .
H2N H 0.262(4) 0.245(2) 0.3376(10) 0.048(9) Uiso 1 1 d . . .
C1 C 0.5195(2) 0.21346(14) 0.24057(8) 0.0260(5) Uani 1 1 d . . .
H1 H 0.4986 0.2013 0.2074 0.031 Uiso 1 1 calc R . . .
C2 C 0.3624(2) 0.31031(15) 0.29255(9) 0.0282(5) Uani 1 1 d . . .
C3 C 0.3595(3) 0.14890(15) 0.30495(9) 0.0305(6) Uani 1 1 d . . .
C4 C 0.4568(3) 0.13583(14) 0.26901(9) 0.0269(5) Uani 1 1 d . . .
C5 C 0.2834(3) 0.07902(17) 0.33474(10) 0.0430(7) Uani 1 1 d . . .
H51 H 0.2388 0.0340 0.3149 0.052 Uiso 1 1 calc R . . .
H52 H 0.2055 0.1067 0.3534 0.052 Uiso 1 1 calc R . . .
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C6 C 0.5035(3) 0.04510(15) 0.25543(9) 0.0291(5) Uani 1 1 d . . .
O2' O 0.73108(18) 0.26758(11) 0.16606(5) 0.0304(4) Uani 1 1 d . . .
O3' O 0.96367(18) 0.38778(11) 0.19253(6) 0.0356(4) Uani 1 1 d . . .
O4' O 0.87278(19) 0.41542(12) 0.28698(7) 0.0413(4) Uani 1 1 d . . .
O5' O 0.71918(17) 0.24828(11) 0.29396(5) 0.0309(4) Uani 1 1 d . . .
O6' O 1.03795(19) 0.28249(13) 0.37048(6) 0.0418(5) Uani 1 1 d . . .
C1' C 0.6915(2) 0.22575(16) 0.24610(8) 0.0268(5) Uani 1 1 d . . .
H1' H 0.7421 0.1687 0.2390 0.032 Uiso 1 1 calc R . . .
C2' C 0.7533(2) 0.29827(15) 0.21325(8) 0.0268(5) Uani 1 1 d . . .
H2' H 0.6969 0.3543 0.2181 0.032 Uiso 1 1 calc R . . .
C3' C 0.9213(3) 0.31449(16) 0.22219(8) 0.0299(5) Uani 1 1 d . . .
H3' H 0.9792 0.2609 0.2132 0.036 Uiso 1 1 calc R . . .
C4' C 0.9460(3) 0.33375(16) 0.27436(9) 0.0324(6) Uani 1 1 d . . .
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C5' C 0.8776(3) 0.25913(17) 0.30398(8) 0.0327(6) Uani 1 1 d . . .
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H6'A H 0.8315 0.3341 0.3629 0.053 Uiso 1 1 calc R . . .
H6'B H 0.8307 0.2302 0.3730 0.053 Uiso 1 1 calc R . . .
C7 C 0.6416(3) 0.32601(18) 0.13817(9) 0.0406(7) Uani 1 1 d . . .
H71 H 0.6918 0.3838 0.1355 0.049 Uiso 1 1 calc R . . .
H72 H 0.5438 0.3354 0.1532 0.049 Uiso 1 1 calc R . . .
C8 C 0.6180(3) 0.28708(19) 0.09022(9) 0.0401(6) Uani 1 1 d . . .
C9 C 0.6567(3) 0.2005(2) 0.07864(10) 0.0500(8) Uani 1 1 d . . .
H9 H 0.7031 0.1640 0.1009 0.060 Uiso 1 1 calc R . . .
C10 C 0.6275(5) 0.1667(2) 0.03430(12) 0.0730(11) Uani 1 1 d . . .
H10 H 0.6559 0.1082 0.0269 0.088 Uiso 1 1 calc R . . .
C11 C 0.5574(6) 0.2186(3) 0.00138(14) 0.1014(16) Uani 1 1 d . . .
H11 H 0.5359 0.1955 -0.0282 0.122 Uiso 1 1 calc R . . .
C12 C 0.5192(7) 0.3052(3) 0.01245(15) 0.1144(18) Uani 1 1 d . . .
H12 H 0.4726 0.3411 -0.0100 0.137 Uiso 1 1 calc R . . .
C13 C 0.5487(5) 0.3401(3) 0.05651(13) 0.0811(12) Uani 1 1 d . . .
H13 H 0.5221 0.3991 0.0635 0.097 Uiso 1 1 calc R . . .
C14 C 1.1208(3) 0.3947(2) 0.18210(10) 0.0422(7) Uani 1 1 d . . .
H141 H 1.1630 0.3355 0.1764 0.051 Uiso 1 1 calc R . . .
H142 H 1.1744 0.4213 0.2084 0.051 Uiso 1 1 calc R . . .
C15 C 1.1397(3) 0.45273(18) 0.13905(9) 0.0378(6) Uani 1 1 d . . .
C16 C 1.0350(4) 0.4520(2) 0.10288(10) 0.0513(7) Uani 1 1 d . . .
H16 H 0.9492 0.4158 0.1052 0.062 Uiso 1 1 calc R . . .
C17 C 1.0559(4) 0.5045(2) 0.06321(11) 0.0602(9) Uani 1 1 d . . .
H17 H 0.9844 0.5031 0.0392 0.072 Uiso 1 1 calc R . . .
C18 C 1.1817(4) 0.5585(2) 0.05925(12) 0.0636(9) Uani 1 1 d . . .
H18 H 1.1959 0.5936 0.0326 0.076 Uiso 1 1 calc R . . .
C19 C 1.2855(4) 0.5601(2) 0.09477(13) 0.0699(10) Uani 1 1 d . . .
H19 H 1.3710 0.5966 0.0923 0.084 Uiso 1 1 calc R . . .
C20 C 1.2647(4) 0.5078(2) 0.13463(11) 0.0556(8) Uani 1 1 d . . .
H20 H 1.3362 0.5100 0.1587 0.067 Uiso 1 1 calc R . . .
C21 C 0.9693(3) 0.4895(2) 0.29391(12) 0.0560(8) Uani 1 1 d . . .
H211 H 0.9840 0.5208 0.2644 0.067 Uiso 1 1 calc R . . .
H212 H 1.0677 0.4688 0.3048 0.067 Uiso 1 1 calc R . . .
C22 C 0.9024(3) 0.55252(17) 0.32922(9) 0.0364(6) Uani 1 1 d . . .
C23 C 0.7496(3) 0.5495(2) 0.34073(11) 0.0528(8) Uani 1 1 d . . .
H23 H 0.6875 0.5059 0.3273 0.063 Uiso 1 1 calc R . . .
C24 C 0.6892(4) 0.6102(2) 0.37176(13) 0.0690(10) Uani 1 1 d . . .
H24 H 0.5865 0.6073 0.3793 0.083 Uiso 1 1 calc R . . .
C25 C 0.7775(5) 0.6739(2) 0.39138(14) 0.0747(11) Uani 1 1 d . . .
H25 H 0.7351 0.7153 0.4121 0.090 Uiso 1 1 calc R . . .
C26 C 0.9308(5) 0.6781(2) 0.38087(12) 0.0686(10) Uani 1 1 d . . .
H26 H 0.9919 0.7218 0.3946 0.082 Uiso 1 1 calc R . . .
C27 C 0.9925(3) 0.61698(19) 0.34983(10) 0.0484(7) Uani 1 1 d . . .
H27 H 1.0956 0.6194 0.3428 0.058 Uiso 1 1 calc R . . .
C28 C 1.0512(3) 0.3132(3) 0.41760(11) 0.0734(11) Uani 1 1 d . . .
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H282 H 1.0072 0.3727 0.4206 0.088 Uiso 1 1 calc R . . .
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C30 C 1.3055(4) 0.3895(3) 0.42067(12) 0.0729(11) Uani 1 1 d . . .
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 C32 C 1.5259(5) 0.3131(6) 0.44781(16) 0.118(2) Uani 1 1 d . . .
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 C33 C 1.4407(6) 0.2398(4) 0.45778(13) 0.0947(16) Uani 1 1 d . . .
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 C34 C 1.2860(4) 0.2413(3) 0.44840(11) 0.0696(10) Uani 1 1 d . . .
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 C9 0.066(2) 0.0475(18) 0.0360(16) -0.0006(14) -0.0037(13) -0.0055(15)
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 C12 0.198(5) 0.088(3) 0.058(3) 0.005(2) -0.058(3) 0.022(4)
 C13 0.128(3) 0.063(2) 0.052(2) 0.0031(18) -0.029(2) 0.021(2)
 C14 0.0321(15) 0.0492(17) 0.0452(17) 0.0062(14) 0.0046(12) -0.0029(13)
 C15 0.0415(15) 0.0386(15) 0.0334(15) 0.0017(12) 0.0074(12) 0.0022(12)
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 C31 0.084(3) 0.179(6) 0.057(3) -0.018(3) 0.002(2) -0.067(4)
 C32 0.051(3) 0.254(8) 0.049(3) -0.032(4) -0.004(2) 0.004(4)
 C33 0.086(3) 0.156(5) 0.042(2) -0.021(3) -0.014(2) 0.058(3)
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All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix. The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry. An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.

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