S1 Table

Crystal data and details of the structure determination (1-4)

Crystal data

2 ($C_{15}H_{17}N\ O_{7)}, CH_4O$	δ = 86.298(3) º
Mr = 678.63	V = 1518.6(2) Å^3
Triclinic, P-1 (Nº 2)	Z = 2
a = 7.7008(6) Å	Mo$K\alpha$ radiation
b =13.8964(11) Å	μ = 0.119 mm^{-1}
c =15.3172(13) Å	T = 100 K
α = 68.684(3) º	0.03 x 0.12 x 0.12 mm
β = 84.244(3) º	

Data collection

Bruker-Nonius diffractometer	5042 reflections with $I > 2\sigma(I)$
6881 measured reflections	R_{int} = 0.113
6881 independent reflections	Theta min-max (deg) 1.6-27.6

Refinement

R [($F^2 > 2\sigma(F^2)$] = 0.0654	H-atom parameters constrained
*w*R(F^2) = 0.1852	444 parameters
S = 1.06	$\Delta\rho_{max}$ = 0.75 e Å^{-3}
F(000) = 716	$\Delta\rho_{mim}$ = -0.42 e Å^{-3}

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