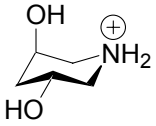
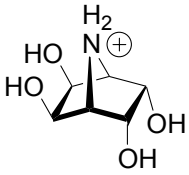
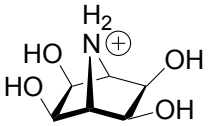
Supplementary Material for Organic & Biomolecular Chemistry

Supporting information

Anette Gregersen, Christian Marcus Pedersen, Henrik Helligsø Jensen and Mikael Bols* "On the electronic effects from OH groups. Synthesis and investigation of tetrahydroxylated azabicycloheptanes."

Table S1. Angles and distances in molecules **1**, **2** and **27**. The values were obtained by from the chem3D pro 6.0 models, which were energy minimized in MOPAC, PM3. The NO distance and NCO angle can be determined directly from the program, while the distance and angle to the CO bond middle was obtained by simple geometric calculations.

PM3	 **27**		 **2**	 **1**
	eq	*ax*	*endo*	*exo*
Distance N---O	3.693 Å	2.886 Å	3.627 Å	2.993 Å
Distance N---(CO) bond middle	3.106 Å	2.702 Å	3.016 Å	2.700 Å
Angle O-C----N	138.5°	90°	144.2°	100.3°
Angle O-(CO) bond middle ----N	145.8°	104.7°	151.0°	114.0°
Charge dipole interaction ($e\mu\cos(\alpha)/r^2$; D_E; = 13)	0.78 kcal/mol	0.31 kcal/mol	0.87 kcal/mol	0.50 kcal/mol
Ratio eq/ax or endo/exo	2.5		1.7	
Measured substituent effect ($RT\ln\sigma_s$)	0.77 kcal/mol	0.30 kcal/mol	0.73 kcal/mol	0.56 kcal/mol
Ratio of measured substituent effects	2.6		1.3	