Electronic Supplementary Material (ESI) for New Journal of Chemistry.

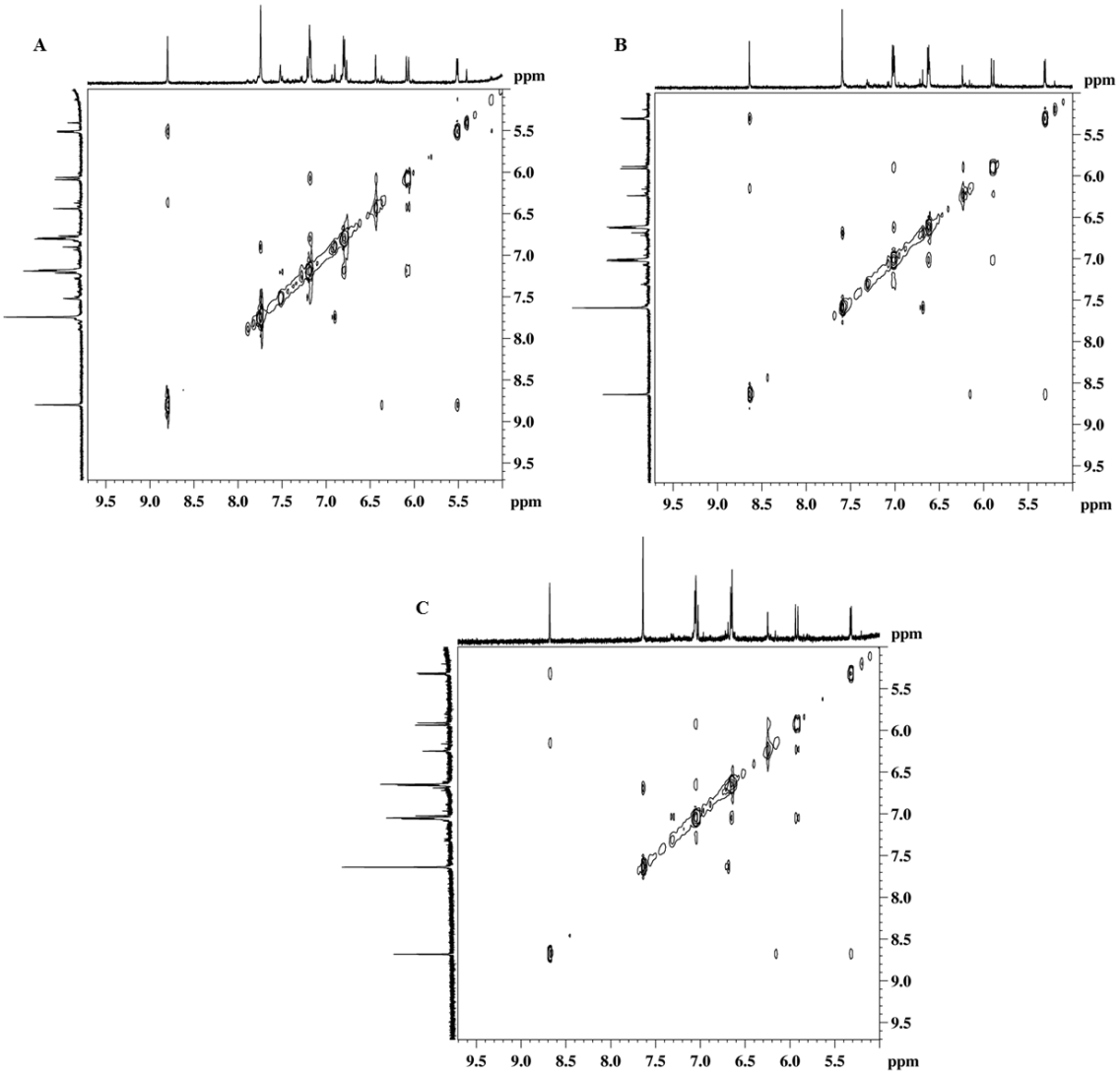


Fig. SI-1 Portion of the 2D NOESY spectra of mv3cumglc (1.8 mM (A); 1.0 mM (B)and 0.6 mM (C)) acquired in D_2O/DMSO (7:3) with a mixing time of 400 ms.

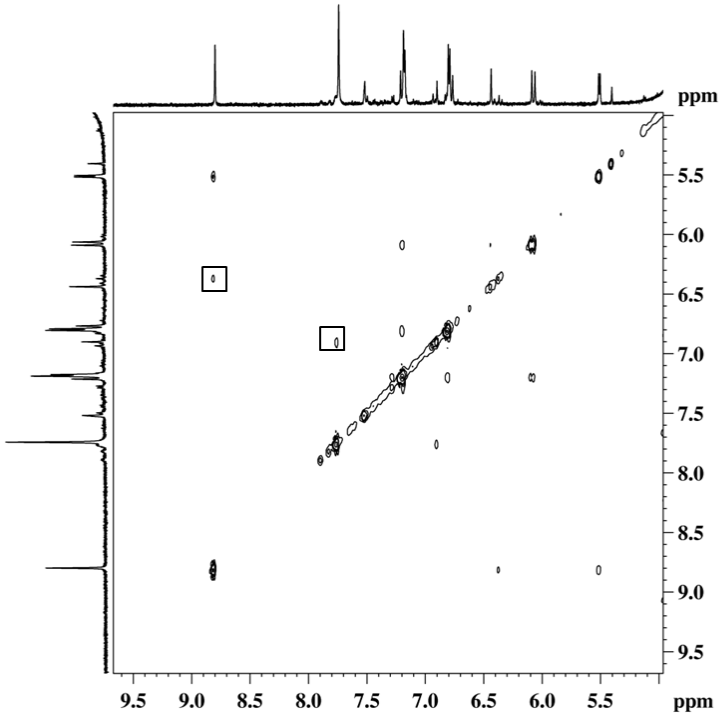


Fig. 2 SI Portion of the 2D ROESY spectra of mv3cumglc (1.8 mM) acquired in D_2O/DMSO (7:3) with a mixing time of 400 ms, showing NOE interactions and chemical exchange peaks (in boxes).

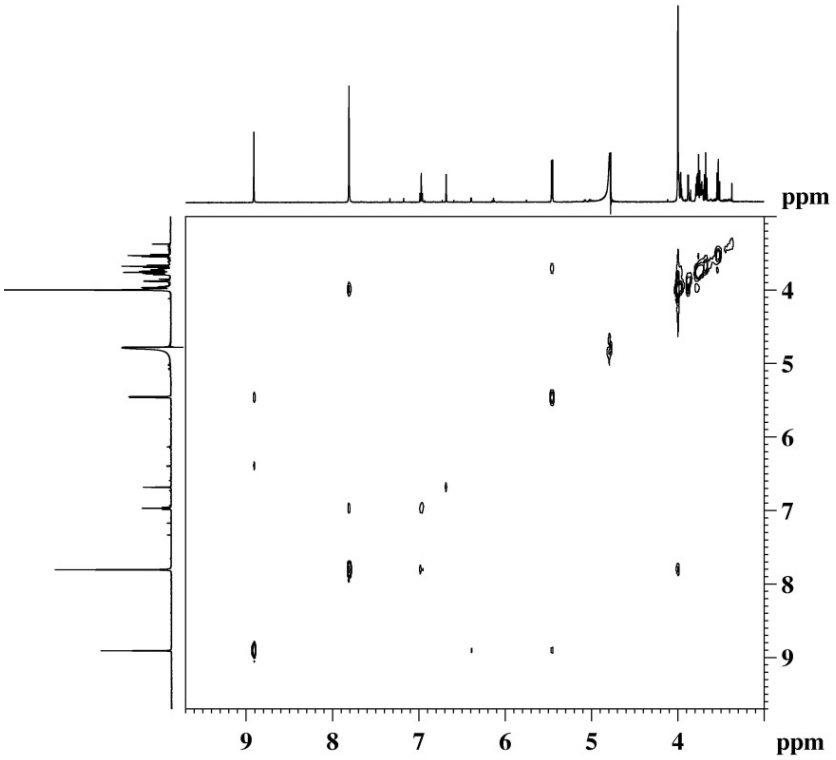
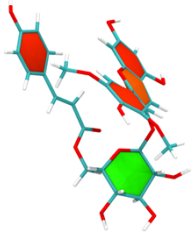
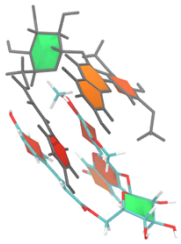
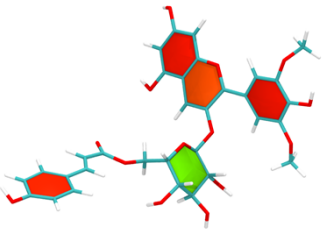
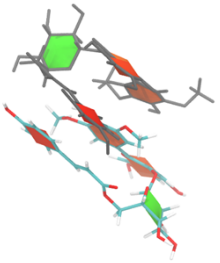
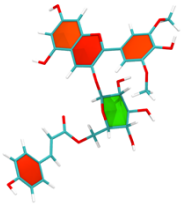
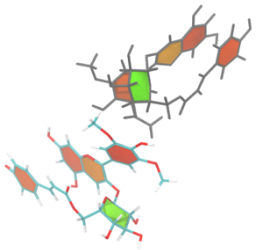
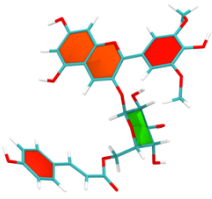
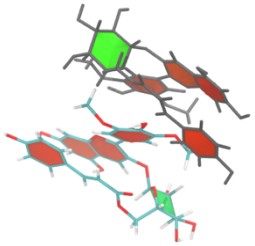
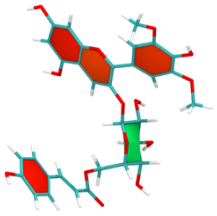
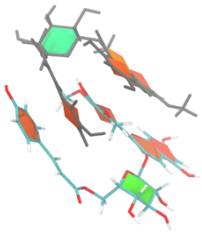


Fig. 3 SI Portion of the 2D NOESY spectra of mv3glc (2.0 mM) acquired in D_2O/DMSO (7:3) with a mixing time of 400 ms.

ΔEnergy / kcal mol^{-1}	Mv3cumglc	ΔEnergy kcal mol^{-}	(Mv3cumglc)$_2$
0.0		0.0	
1.3		0.4	
4.9		8.5	
5.5		9.6	
5.7		10.2	

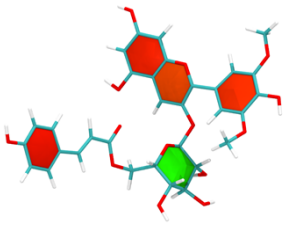
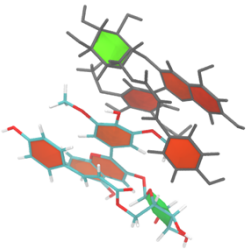
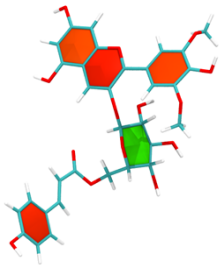
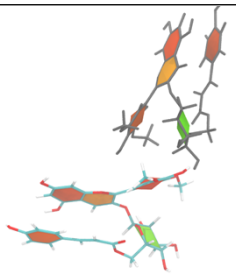
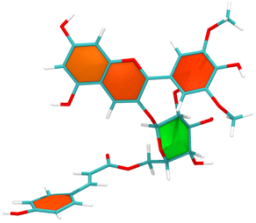
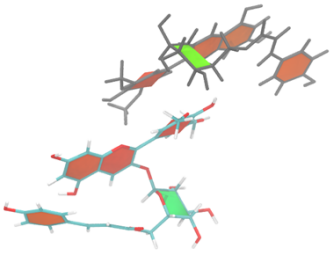
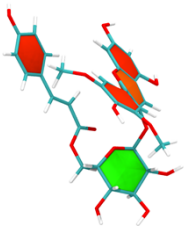
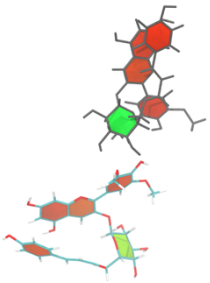
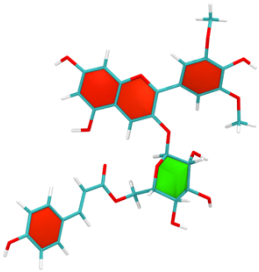
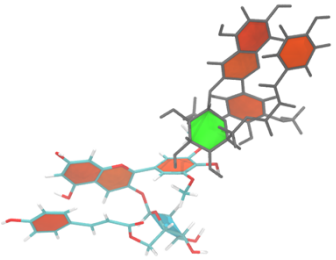
6.2		10.7	
8.6		14.2	
9.3		14.8	
9.3		29.5	
9.8		29.6	

Fig SI-4 Representation of the optimized representative geometries adopted by mv3cumglc and $(mv3cumglc)_2$ compounds along MD simulations. ΔEnergy values are also presented, relatively to the most stable structure (1st table line).