Orientation of the GM1 ganglioside in Langmuir-Blodgett monolayers: a PM IRRAS and computational study

SUPPLEMENTARY INFORMATION

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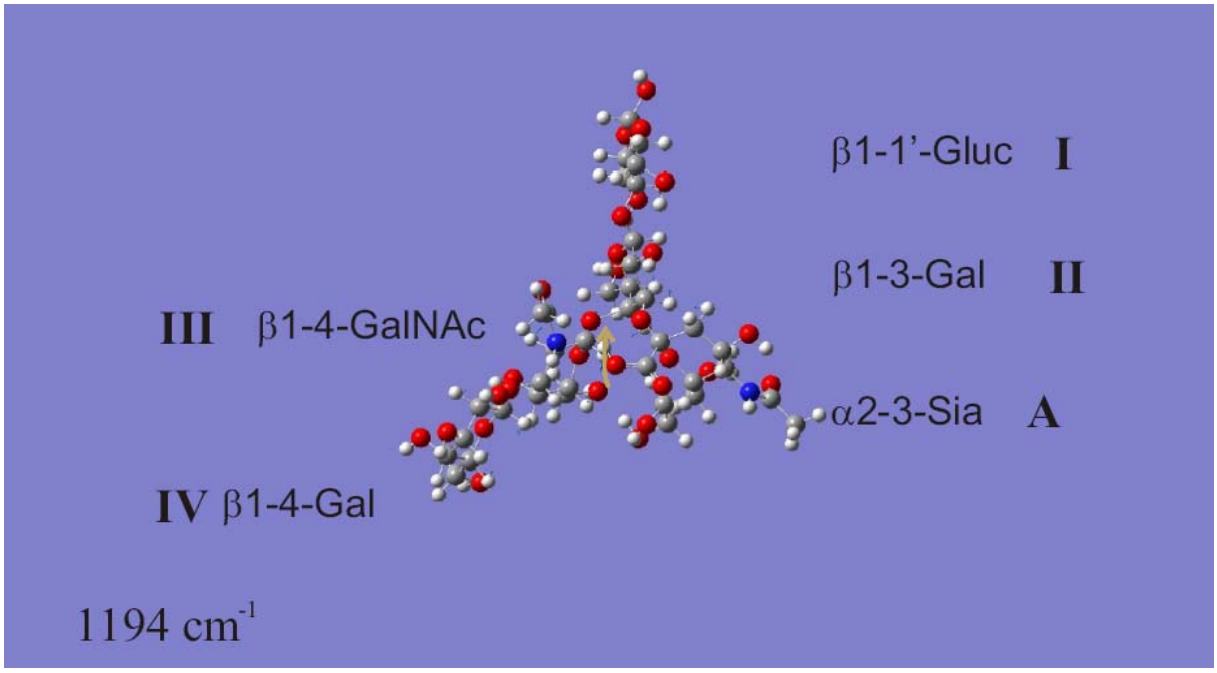
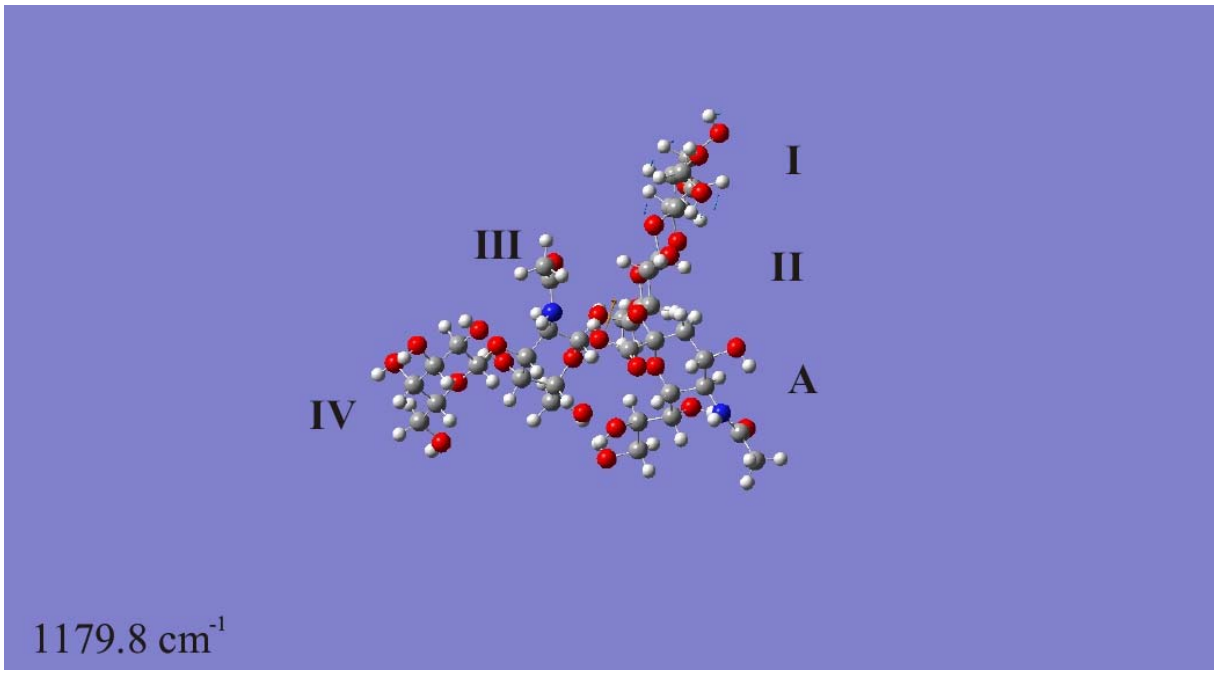
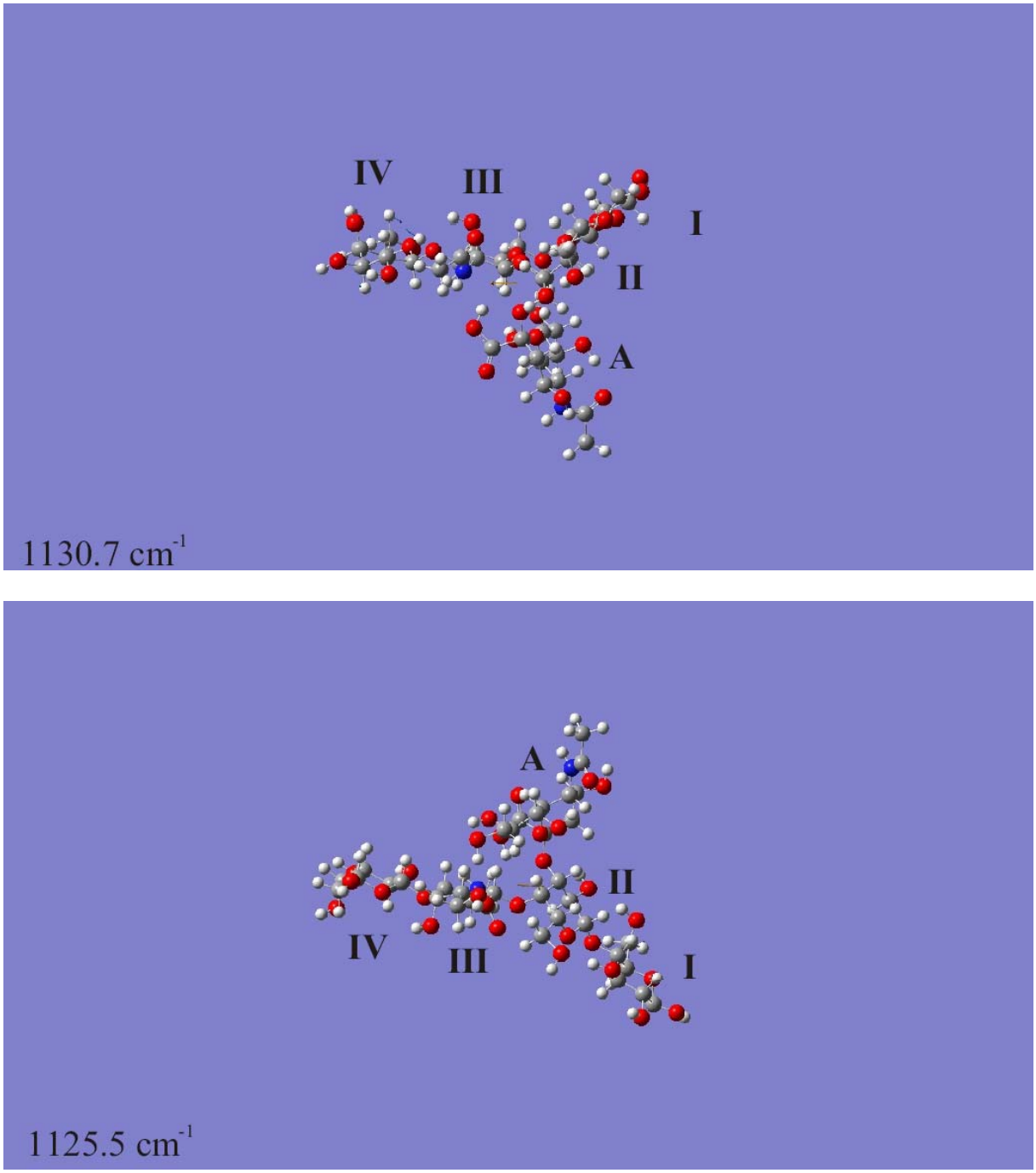
A quantum chemical calculation on the B3LYP/6-31G(d) level of theory was performed to find the conformation and an IR spectrum of the polar head group of the GM1 ganglioside. The polar head group of the GM1 molecule is composed of five sugar residues: βGlc-(1-1) (I);β-Gal-(1-4) (II); α-Nue5Ac-(2-3) (A); β-GalNAc-(1-4) (III) and β-Gal-(1-3) (IV). In the IR spectrum the bulky head group of GM1 ganglioside gives rise to many absorption bands. The strong asymmetric ν_{as}(COC) stretching modes arising from various sugar residues in the ganglioside molecule can be used to discuss in detail the orientation of individual sugar residues of the polar head group of the GM1 molecule in a monolayer. Figures presented below show the structure of the pentasaccharide head group of the GM1 molecule with marked sugar residues and direction of the dipole moment vector of the ν_{as}(COC) stretching modes at various wavenumbers, as discussed in the article.



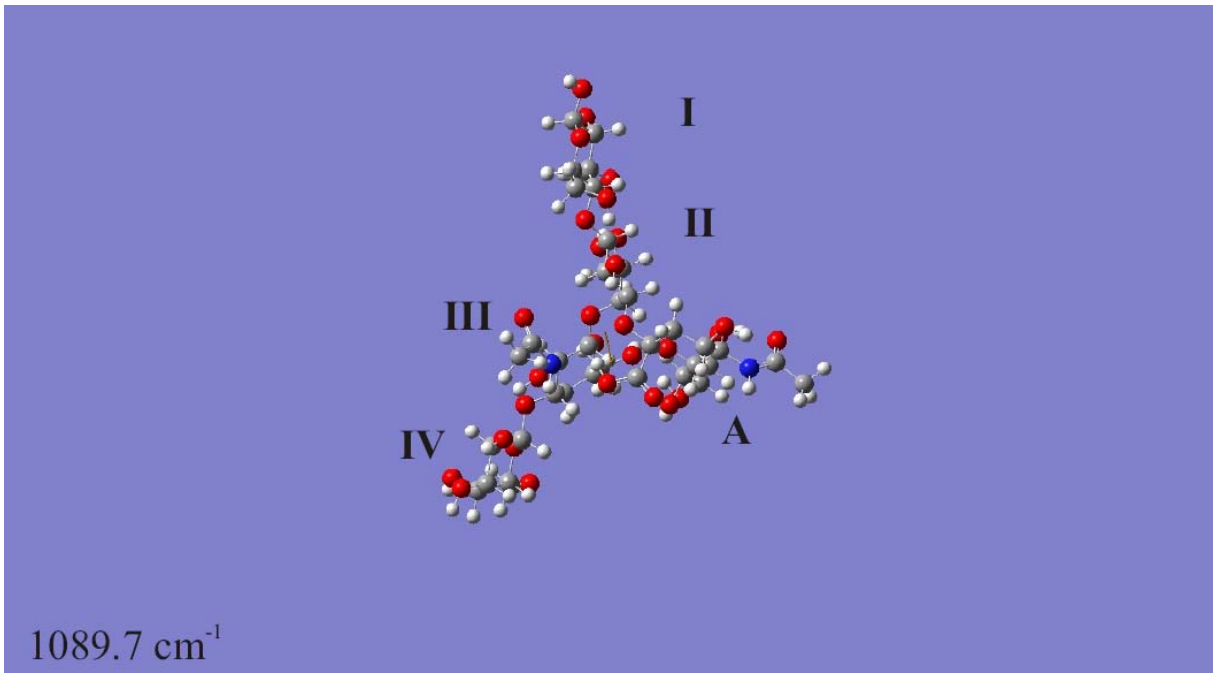
S.I. 1 The orientation of the polar head group of the GM1 molecule and the orientation of the transition dipole moment of the ν_{as}(COC) stretching mode at 1194.0 cm^{-1}.



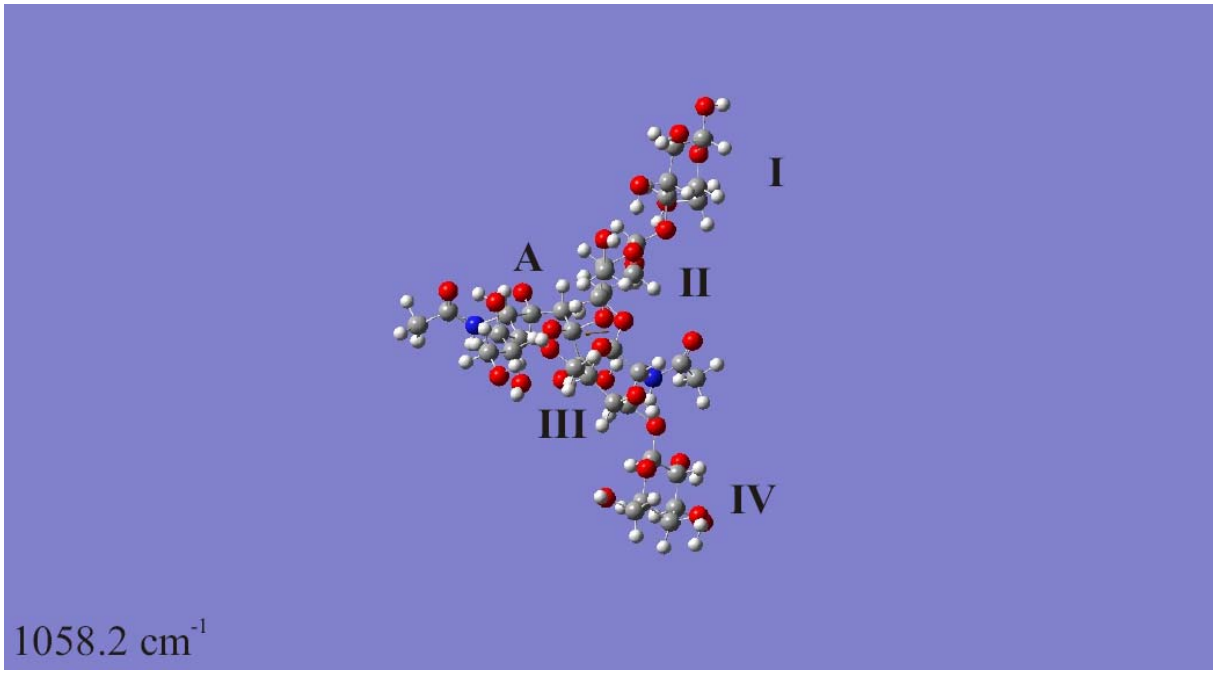
S.I. 2 The orientation of the polar head group of the GM1 molecule and the orientation of the transition dipole moment of the ν_{as}(COC) stretching mode at 1179.8 cm^{-1}.



S.I. 3 The orientation of the polar head group of the GM1 molecule and the orientation of the transition dipole moment of the ν_{as}(COC) stretching mode at 1130.7 and 1125.5 cm^{-1}.



S.I. 4 The orientation of the polar head group of the GM1 molecule and the orientation of the transition dipole moment of the ν_{as}(COC) stretching mode at 1089.7 cm^{-1}.



S.I. 5 The orientation of the polar head group of the GM1 molecule and the orientation of the transition dipole moment of the ν_{as}(COC) stretching mode at 1058.9 cm^{-1}.