

Supplemental Table S1 : Characterization of GluCer species by mass spectrometry.

Exact mass measurements (MS mode) and fragment ions obtained by MS² (a) and MS³ (b) modes for singly charged ions (lithium adducts) of DRM GluCer produced in the electrospray ionisation mode. Nomenclature of ceramide fragment ions is according to Domon and Costello (1988), Adams and Ann (1993) and Levery et al. (2000).

fatty acid <i>sphingosine</i> (formula)	Measured m/z (M+Li) ⁺ ion	Calculated m/z (M+Li) ⁺ ion	Y0 (a) m/z	Z0 (a) m/z	O (a) m/z	Z0/G (b) m/z	Y0/O (b) m/z	C1 (b) m/z
16:0 <i>d 18:2</i> (C ₄₀ H ₇₅ O ₈ NLi) ⁺	704.5705	704.5653	542.5	524.3	450.4	304.3	304.3	187.1
h 16:0 <i>d 18:2</i> (C ₄₀ H ₇₅ O ₉ NLi) ⁺	720.5617	720.5602	558.5	540.5	466.4	304.3	304.3	187.1
h 16:0-OH <i>d 18:2</i> (C ₄₀ H ₇₅ O ₁₀ NLi) ⁺	736.5450	736.5551	574.5	556.5	482.4	304.3	320.3	187.1

Adams J, Ann Q (1993) Structure determination of sphingolipids by mass spectrometry. *Mass Spectrom Rev.* 12: 51-85

Domon B, Costello CE (1988) Structure elucidation of glycosphingolipids and gangliosides using high-performance tandem mass spectrometry. *Biochemistry* 27:1534-1543

Levery SB, Toledo MS, Doong RL, Straus AH, Takahashi HK (2000). Comparative analysis of ceramide structural modification found in fungal cerebrosides by electrospray tandem mass spectrometry with low energy collision-induced dissociation of Li⁺ adduct ions. *Rapid Commun Mass Spectrom.* 14:551-563.