

Supplementary Data 3 (1/7) - Distribution of GSLs

No.	Scheme	Structures	exact mass	Ceramide		Organs							
		theoretical <i>m/z</i>	mass	SB, FA		skin [sk]	gill [gi]	brain [br]	heart [he]	liver [li]	intestine [in]	testis [te]	ovary [ov]
GL1	Cer	806,6	548	d18:1, C16:0	✓	✓						✓	✓
GL2		808,6	550	d18:0, C16:0									✓
GL3		836,6	578	t18:0, C16:1	✓	✓							
GL4		838,6	580	t18:0, C16:0	✓	✓							
GL5		866,7	608	t18:0, C18:0								✓	
GL6		890,7	632	t18:0, C20:2	✓								
GL7		892,7	634	t18:0, C20:1	✓		✓						
GL8		894,7	636	t18:0, C20:0	✓	✓							
GL9		916,7	658	d18:1, 24:1	✓		✓	✓					
GL10		918,7	660	d18:1, 24:0	✓		✓	✓					
GL11		920,7	662	t18:0, C22:1	✓		✓	✓					
GL12		922,7	664	t18:0, C22:0			✓	✓					
GL13		934,7	676	t18:0, C23:1						✓			
GL14		946,7	688	d18:1, C26:0			✓	✓					
GL15		948,7	690	t18:0, C24:1	✓	✓	✓	✓	✓	✓		✓	
GL16		962,8	704	t18:0, C25:1				✓					
GL17		964,8	706	t18:0, C25:0					✓				
GL18		966,8	708	t18:0, hC23:0						✓			
GL19		976,8	718	t18:0, C26:1				✓					
GL20		978,8	720	t18:0, C26:0						✓			
GL21		980,8	722	t18:0, hC24:0					✓	✓			
GL22		1004,9	746	t18:1, C28:0								✓	
GL23		1006,9	748	t18:0, C28:0								✓	
GL24		1008,8	750	t18:0, hC26:0					✓	✓			
GL25	Cer	1281,9	662	t18:0, C22:1				✓	✓				
GL26		1295,9	676	t18:0, C23:1				✓	✓				
GL27		1299,9	680	t18:0, hC20:0						✓			
GL28		1310,0	690	t18:0, C24:1				✓	✓				

Supplementary Data 3 (2/7)

No.	Scheme	theoretical <i>m/z</i>	mass	SB, FA	skin [sk]	gill [gi]	brain [br]	heart [he]	liver [li]	intestine [in]	testis [te]	ovary [ov]
GL29	◆—○Cer	1314,0	694	t18:0, hC22:0						✓		
GL30		1324,0	704	t18:0, C25:1				✓	✓			
GL31		1328,0	708	t18:0, hC23:0						✓		
GL32		1338,0	718	t18:0, C26:1				✓	✓			
GL33		1366,0	746	t18:0, C28:1					✓			
GL34	◆—○Cer	1312,0	662	t18:0, C22:1				✓	✓			
GL35		1326,0	676	t18:0, C23:1				✓		✓		
GL36		1329,0	680	t18:0, hC20:0						✓		
GL37		1340,0	690	t18:0, C24:1				✓				
GL38		1368,0	718	t18:0, C28:1					✓			
GL39		1372,0	722	t18:0, hC24:0						✓		
GL40	◆—○Cer	1272,9	694	t18:0, hC22:0						✓		
GL41		1286,9	708	t18:0, hC23:0						✓		
GL42		1299,9	720	t18:0, C26:0						✓		
GL43		1301,0	722	t18:0, hC24:0						✓		
GL44		1313,0	734	t18:0, C27:0						✓		
GL45		1315,0	736	t18:0, hC25:0						✓		
GL46		1329,0	750	t18:0, hC26:0						✓		
GL47	○—●Cer	1008,7	546	d18:1, C16:1				✓		✓		
GL48		1010,8	548	d18:1, C16:0		✓			✓	✓		✓
GL49		1012,8	550	d18:0, C16:0								✓
GL50		1092,8	630	d18:1, C22:1		✓						
GL51		1094,8	632	d18:1, C22:0		✓						
GL52		1120,9	658	d18:1, C24:1	✓	✓	✓	✓		✓		
GL53		1122,9	660	d18:1, C24:0		✓	✓	✓		✓		✓
GL54		1124,9	662	t18:0, C22:1						✓		
GL55	◆—○—●Cer	1372,0	548	d18:1, C16:0	✓	✓		✓		✓	✓	

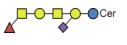
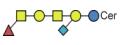
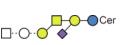
Supplementary Data 3 (3/7)

No.	Scheme	theoretical <i>m/z</i>	mass	SB, FA	skin [sk]	gill [gi]	brain [br]	heart [he]	liver [li]	intestine [in]	testis [te]	ovary [ov]
GL56		1456,0	632	d18:1, C22:0		✓				✓	✓	
GL57		1482,0	658	d18:1, C24:1	✓			✓			✓	
GL58		1484,0	660	d18:1, C24:0	✓						✓	
GL59		1544,1	720	t18:0, C26:0		✓						
GL60		1761,1	576	d18:1, C18:0			✓					
GL61		1821,2	636	t18:0, C20:0						✓		
GL62		1903,2	718	t18:0, C26:1							✓	
GL63		2123,3	576	d18:1, C18:0			✓					
GL64		2153,3	576	d18:1, C18:0			✓					
GL65		2153,3	576	d18:1, C18:0			✓					
GL66		2153,3	576	d18:1, C18:0			✓					
GL67		1617,1	548	d18:1, C16:0	✓	✓		✓	✓	✓	✓	✓
GL68		1647,1	578	t18:0, C16:1	✓	✓					✓	✓
GL69		1701,1	632	d18:1, C22:0	✓	✓		✓			✓	
GL70		1727,2	658	d18:1, C24:1		✓		✓	✓	✓	✓	✓
GL71		1729,2	660	d18:1, C24:0	✓	✓				✓	✓	✓
GL72		1757,2	688	d18:1, C26:0	✓						✓	✓
GL73		1759,2	690	t18:0, C24:1							✓	✓
GL74		1647,1	548	d18:1, C16:0				✓		✓	✓	✓
GL75		1757,2	658	d18:1, C24:1	✓			✓		✓	✓	
GL76		1759,2	660	d18:1, C24:0	✓			✓		✓	✓	
GL77		1460,0	548	d18:1, C16:0		✓					✓	
GL78		1520,0	608	t18:0, C18:0							✓	
GL79		1544,1	632	d18:1, C22:0		✓						
GL80		1604,1	692	t18:0, C24:0		✓						
GL81		1819,1	546	d18:1, C16:1								✓
GL82		1821,2	548	d18:1, C16:0	✓	✓			✓	✓	✓	✓

Supplementary Data 3 (4/7)

No.	Scheme	theoretical <i>m/z</i>	mass	SB, FA	skin [sk]	gill [gi]	brain [br]	heart [he]	liver [li]	intestine [in]	testis [te]	ovary [ov]
GL83		1850,2	576	d18:1, C18:0			✓					
GL84		1933,3	660	d18:1, C24:0	✓	✓		✓		✓		
GL85		1851,2	548	d18:1, C16:0					✓			
GL86		1821,2	548	d18:1, C16:0	✓	✓					✓	
GL87		1850,2	576	d18:1, C18:0			✓					
GL88		1933,3	660	d18:1, C24:0		✓						
GL89		2210,3	576	d18:1, C18:0			✓					
GL90		2270,4	636	t18:0, C20:0	✓							
GL91		2294,5	660	d18:1, C24:0	✓							
GL92		2296,4	662	t18:0, C22:1	✓							
GL93		2322,5	688	d18:1, C26:0	✓							
GL94		2324,5	690	t18:0, C24:1	✓							
GL95		2210,3	576	d18:1, C18:0			✓					
GL96		2572,5	576	d18:1, C18:0			✓					
GL97		2572,5	576	d18:1, C18:0			✓					
GL98		2602,2	576	d18:1, C18:0			✓					
GL99		2602,2	576	d18:1, C18:0			✓					
GL100		2602,2	576	d18:1, C18:0			✓					
GL101		2602,2	576	d18:1, C18:0			✓					
GL102		2933,7	576	d18:1, C18:0			✓					
GL103		2963,7	576	d18:1, C18:0			✓					
GL104		2963,7	576	d18:1, C18:0			✓					
GL105		3294,8	576	d18:1, C18:0			✓					
GL106		3294,8	576	d18:1, C18:0			✓					
GL107		1879,2	548	d18:1, C16:0						✓		
GL108		1879,2	548	d18:1, C16:0						✓		
GL109		2066,3	548	d18:1, C16:0		✓				✓	✓	

Supplementary Data 3 (5/7)

No.	Scheme	theoretical <i>m/z</i>	mass	SB, FA	skin [sk]	gill [gi]	brain [br]	heart [he]	liver [li]	intestine [in]	testis [te]	ovary [ov]
GL110		2096,3	578	t18:0, C16:1							✓	
GL111		2066,3	548	d18:1, C16:0	✓	✓		✓			✓	✓
GL112		2096,3	578	t18:0, C16:1							✓	
GL113		2238,4	546	d18:1, C16:1						✓		
GL114		2240,4	548	d18:1, C16:0	✓	✓			✓	✓	✓	
GL115		2270,4	578	t18:0, C16:1	✓							
GL116		2272,4	580	t18:0, C16:0					✓			
GL117		2350,5	658	d18:1, C24:1	✓			✓				
GL118		2352,5	660	d18:1, C24:0	✓			✓	✓		✓	
GL119		2382,5	690	t18:0, C24:1							✓	
GL120		2270,4	548	d18:1, C16:0					✓		✓	
GL121		2382,5	660	d18:1, C24:0							✓	
GL122		2270,4	548	d18:1, C16:0							✓	
GL123		1501,0	548	d18:1, C16:0							✓	✓
GL124		1705,1	548	d18:1, C16:0							✓	
GL125		1817,2	660	d18:1, C24:0								✓
GL126		1819,2	662	t18:0, C22:1								✓
GL127		1821,2	664	t18:0, C22:0								✓
GL128		2066,3	548	d18:1, C16:0		✓					✓	✓
GL129		2096,3	578	t18:0, C16:1							✓	
GL130		2124,3	548	d18:1, C16:0							✓	
GL131		2156,3	580	t18:0, C16:0		✓						
GL132		2180,3	604	d18:1, C18:0	✓							
GL133		2186,3	610	t18:0, hC16:0	✓							
GL134		2212,4	636	t18:0, C20:0		✓						
GL135		2226,3	650	t18:0, C21:0		✓						
GL136		2240,3	664	t18:0, C22:0	✓	✓						

Supplementary Data 3 (6/7)

Supplementary Data 3 (7/7)

No.	Scheme	theoretical <i>m/z</i>	mass	SB, FA	skin [sk]	gill [gi]	brain [br]	heart [he]	liver [li]	intestine [in]	testis [te]	ovary [ov]
GL163		2732,8	748	t18:0, C28:0							✓	
GL164		2738,6	580	t18:0, C16:0							✓	
GL165		2808,7	650	t18:0, C21:0								
GL166		2848,7	690	t18:0, C24:1							✓	
GL167		2878,8	720	t18:0, C26:0							✓	
GL168		2904,8	746	t18:0, C28:1							✓	
GL169		2983,8	580	t18:0, C16:0							✓	
GL170		3095,9	692	t18:0, C24:0							✓	
GL171		3545,1	692	t18:0, C24:0							✓	
GL172		2747,7	548	d18:1, C16:0							✓	

Supplementary Data 3 - The inclusion criteria of individual molecules in an organ were (1) observation of corresponding MS signal in three independent experiments and (2) confirmation of individual compounds by MS/MS analysis of permethylated glycans. The sequence of carbohydrate moieties and the nature of ceramides were established by CID MS/MS fragmentation of permethylated GSLs in positive mode. Values in “mass” column correspond to the diagnostic Z fragmentation ions for the methylated ceramide moiety. Most probable combinations of sphingoid bases and fatty acids based on composition and Z fragment ions are provided in the “SB, FA” column. Graphical representation is based on accepted conventions for GSLs and monosaccharide nomenclature.^{1,2} The interglycosidic bonds between monosaccharides are represented using the conventional positions as I, C2 position; /, C3 position; —, C4 position; \, C6 position, except for (α 2,8) linkages between sialic acids which do not follow any convention. Whenever linkages could not be deduced from specific CID MS/MS fragmentation pattern and literature, they are shown as dotted lines.

Supplementary References

1. *Essentials of Glycobiology*. (Cold Spring Harbor Laboratory Press, 2015).
2. Varki, A. et al. Symbol Nomenclature for Graphical Representations of Glycans. *Glycobiology* **25**, 1323–1324 (2015).