

SUPPLEMENTARY MATERIALS

TABLE

Table S1. Amino acid sequences of β -chain CDR expressed by iNKT cell hybridomas used in this study						
Hybridoma	TCR β^a	CDR1 $\beta^{b,c}$	CDR2 $\beta^{b,c}$	CDR3 β^c	J β	
H41-2D9/V α 14	TRBV19*01 (V β 6)	qqn FNHDT myw	iyy SITEND lqk	cass IARATE vffg	1.1	
V α 14/ V β 7	TRBV29*02 (V β 7)	gqd MSJET myw	iyi SYDVDS nse	cass LRGQNT lyfg	2.4	
V α 14/DO β	TRBV13-2*01 (V β 8.2)	nqt NNHNN myw	ihy SYGAGS tek	casg SGTNT evfg	1.1	
N38-3C3				casg DQITGQ lyfg	2.2	
DN32-D3				casg DPDIQNT lyfg	2.4	
N38-2C12				casg DEGYT qyfg	2.5	
N37-1H5a				casg AQGLSSYE qyfg	2.6	
N57-2C12	TRBV31*02 (V β 14)	tik GKSSPN lyw	lfy SITVG gev	caws RTANSND ytfg	1.2i	
N57-2B6				caws SNSD ytfg	1.2ii	
H41-2C9				caws TGDE qyfg	2.5	
H41-3C5				cawt GGQGQDT qyfg	2.6	
^a IMGT nomenclature; old designation in parenthesis ^b sequences obtained from IMGT (http://www.imgt.org/textes/IMGTrepertoire/) ^c amino acid residues flanking the CDR are in lower case; from http://www.imgt.org/textes/IMGTrepertoire/						

Supplementary Figure Legends

Figure S1: Structures of glycolipids and their variants used in this study.

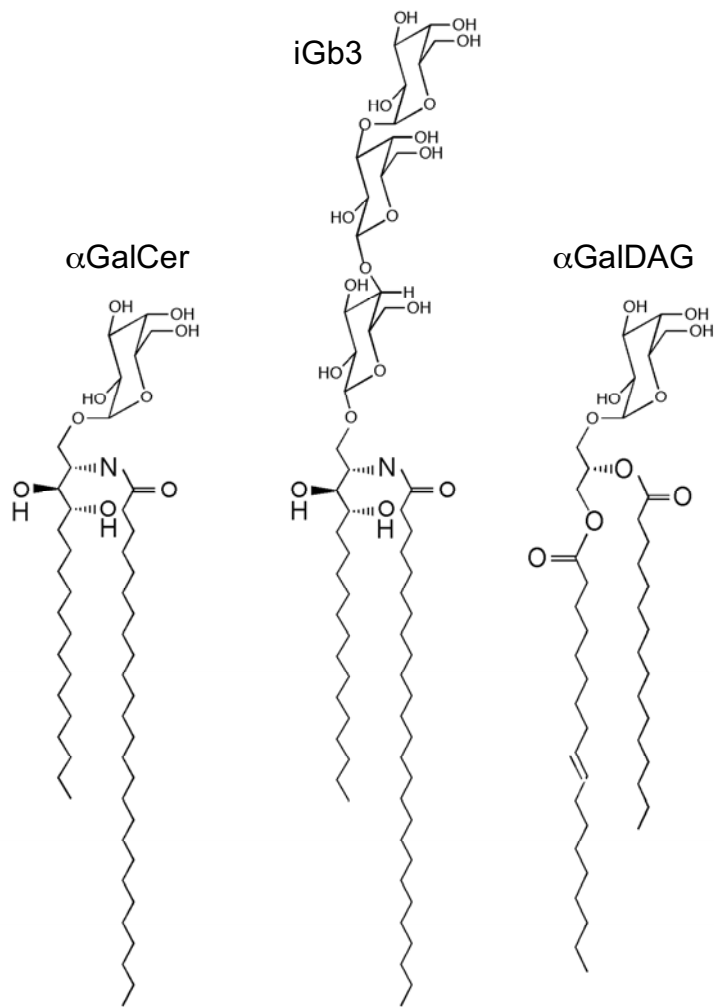
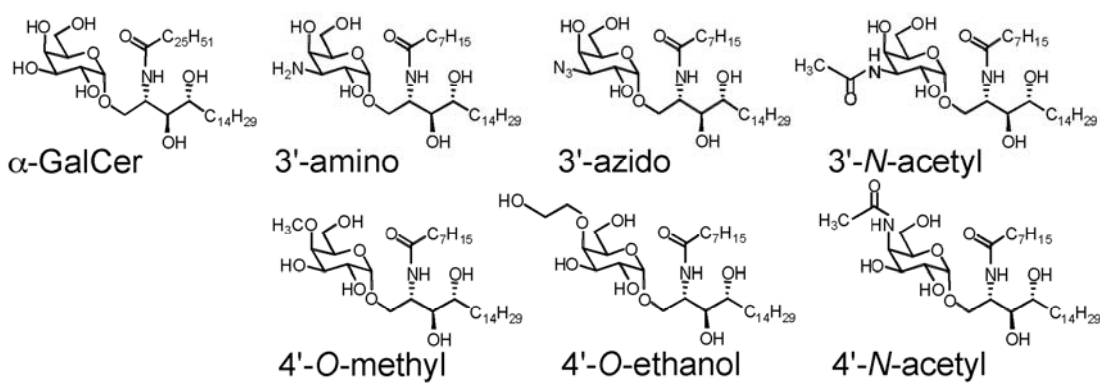
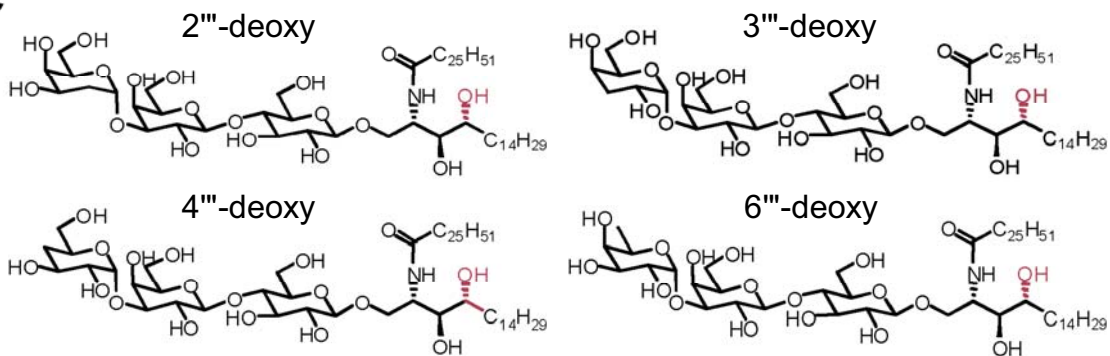
(A) Structure of native glycolipid antigens. (B) Structures of 3' and 4' α GalCer variants. (C) Structures of terminal α 1,3Gal variants of iGb3.

Figure S2: Schematic rendition of NKTcr/CD1d- GalCer interactions. Mouse

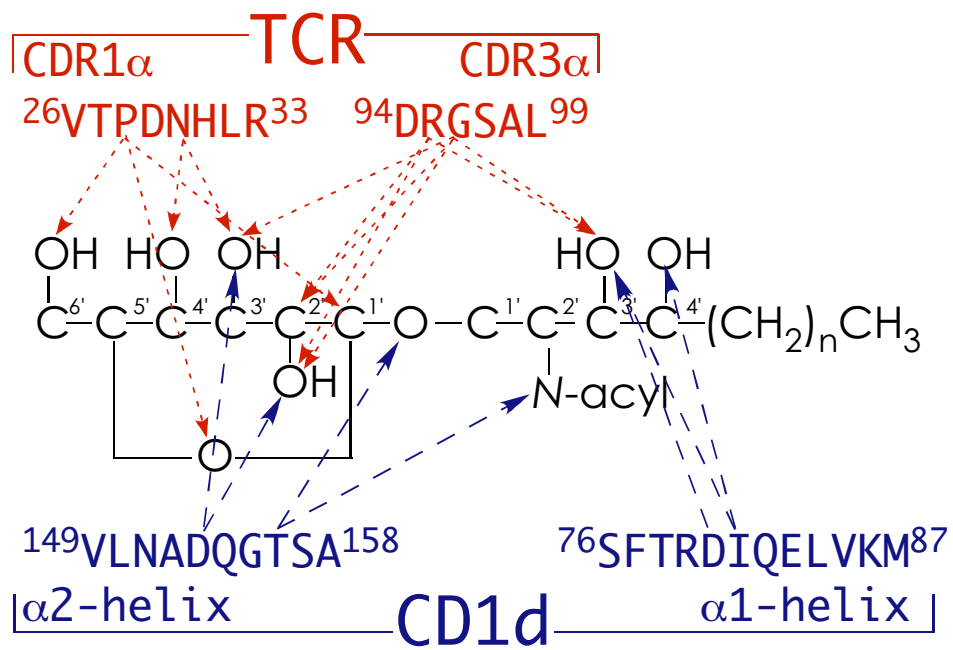
CD1d- α GalCer interactions are based on the reported crystal structure (Zajonc et al., 2005). NKTcr/CD1d- α GalCer interactions are adapted from the recently reported crystal structure of the mouse V α 14-V β 8.2 NKTcr/CD1d- α GalCer co-complex (Pellicci et al., 2009). Blue, mouse CD1d residues; red, V α 14 residues; black, α GalCer.

References

- Pellicci, D.G., Patel, O., Kjer-Nielsen, L., Pang, S.S., Sullivan, L.C., Kyparissoudis, K., Brooks, A.G., Reid, H.H., Gras, S., Lucet, I., Koh, R., Smyth, M.J., Mallevaey, T., Matsuda, J.L., Gapin, L., McCluskey, J., Godfrey, D.I. and Rossjohn, J. (2009) Differential recognition of CD1d- α -galactosyl ceramide by the V β 8.2 and V β 7 semi-invariant NKT T-cell receptors. *Immunity*, **31**, 47-59.
- Zajonc, D.M., Cantu, C., 3rd, Mattner, J., Zhou, D., Savage, P.B., Bendelac, A., Wilson, I.A. and Teyton, L. (2005) Structure and function of a potent agonist for the semi-invariant natural killer T cell receptor. *Nat Immunol*, **6**, 810-818.

A**B****C**

Supplementary Figure 1



Supplementary Figure 2