Supplementary Data

Supplementary Figure 1. Omit map of α-*C*-GalCer in mouse CD1d binding cleft.

Omit map contoured at 1 sigma. α-*C*-GalCer, blue; CDR1α, purple; CDR3α, yellow; mCD1d, grey.

Supplementary Figure 2. Differential affinity binding kinetics of Vβ8.2 and Vβ7 to CD1d-Ag.

Binding of increasing concentrations of Vβ8.2 TCR to CD1d-α-GalCer (A) or CD1d-α-*C*-GalCer (B). Binding of Vβ7 TCR to CD1d-α-GalCer (C) or CD1d-α-*C*-GalCer (D). All results are shown as one representative experiment of two.

Supplementary Table 1

Data collection and refinement statistics

Supplementary Table 1 Data collection and refinement statistics

	mVα14Vβ8.2TCR-CD1d-α-*C*-GalCer
Data collection	
Temperature	100K
Resolution limits (Å)	50-3.2 (3.37-3.20)
Space Group	$P2_12_12_1$
Cell dimensions (Å)	*a*=59.17, *b*=86.37, *c*= 236.40
Total N$^{o.}$ observations	168608
N$^{o.}$ unique observations	20725
Multiplicity	8.1 (9.8)
Data completeness	100 (100)
I/σ_1	7.2 (2.2)
$R_{p.i.m}$[1] (%)	9.8 (37.7)
Refinement statistics	
R_{factor}[2] (%)	22.6
R_{free}[3] (%)	28.9
Non hydrogen atoms[4]	
- protein	6587
- lipid	60
- other	56
Ramachandran plot	
- Most favoured	88.4
- Allowed region (%)	11.3
- Generously allowed region (%)	0.3%
B-factors (Å^2)	
- Average main chain	80.5
- Average side chain	82.0
- α-GalCer	76.1
rmsd bonds (Å)	0.007
rmsd angles (°)	1.007

[1] $R_{p.i.m} = \Sigma_{hkl} [1/(N-1)]^{1/2} \Sigma_i \mid I_{hkl,\,i} - \langle I_{hkl} \rangle \mid / \Sigma_{hkl} \langle I_{hkl} \rangle$

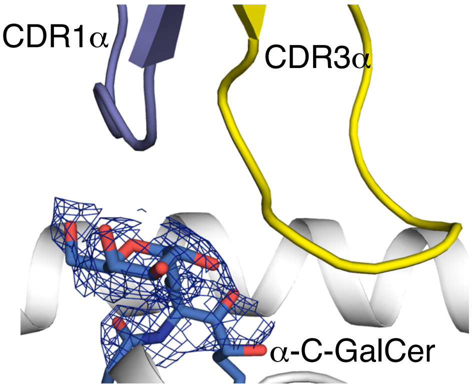
[2] $R_{factor} = (\Sigma \mid |F_o| - |F_c| \mid) / (\Sigma |F_o|)$ - for all data except as indicated in footnote 3.

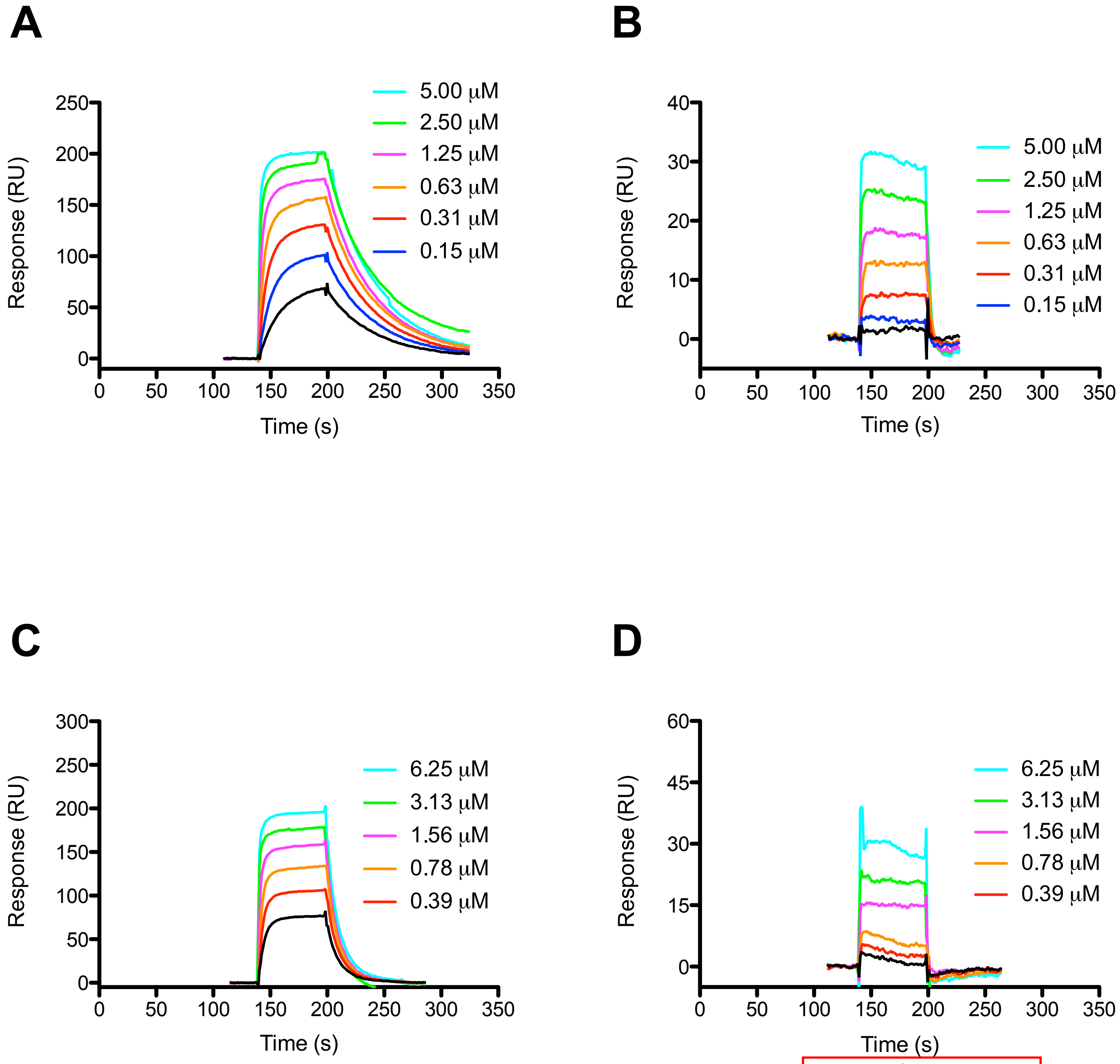
[3] 5% of data was used for the R_{free} calculation

Values in parentheses refer to the highest resolution bin.

[4] The residues that could not be modelled in the structures were CD1d: residues 1-6, 300-302; β_2m: residue 1; TCR α chain: residues 1, 135-135, 209-210; TCR β chain: residues 1-2, CDR3β loop 96-102.

SUPPLEMENTARY FIGURE 1




A
Response (RU)
250
200
150
100
50
0
0
50
100
150
200
250
300
350
Time (s)
5.00 μM
2.50 μM
1.25 μM
0.63 μM
0.31 μM
0.15 μM
B
Response (RU)
40
30
20
10
0
-5
0
50
100
150
200
250
300
350
Time (s)
5.00 μM
2.50 μM
1.25 μM
0.63 μM
0.31 μM
0.15 μM
C
Response (RU)
300
250
200
150
100
50
0
0
50
100
150
200
250
300
350
Time (s)
6.25 μM
3.13 μM
1.56 μM
0.78 μM
0.39 μM
D
Response (RU)
60
45
30
15
0
0
50
100
150
200
250
300
350
Time (s)
6.25 μM
3.13 μM
1.56 μM
0.78 μM
0.39 μM

Supp. Fig. 2