Table S1. Data collection and refinement statistics.

Data set	DPP-IV + Fab	DPP-IV + Fab + sitagliptin
Data collection		
Wavelength (Å)	1.000	1.000
Space group	$P2_1$	$P2_1$
Unit cell dimensions		
a,b,c (Å)	97.26, 201.72, 97.28	97.77, 200.86, 97.93
α, β, γ (°)	90.00, 93.71, 90.00	90.00, 93.64, 90.00
Resolution (Å)	40-2.4 (2.53-2.40)	40-2.9 (3.06-2.90)
No. of total reflections	532468 (73584)	308152 (45665)
No. of unique	143426 (20726)	82544 (12065)
Wilson B factor ($Å^2$)	36.51	69.07
Average Multiplicity	3.7 (3.6)	3.7 (3.8)
Completeness (%)	98.6 (97.8)	99.2 (99.2)
Intensity I/σI	9.8 (2.2)	10.5 (2.7)
R_{sym}[a]	0.101 (0.589)	0.080 (0.422)
Refinement		
Resolution (Å)	30-2.4 (2.49-2.40)	30-2.9 (3.02-2.9)
R_{factor}/ R_{free}[b]	0.270 (0.300)	0.275 (0.308)
No. of Atoms		
Protein	18291	18371
Water	222	42
Ligand	-	56
Ramachandran statistics		
Residues in favored regions	93.0%	91.0%
Residues in allowed regions	5.7%	7.5%
Residues in disallowed regions	1.3%	1.5%
Avg. *B*-factors ($Å^2$)		
Protein-DPPIV	35.3	72.5
Protein-Fab	88.3	134.9
Solvent	28.3	53.8
ligand	-	77.1
r.m.s.d. in bond length (Å)[c]	0.005	0.004
r.m.s.d. in bond angles (°)[c]	1.04	0.95

Values in parentheses are for the highest resolution shell.

[a] $R_{sym} = \sum | I_{avg} - I_j | / \sum I_j$., where I_i is the observed intensity for the ith measurement and I_{avg} is the average intensity of all measurements.

[b] $R_{factor} = \sum | F_o - F_c | / \sum F_o$, where F_o and F_c are observed and calculated structure factors, respectively, R_{free} was calculated from a randomly chosen 5% of reflections excluded from the refinement, and R_{factor} was calculated from the remaining 95% of reflections.

[c] r.m.s.d. is the root-mean-square deviation from ideal geometry.

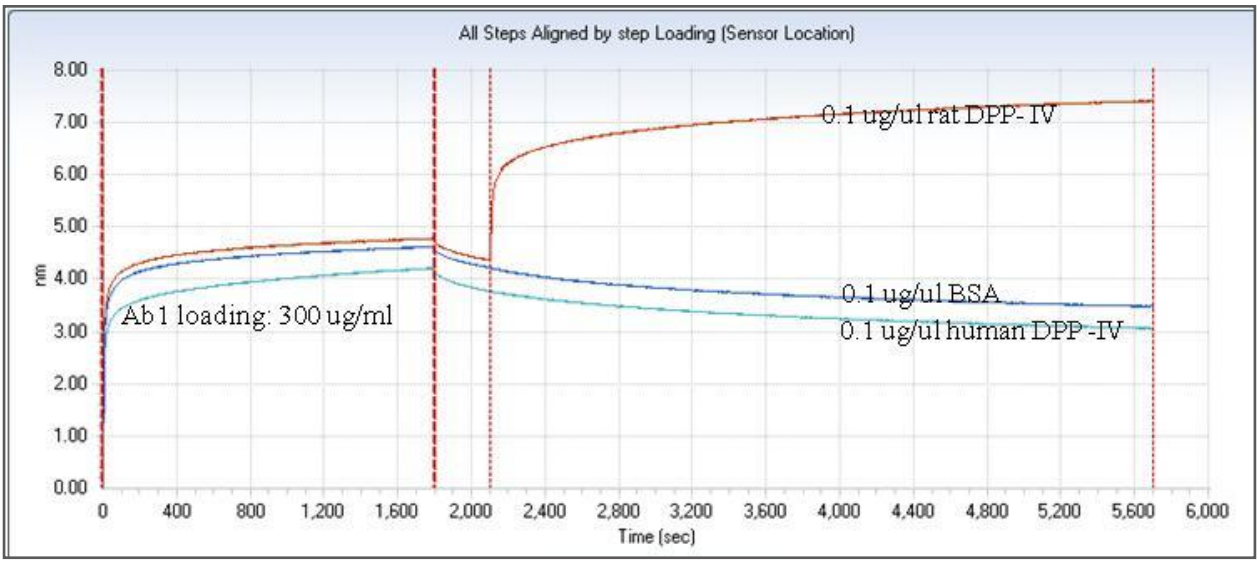
SUPPLIMENTAL FIGURE LEGENDS

Figure S1. Binding specificity of Ab1. A) Octet binding analysis of Ab1 to rat and human DPP-IV in HBS. B) Octet binding analysis of Ab1 to targets mixed with 293 cell lysate in HBS. Key recognition epitope for Ab1's specificity is high-lighted with a text box in the sequence-alignment panel of dipeptityl peptidases.

Figure S2. Inhibition of rat DPP-IV activity against its natural substrates (GLP-1 and GIP) by Ab1. A) GLP-1 as substrate. B) GIP as substrate. C) GP-pNA as substrate.

Figure S1.

A.


All Steps Aligned by step Loading (Sensor Location)
0.1 ug/ul rat DPP-IV
0.1 ug/ul BSA
0.1 ug/ul human DPP-IV
Ab1 loading: 300 ug/ml
nm
Time (sec)

B.

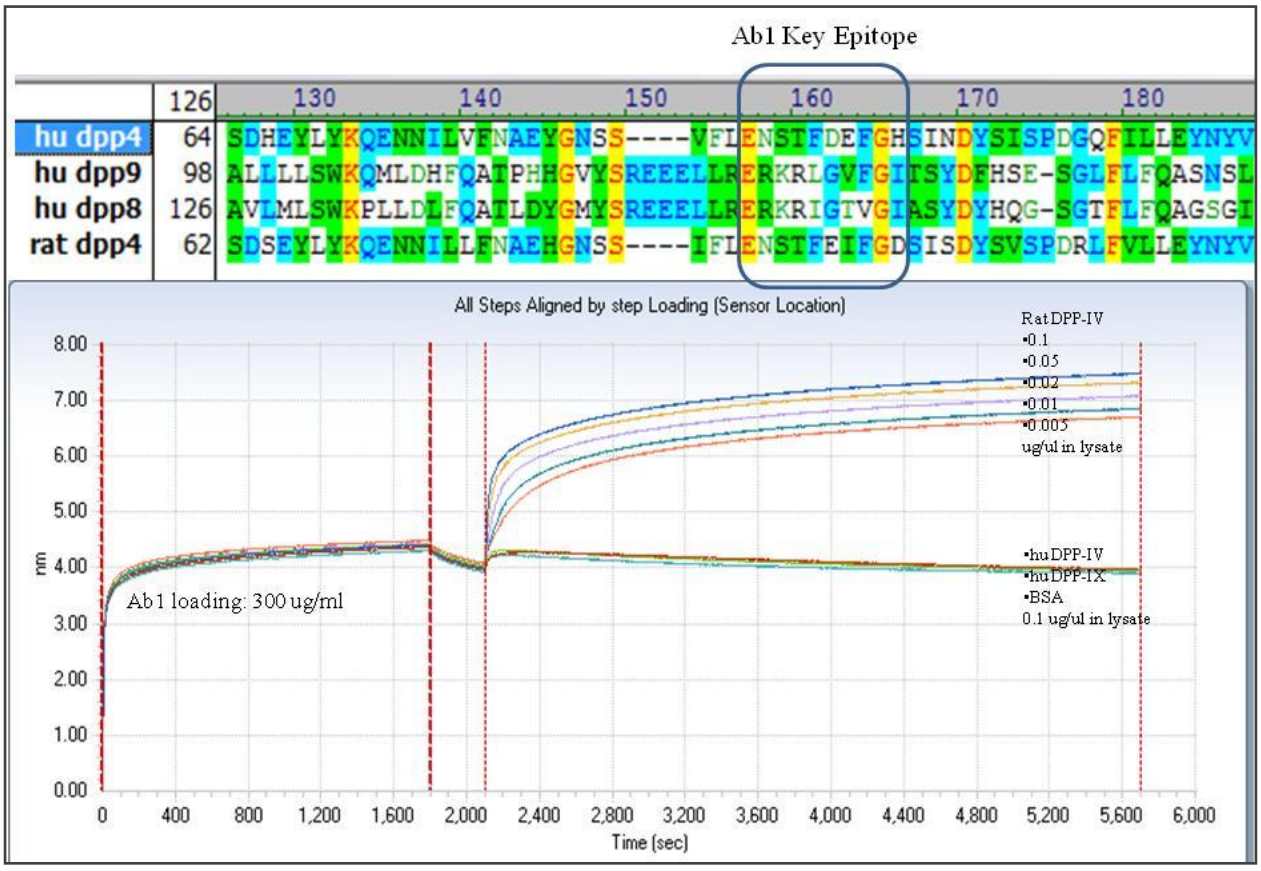
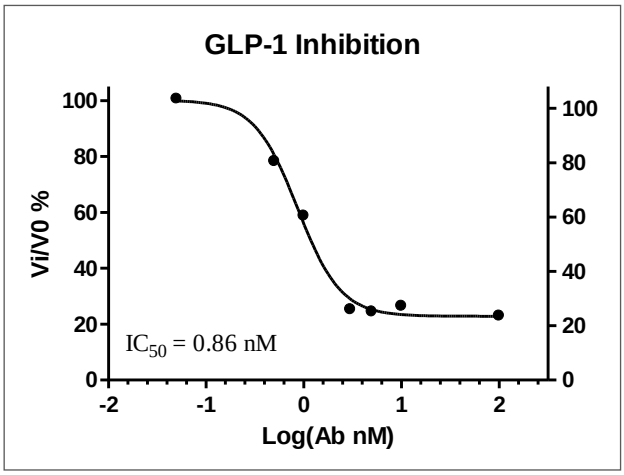
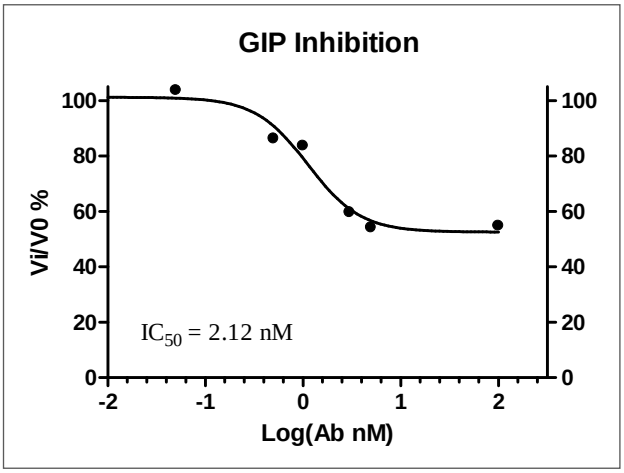

Ab1 Key Epitope
126
130
140
150
160
170
180
hu dpp4 64 SDHEYLYKQENNILVFNAEYGNSS----VFLENSTFDEFGHSINDYSISPDGQFILLEYNYV
hu dpp9 98 ALLLLSWKQMLDHFQATPHHGVYSREEELLRERKRLGVFGITSYDFHSE-SGLFLFQASNSL
hu dpp8 126 AVLMLSWKPLLDLFQATLDYGMYSREEELLRERKRIGTVGIASYDYHQG-SGTFLFQAGSGI
rat dpp4 62 SDSEYLYKQENNILLFNAEHGNSS----IFLENSTFEIFGDSISDYSVSPDRLFVLLEYNYV
All Steps Aligned by step Loading (Sensor Location)
Rat DPP-IV
•0.1
•0.05
•0.02
•0.01
•0.005
ug/ul in lysate
•huDPP-IV
•huDPP-IX
•BSA
0.1 ug/ul in lysate
Ab1 loading: 300 ug/ml
nm
Time (sec)

Figure S2.

A.



B.



C.