S3 Table. Affinities to mfT1r2a/T1r3LBD derived from the DSF results and physicochemical parameters for the α-substituent group of amino acids.

	Affinity	Physicochemical parameters						
L-amino acid	$pK_{d\text{-}app}$ [a]	π_{α} [b]	E_s' [c] [c]	HP [d]	logK_d_CW [e]	ΔMgVol [f]	Hydropathy Index [g]	pI [h]
Gly	2.65	0	0	2.39	-0.69	0	-0.4	5.97
Ala	3.95	0.28	-0.2	1.94	-1.33	0.32	1.8	6
Ser	3.02	-0.19	-0.48	-5.06	2.49	0.38	-0.8	5.68
Thr	2.97	0.07	-0.73	-4.88	1.89	0.52	-0.7	5.6
Asn	2.52	-0.52	-0.98	-9.68	4.88	0.58	-3.5	5.41
Gln	4.85	-0.52	-0.82	-9.38	4.07	0.72	-3.5	5.65
Asp	1.46	0.05	-0.98	-10.95	3.27	0.53	-3.5	2.77
Glu	2.98	0.02	-0.82	-10.2	2.25	0.68	-3.5	3.22
Arg	3.56	-0.42	-0.82	-19.92	4.32	1	-4.5	10.76
Val	3.10	1	-1.29	1.99	-2.97	0.6	4.2	5.96
Leu	2.96	1.52	-1.44	2.28	-3.62	0.74	3.8	5.98
Ile	2.22	1.43	-1.81	2.15	-3.62	0.74	4.5	6.02
Met	3.25	0.99	-1.03	-1.48	-1.73	0.76	1.9	5.74
His	2.78	0.17	-0.86	-10.27	3.34	0.75	-3.2	7.59
Phe	2.36	1.78	-0.9	-0.76	-2.19	0.93	2.8	5.48

[a]Converted from the values in Supplementary Table 1. [b]For hydrophobicity. Cited from Akamatsu *et al., J. Pharm. Sci.*, 83, 1026 (1994). [c]For steric effects. Cited from Akamatsu *et al., J. Pharm. Sci.*, 83, 1026 (1994). [d]For hydration potential. Cited from Wolfenden *et al., Biochemistry,* 20, 849 (1981). [e]For polarity. Cited from Radzicka & Wolfenden, *Biochemistry*, 27, 1664 (1988), free energies for transfer from cyclohexane to an aqueous solution. [f]McGowan volumes [ref.: McGowan, *J. Appl. Chem. Biotechnol.*, 28, 599 (1978)] calculated by BioLoom (BioByte, Claremont, CA, USA). [g]For hydrophobicity/hydrophilicity. Cited from Kyte & Doolittle, *J. Mol. Biol.*, 157, 105 (1982). [h]Cited from Handbook of Chemistry and Physics, CRC Press.