Supplementary data

Helical structures of homo-chiral isotope-labeled α-aminoisobutyric acid peptides

Atsushi Ueda[a], Makoto Oba[a], Yuki Izumi[a], Yasuhito Sueyoshi[a], Mitsunobu Doi[b], Yosuke Demizu[c], Masaaki Kurihara[c], and Masakazu Tanaka[a,*]

[a] *Graduate School of Biomedical Sciences, Nagasaki University, 1-14 Bunkyo-machi, Nagasaki 852-8521, Japan*

[b] *Osaka University of Pharmaceutical Sciences, Osaka 569-1094, Japan*

[c] *Division of Organic Chemistry, National Institute of Health Sciences, Tokyo 158-8501, Japan*

matanaka@nagasaki-u.ac.jp

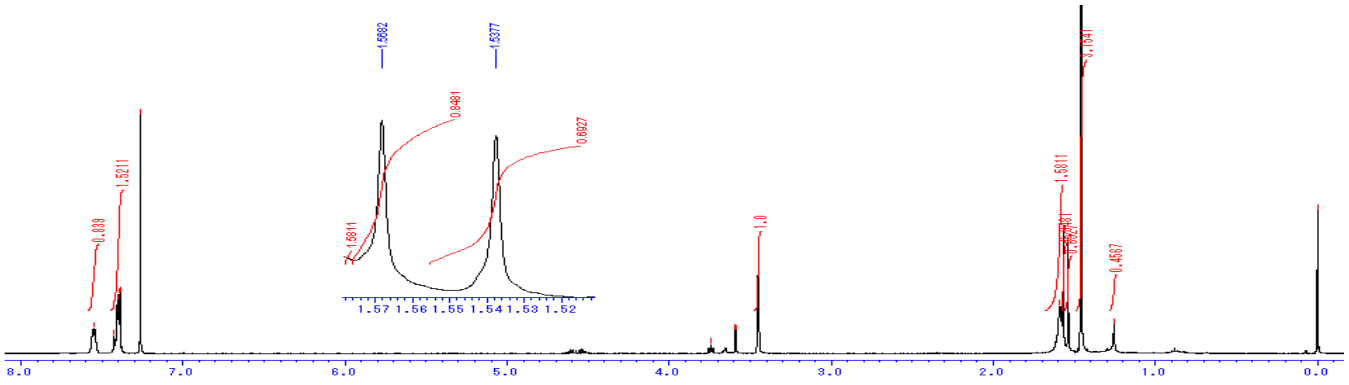
* Corresponding author. Tel. & fax: +81-95-819-2423; e-mail: matanaka@nagasaki-u.ac.jp

Table S1. Crystal and diffraction parameters of peptides **7a** and **10a**.

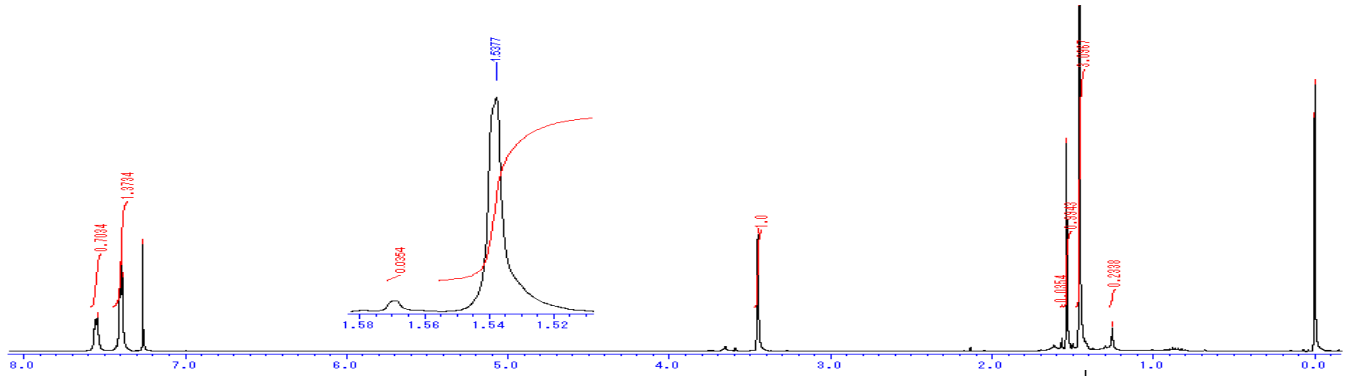
	Tetrapeptide **7a**	Octapeptide **10a**
empirical formula	$C_{28}H_{44}N_4O_7$, CH_4O	$4(C_{44}H_{72}N_8O_{11})$, $3(C_2H_8O_2)$
*M*r	580.71	917.13
crystal dimensions [mm]	0.28×0.25×0.19	0.25×0.25×0.20
Temperature [K]	93	93
crystal system	monoclinic	triclinic
lattice parameters:		
a, *b*, *c* [Å]	9.6765, 18.093, 18.553	14.585, 17.456, 21.012
α, β, γ [°]	90, 92.35, 90	99.876, 93.407, 92.640
V [Å^3]	3245.4	5252.4
space group	*P21/n*	*P1*
Z value	4	4
D_{calc} [g/cm^3]	1.189	1.160
μ(Mo$K\alpha$) [cm^{-1}]	0.87	0.84
no. of observations ($I > -10.0\ \sigma I$)	5146	11572
no. of variables	372	2401
R_1, R_W	0.0439, 0.1066	0.1004, 0.2229
crystallizing solvent	MeOH/H_2O	MeOH/H_2O

Figure S1. ^{1}H NMR spectra of a) (*R*)-MTPA-(±)-CD_3-Aib-O^{t}Bu, b) (*R*)-MTPA-(*S*)-CD_3-Aib-O^{t}Bu, c) (*R*)-MTPA-(*R*)-CD_3-Aib-O^{t}Bu.

a)



b)



c)

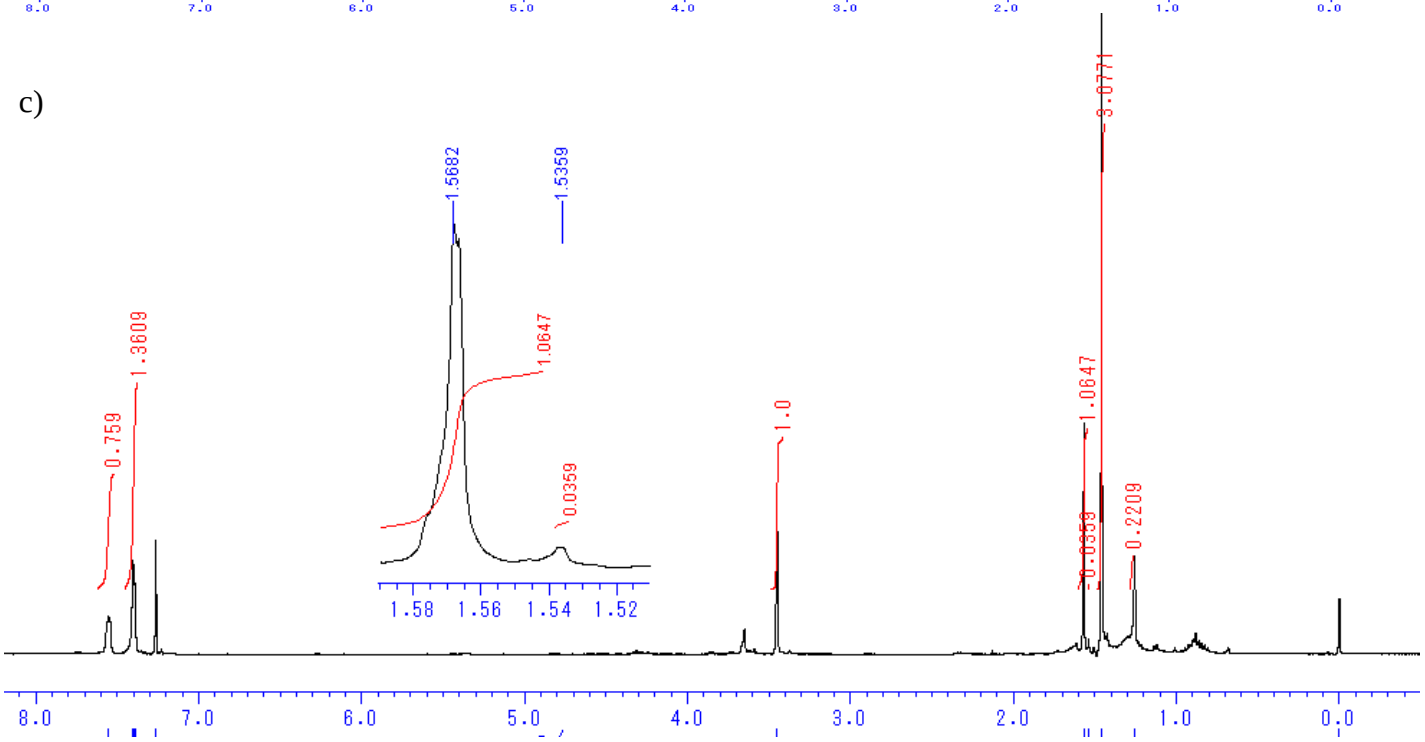
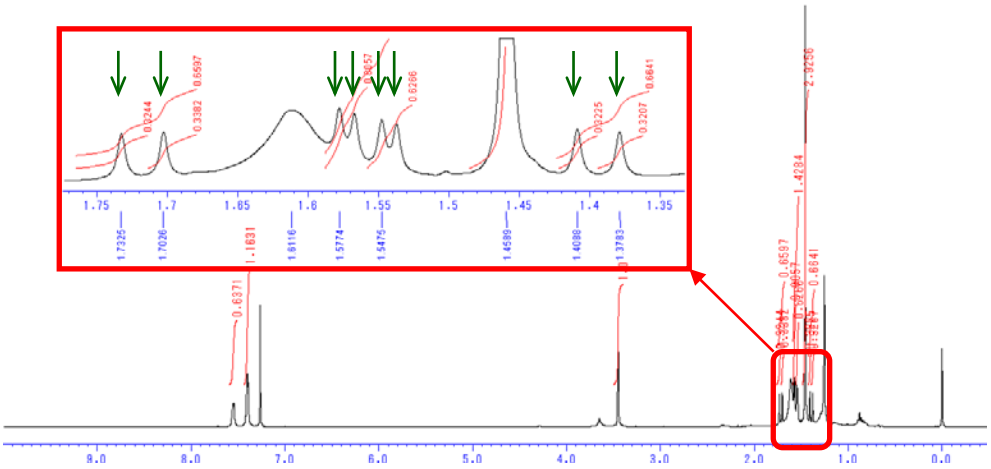
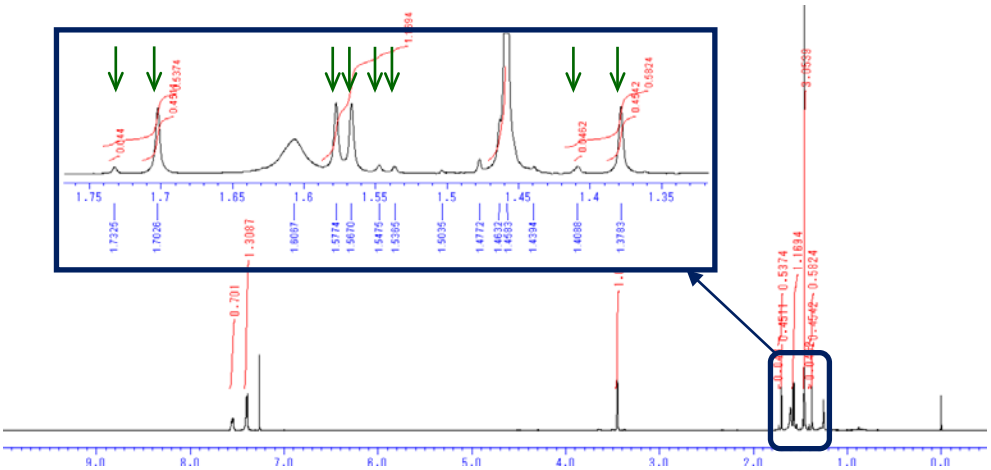


Figure S2. ^{1}H NMR spectra of a) (*R*)-MTPA-(±)-$^{13}CH_3$-Aib-O^{t}Bu, b) (*R*)-MTPA-(*S*)-$^{13}CH_3$-Aib-O^{t}Bu, c) (*R*)-MTPA-(*R*)-$^{13}CH_3$-Aib-O^{t}Bu.

a)



b)



c)

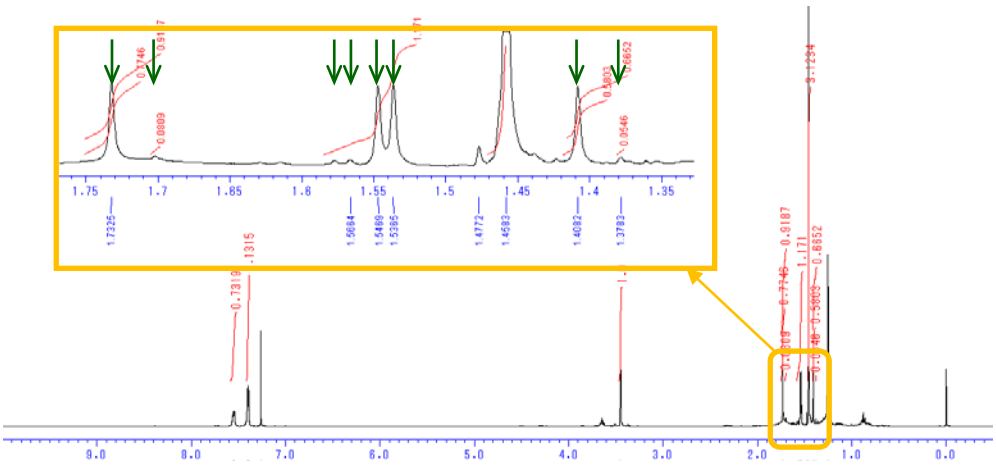


Figure S4. The FT-IR absorption spectra of Cbz-{(*S*)-CD_3-Aib}$_n$-OBu^t in $CDCl_3$ solution (1.0 mM).