Electronic Supplementary Material (ESI) for Molecular BioSystems

Supplemental Data

Supplemental Table S1: Proton chemical shifts (ppm) of $(C18)_2$-L1-R11 in 0.10 M sodium phosphate pH 7.4, evaluated at 298 K and 600 MHz.

A.a	H_N	α	β	γ	others
1)pTyr	8.15	4.53	2.96-2.85		Hδ= 7.06 Hε=7.03
2)Val	8.03	4.02	1.92	0.81-0.79	
3)Asp	8.29	4.52	2.65-2.55		
4)Asn	8.38	4.58	2.72-2.70		6.80-7.54
5)Gln	8.39	4.25	1.91-2.09	2.25	6.73-7.53
6)Ser	8.20	4.28	3.83-3.76		
7)Asp	8.27	4.45	2.58		
8)Gln	8.06	4.09	1.87-1.77	2.08	6.73-7.36
9)Phe	8.06	4.53	3.09-2.96		Hδ=7.14 Hε=7.10
10)Leu	7.99	4.25	1.61-1.49	1.45	0.81-0.76
11)Thr	7.81	4.25	4.19	1.10	

Proton resonance assignments for the C18 alkyl tails:
N**CH_2:** 3.26 and 3.13 ppm
NCH2**CH2(**$CH2)_{15}$ CH3: 1.38, 1.45 ppm
NCH2CH2**$(CH2)_{15}$**CH3: 1.16 ppm
CH3: 0.76, 0.79 ppm
Proton resonance assignments for the linker:
Acyl tail-NCO**CH2**CH2CO: 2.52 ppm
Acyl tail-NCOCH2**CH2**CO: 2.42 ppm
CON**H:** 7.90 ppm
CONH(**CH2CH2**$O)_6$: 3.27, 346, 3.51, 3.55 ppm
O**CH2**CH2CONH-peptide: 3.61 ppm
OCH2**CH2**CONH-peptide: 2.42 ppm