Supporting Information

In situ functionalization of poly(hydroxyethyl methacrylate) cryogels with oligopeptides via *β*-cyclodextrin-adamantane complexation for studying cell-instructive peptide environment

Thai Duong Luong[a±], Mohamed Zoughaib[a±], Ruslan Garifullin[a,b,*], Svetlana Kuznetsova[a], Mustafa O. Guler[c], Timur I. Abdullin[a,*]

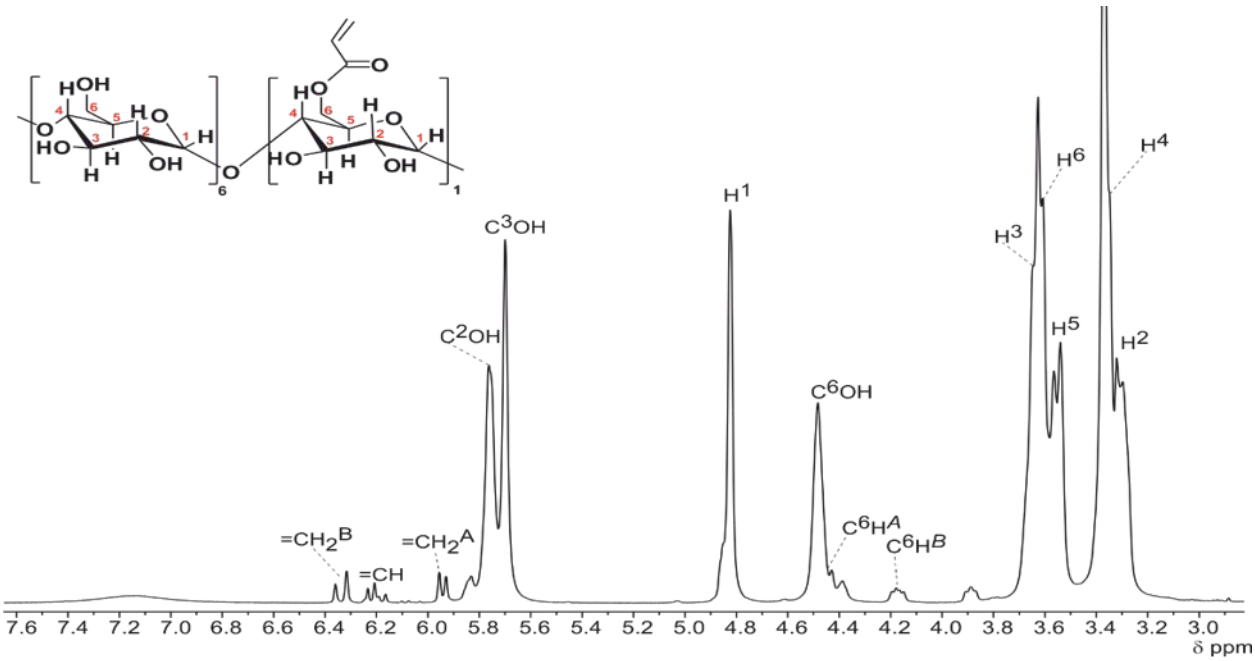
[a]Institute of Fundamental Medicine and Biology, Kazan Federal University, Kazan, Russia
[b]Institute of Materials Science and Nanotechnology, Bilkent University, Ankara, Turkey
[c]Pritzker School of Molecular Engineering, University of Chicago, Chicago, IL, USA

[±] **These authors have equal contribution to this article.**

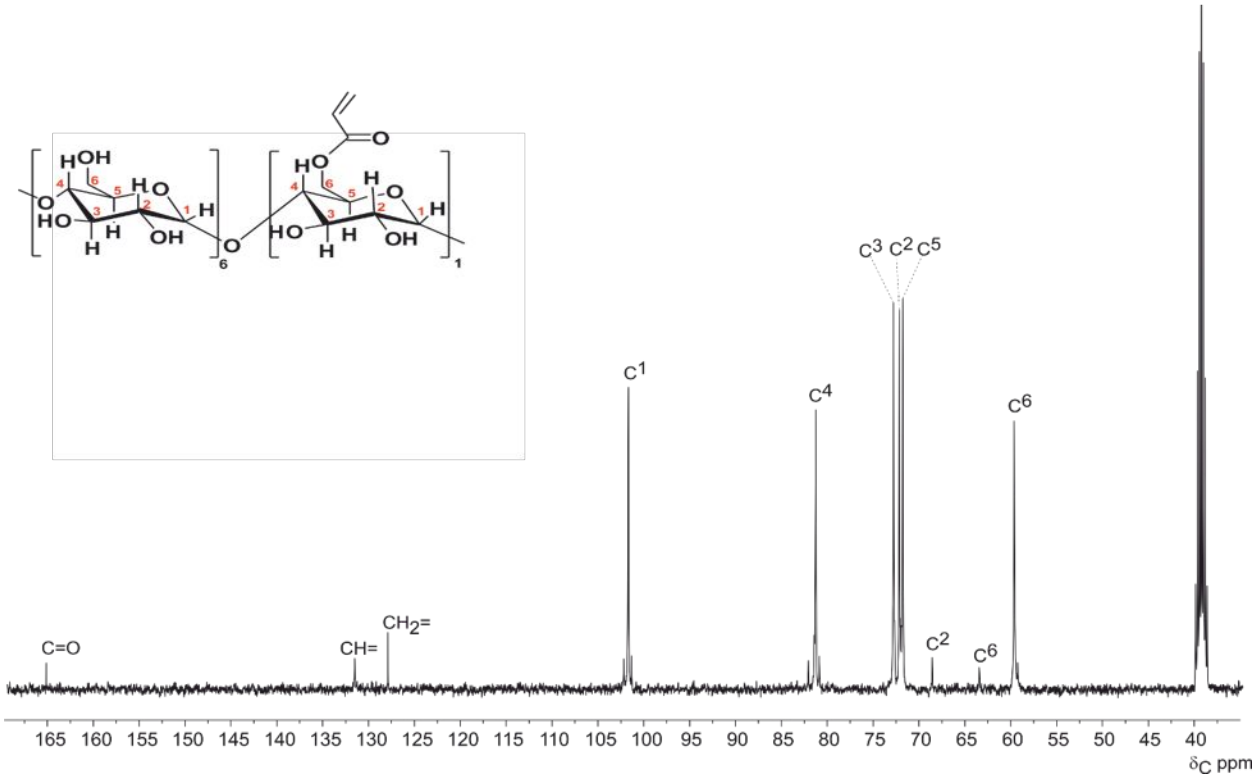
***Corresponding authors:**

T.Abdullin (tabdulli@gmail.com, timur.abdullin@kpfu.ru), R.Garifullin (rigarifullin@kpfu.ru)

A


C3OH
C2OH
H1
C6OH
H3
H6
H4
H5
H2
=CH2B
=CH
=CH2A
C6HA
C6HB
7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0
δ ppm

B


C3 C2 C5
C1
C4
C6
C=O
CH=
CH2=
C2
C6
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40
δC ppm

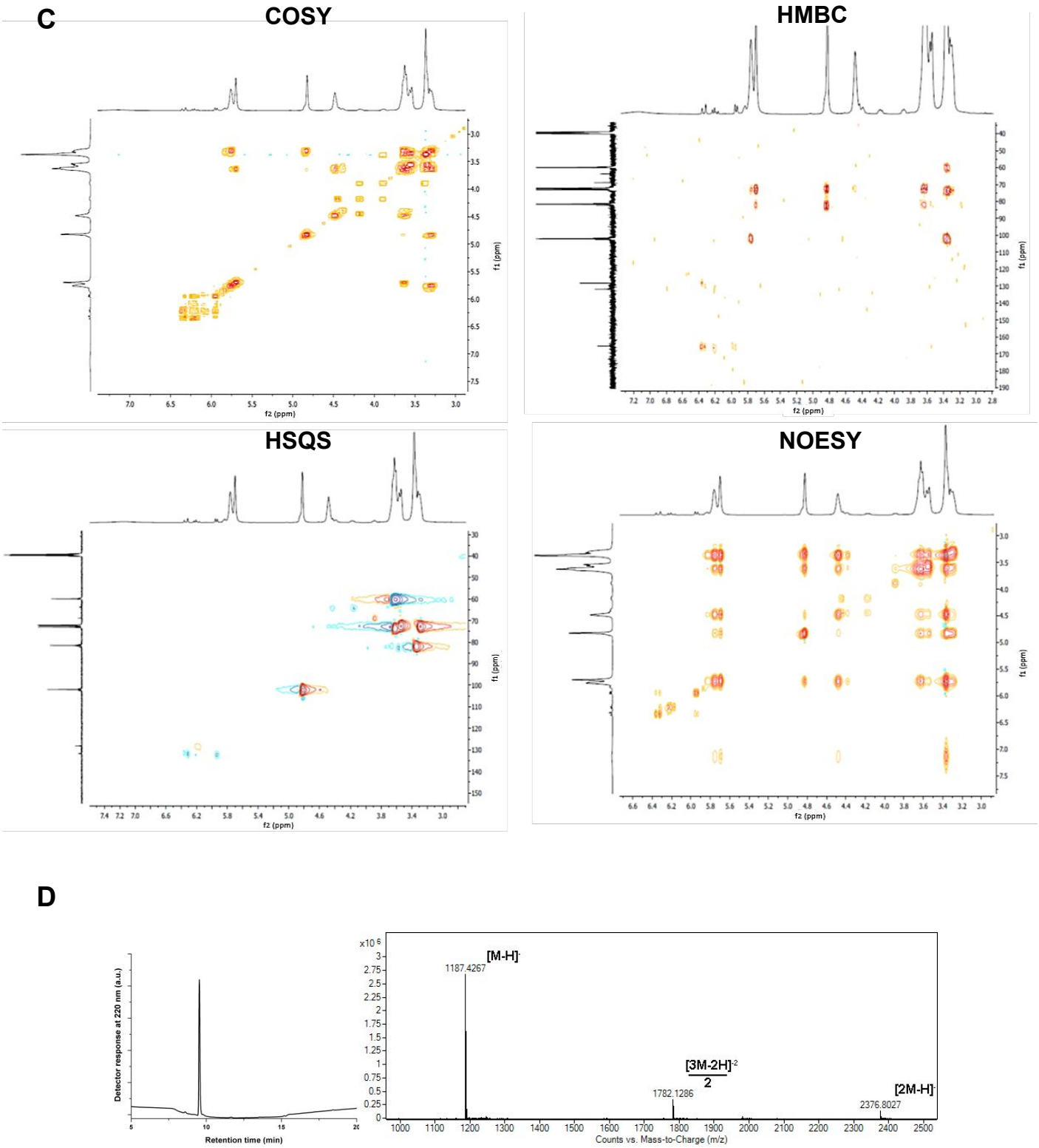


Figure S1. NMR and LC-MS spectra of acryloyl-CD. A. ^{1}H NMR spectrum (400 MHz, DMSO-d_6). The peaks characteristic of the acrylate moiety appeared at chemical shifts range δ: 5.9–6.4 ppm, attributed to CH_2=CH of the methine and methylene protons in the vinyl group. B. ^{13}C NMR spectrum (100.6 MHz, DMSO-d_6). The peaks at 128, 133 and 165 ppm are associated, respectively, with CH_2=, CH= and C=O of the acrylate moiety. C. 2D (COSY, HMBC, HSQS, NOESY) NMR spectra. D. LC-MS spectra of acryloyl-CD.

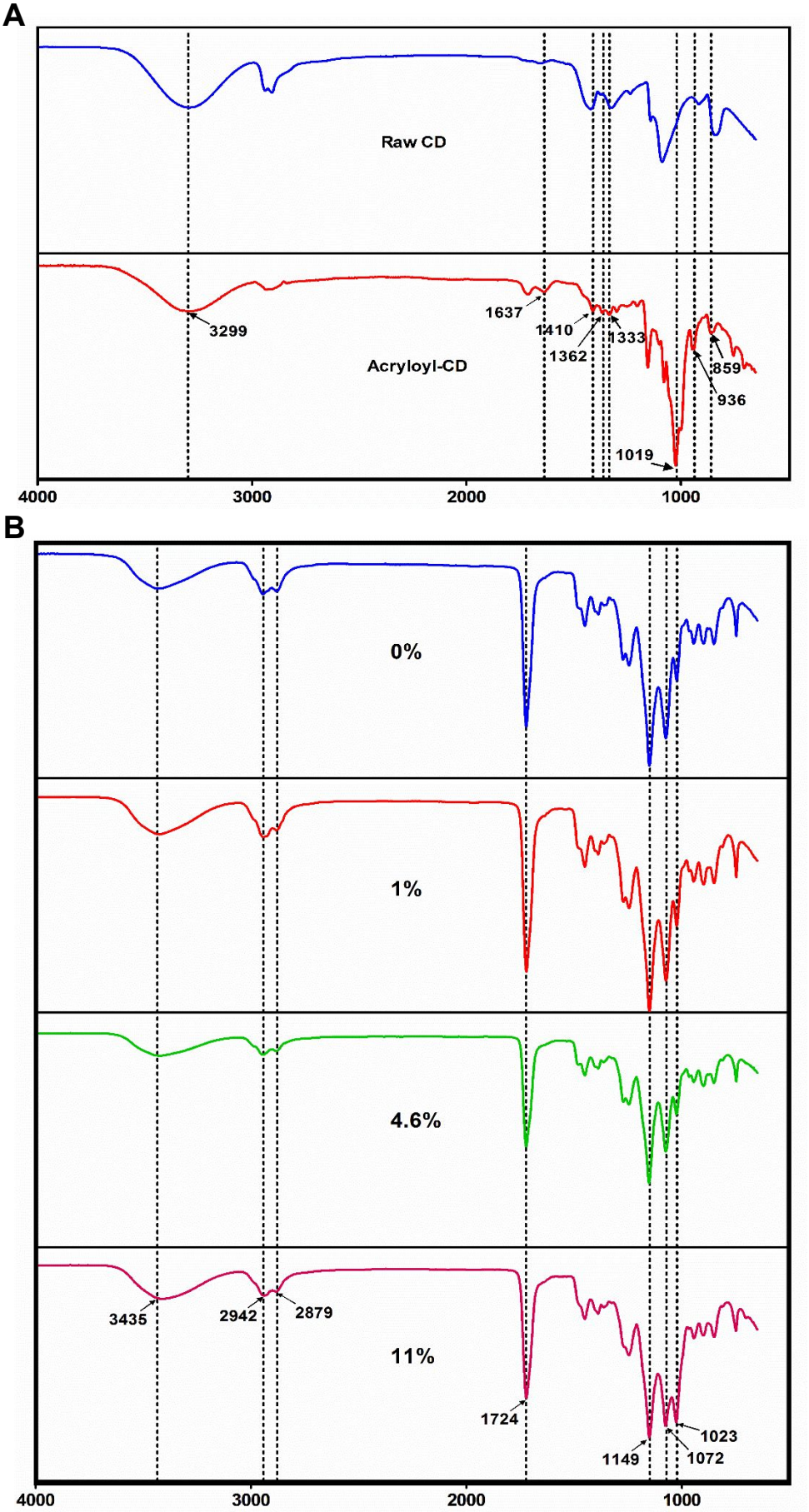


Figure S2. FTIR spectra of (A) β-cyclodextrin (CD)/acryloyl-CD, (B) pHEMA and CD-modified (pHEMA/CD) cryogels prepared with different CD concentrations (0–11%).

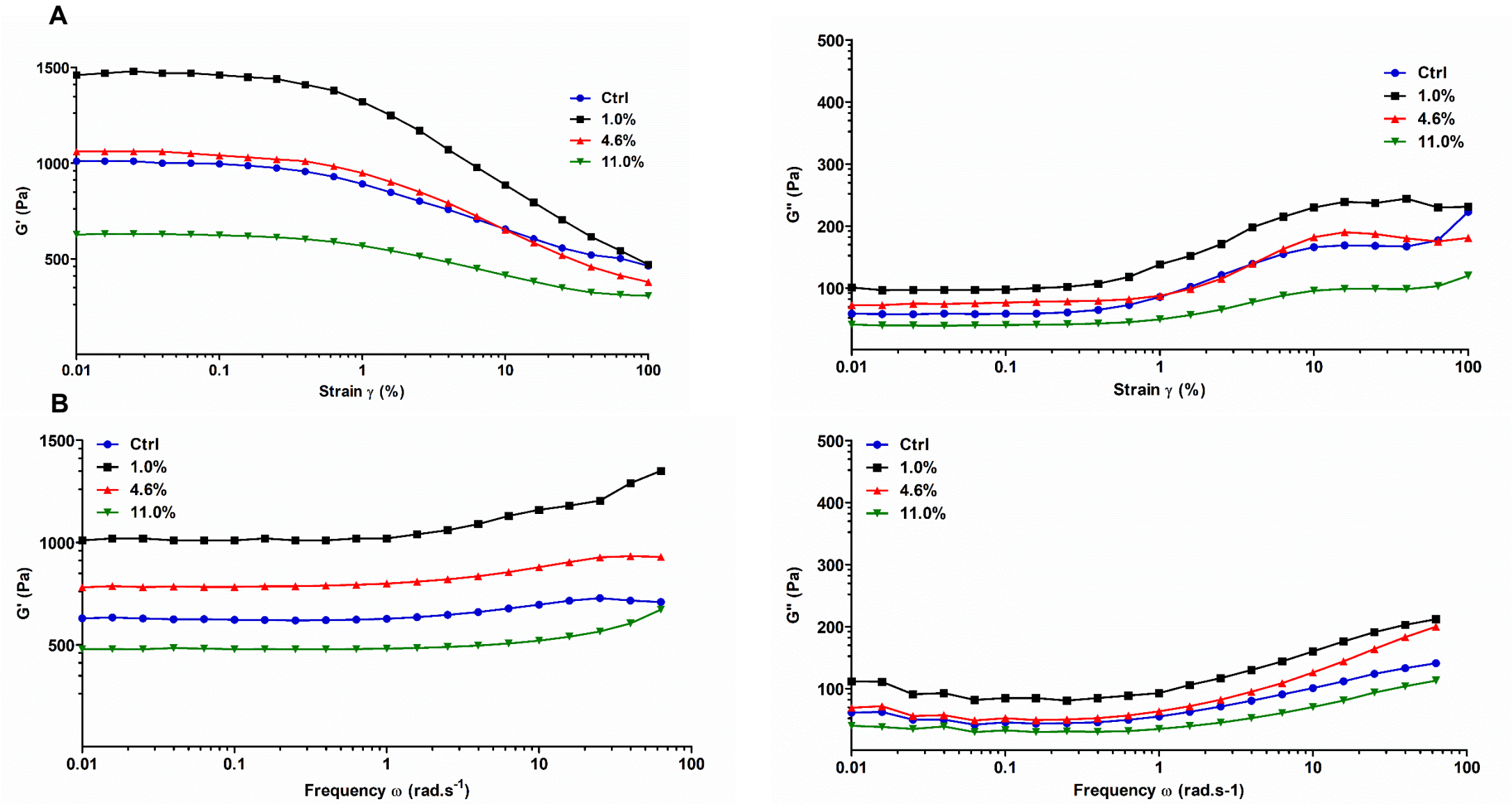


Figure S3. A. Strain amplitude sweep test of the CD-modified pHEMA cryogels. The storage G' and loss G'' moduli are shown as function of strain at angular frequency $\omega = 10$ rad.s^{-1}. B. Frequency sweep test for the same samples. The measurement of frequency dependence of G' and G'' was performed within LVR at δ=1% strain deformation.

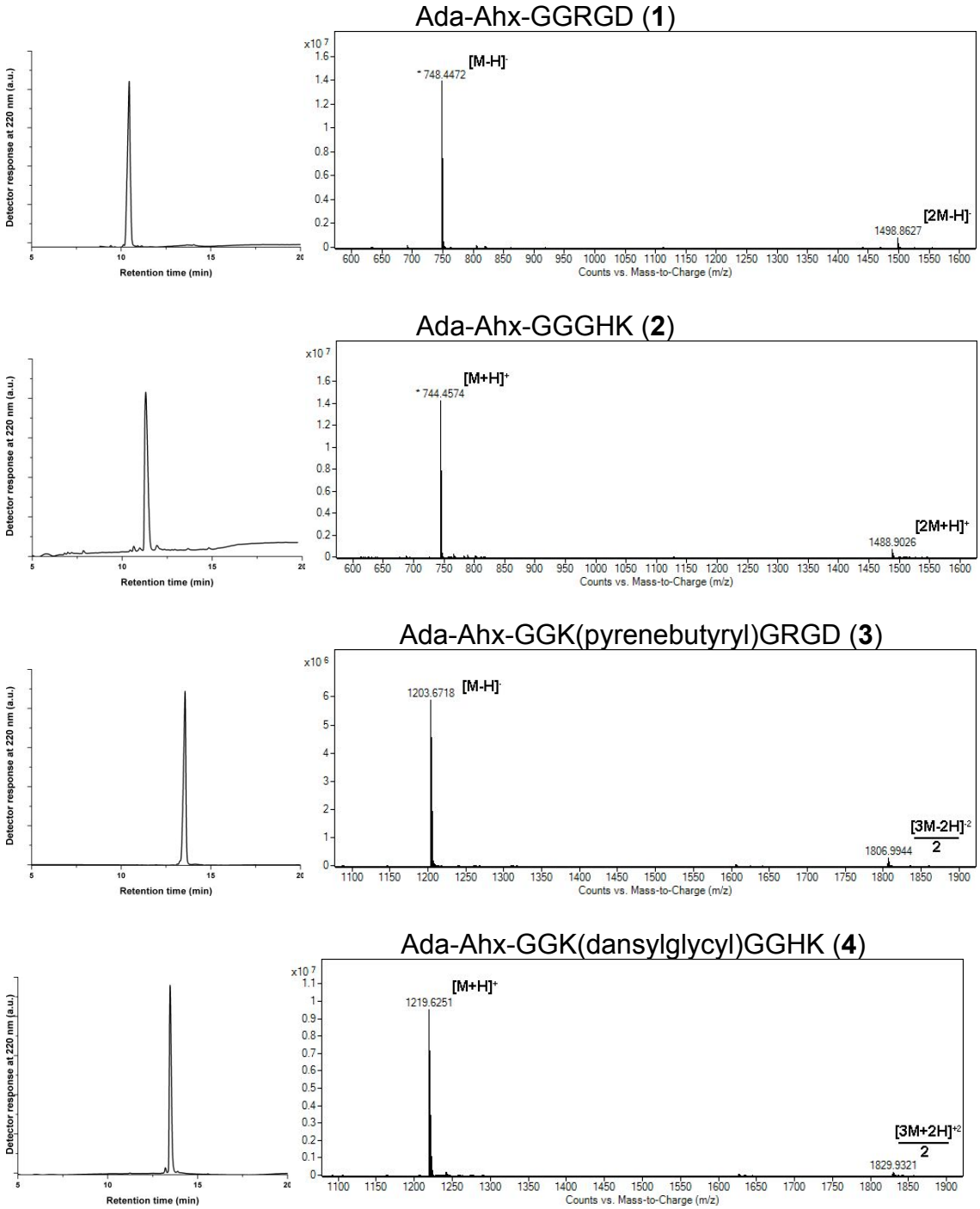


Figure S4. LC-MS spectra of Ada-Ahx-GGRGD (**1**), Ada-Ahx-GGGHK (**2**), Ada-Ahx-GGK(pyrenebutyryl)GRGD (**3**) and Ada-Ahx-GGK(dansylglycyl)GGHK (**4**) peptides.

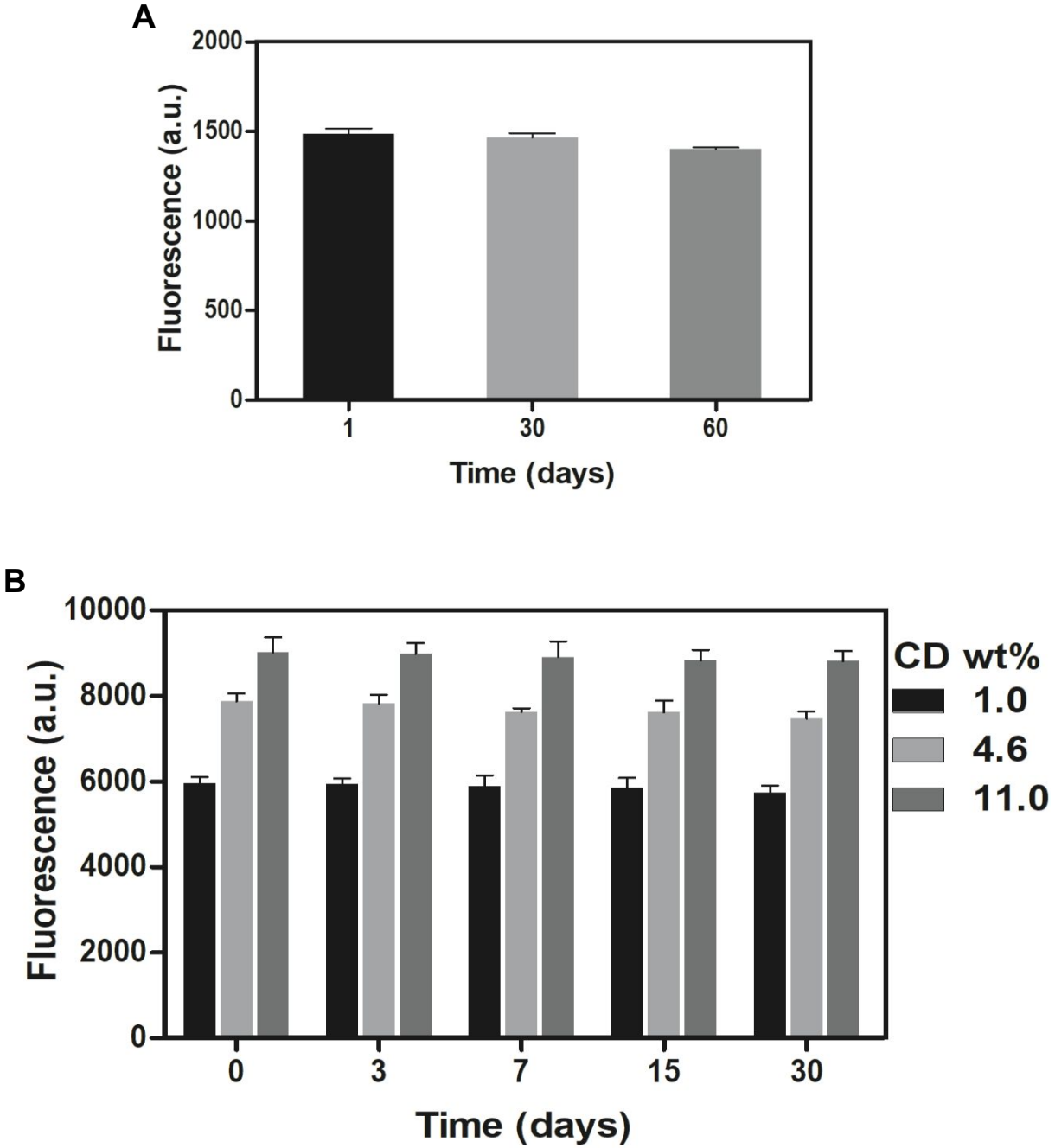


Figure S5. A. Mean fluorescence intensity of modified pHEMA cryogel (4.6% CD) with affinity bound TBO; the material was stored during 60 days followed by staining with TBO. B. Mean fluorescence intensity of CD-modified pHEMA cryogels with affinity bound Ada-Ahx-GGK(pyrenebutyryl)GRGD peptide; the materials functionalization with the peptide was followed by storage during 30 days.