Electronic Supplementary Material (ESI) for Journal of Materials Chemistry B. This journal is © The Royal Society of Chemistry 2014

Brunsveld et al.

Supporting informations

Carborane-beta-cyclodextrin interaction as an efficient strategy to create supramolecular bioactive surface

P. Neirynck, ^a J. Schimer, ^b P. Cigler, ^b P. Jonkheijm, ^c L.-G. Milroy, ^a L. Brunsveld ^a

^a Laboratory of Chemical Biology and Institute of Complex Molecular Systems (ICMS), Department of Biomedical Engineering, Eindhoven University of Technology, Den Dolech 2, 5612 AZ, Eindhoven, The Netherlands Fax: (+31) 40-247-8367; E-mail: I.brunsveld@tue.nl

^b Institute of Organic Chemistry and Biochemistry AS CR, v.v.i., Flemingovo nam. 2, Prague 6, 166 10, Czech Republic, Tel.: +420-220-183-429, Fax: +420-224-310-090, E-mail: cigler@uochb.cas.cz

^c Molecular Nanofabrication Group, MESA⁺ Institute for Nanotechnology, Department of Science and Technology, University of Twente, P.O. Box 217, 7500 AE, Enschede, The Netherlands E-mail: p.jonkheijm@utwente.nl

Telephone: int+31(0)40 247 3737

FAX: int+31(0)40 247 8367

SUPPORTING INFORMATIONS



Figure S1. HRMS of **3**.

Brunsveld et al.

Supporting informations



Figure S2. HRMS of **3** (zoom).

3

Supporting informations



Figure S3. ¹³C NMR of **3** in CD_3CN .

Supporting informations



Figure S4. ¹H NMR of **3** in CD_3CN .

Supporting informations



Figure S5. Analytical HPLC of **3**, R_t = 18.5 min.

Synthesis of cRGD-maleimide 4 and cRAD-maleimide 5



Synthesis of NHS-maleimide linker **10** was carried out following previously described protocol, with a final yield of 43 % after purification.¹

Synthesis of cRGDfK 4' and cRADfK 5' was performed following previously described protocol.²

1 eq of **10** was dissolved together with 1 eq of DIPEA and 1 eq of **4'** or **5'** in DMF:PBS 1:1, pH was adjusted to 7 and reaction was stirred at room temperature for 1 h. Solvents were evaporated and LCMS confirmed the product formation. Product was purified on reverse-phase HPLC equipped with UV detection with a gradient of 10 to 25 % in 20 min, yielding **4** and **5** in respectively 25 and 28 % yield.



Figure S6. LCMS of cRGD-maleimide **4** after purification.



Figure S7. LCMS of carborane-cRGD 6 after purification.



Figure S8. LCMS of carborane-cRAD 7 after purification.