## Efficient microencapsulation of a liquid isocyanate with *in situ* shell functionalization

Le-Thu T. Nguyen,<sup>†,‡</sup> Xander K. D. Hillewaere,<sup>†</sup> Roberto F. A. Teixeira,<sup>†</sup> Otto van den Berg,<sup>†</sup> Filip E. Du Prez<sup>\*,†</sup>

<sup>+</sup> Department of Organic and Macromolecular Chemistry, Polymer Chemistry Research group, Ghent University, Krijgslaan 281 S4, 9000 Gent, and SIM vzw, technologiepark 935, 9052 Zwijnaarde, Belgium

<sup>‡</sup> Department of Polymer Materials, Faculty of Materials Technology, Ho Chi Minh City University of Technology– Vietnam National University, Ly Thuong Kiet 268, District 10, Ho Chi Minh City, Vietnam



## SUPPORTING INFORMATION

Figure S1. Temperature profile applied in the synthesis of microcapsules.



Figure S2. Intensity-concentration Lambert-Beer's law calibration plot of HDI-trimer measured in DMF after solvent signal subtraction.



Figure S3. Intensity-concentration Lambert-Beer 's law calibration plot of MDI-trimer measured in DMF after solvent signal subtraction.

Table S1. Optimal heating time, determined by the shortest reaction time to give well-dispersed stable
microcapsules

Entry	Functionalizing compound	Optimal heating time (min)	Optimal isocyanate core content (%)	Isocyanate core content upon extension of the reaction time for another 5 min (%)	Isocyanate core content after exposure of microcapsules to air at room temperature for one month (%)
1	non-functionalized	20	49	30	15
2	2-ethylhexylamine	20	67	51	62
3	3,4-difluorobenzylamine	15	73	62	68
4	perfluorodecylamine + 2-ethylhexylamine	15	76	69	67
5	3,4-difluorobenzylamine + 2- ethylhexylamine	15	70	59	57
6	HMDS	10	83	62	66



Figure S4. Optical microscopic image of of HDI-trimer containing polyurea microcapsules without shell functionalization in the wet state.



Figure S5. Optical microscopic image of of HDI-trimer containing polyurea microcapsules with shell modification using HMDS in the wet state.



Figure S6. Optical microscopic image of HDI-trimer containing polyurea microcapsules with shell modification using 2-ethylhexylamine in the wet state.



Figure S7. Optical microscopic image of of HDI-trimer containing polyurea microcapsules with shell modification using a 50:50 molar mixture of perfluorodecylamine and 2-ethylhexylamine in the wet state.



Figure S8. Optical microscopic image of of HDI-trimer containing polyurea microcapsules with shell modification using 3,4-difluorobenzylamine in the wet state.



Figure S9. Optical microscopic image of of HDI-trimer containing polyurea microcapsules with shell modification using a 50:50 molar mixture of 3,4-difluorobenzylamine and 2-ethylhexylamine in the wet state.