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High-yielding and scalable method for synthesis of sequence-defined polyurethanes

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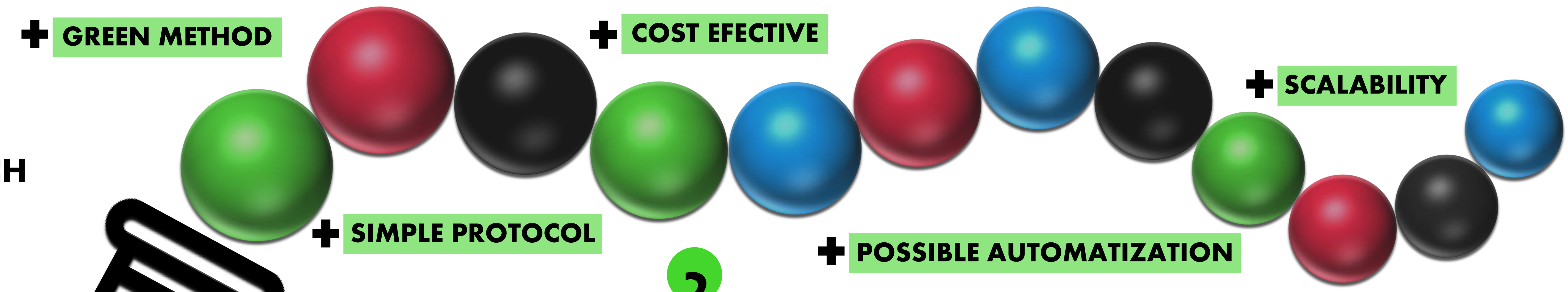
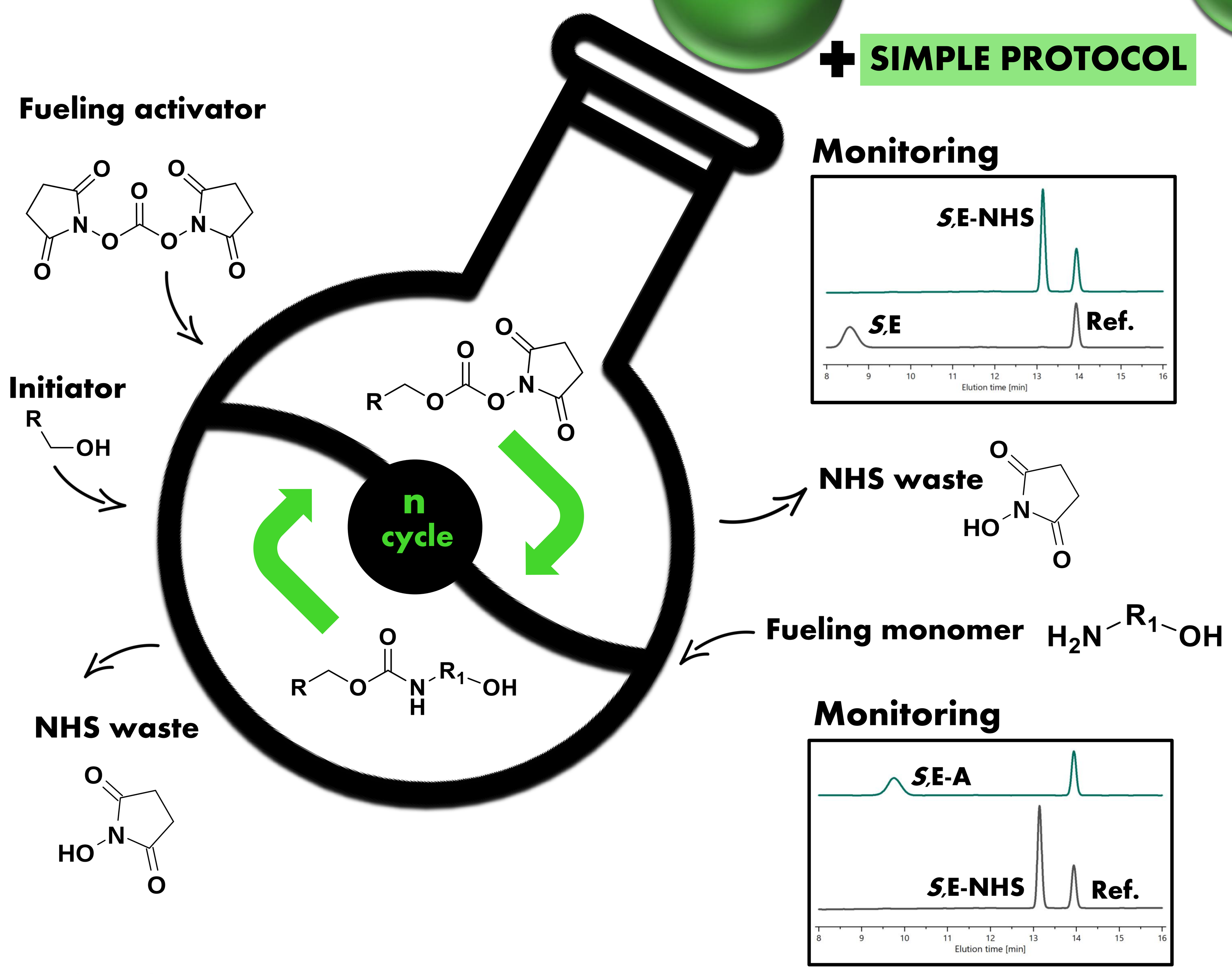
What are the sequence-defined polymers?

Sequence-defined polymers are discrete macromolecules with controlled monomer order. Changing of monomer sequence enables fine-tuning of polymer properties. Therefore, these novel polymers bring new application for materials science [1]. However, available synthesis methods rely on iterative synthesis that have many limitations such as cumbersome protocol, high reagents excess and low overall yield. These difficulties, and especially low yield, make them irrelevant for synthesis of high molar mass polymers[2]. In order to overcome these obstacles we developed the one-pot approach for sequence-defined polyurethanes. High chemoselctivity of applied reactions allows to obtain pure products with high yield [3].



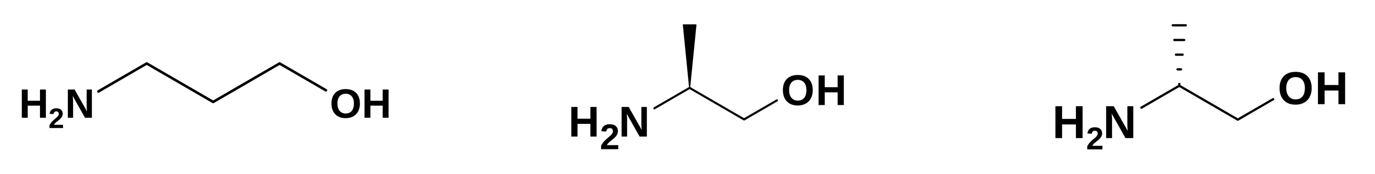
1. REAGENT FUELLED ONE-POT APPROACH



2. SEQUENCE-DEFINED OLIGOURETHANES

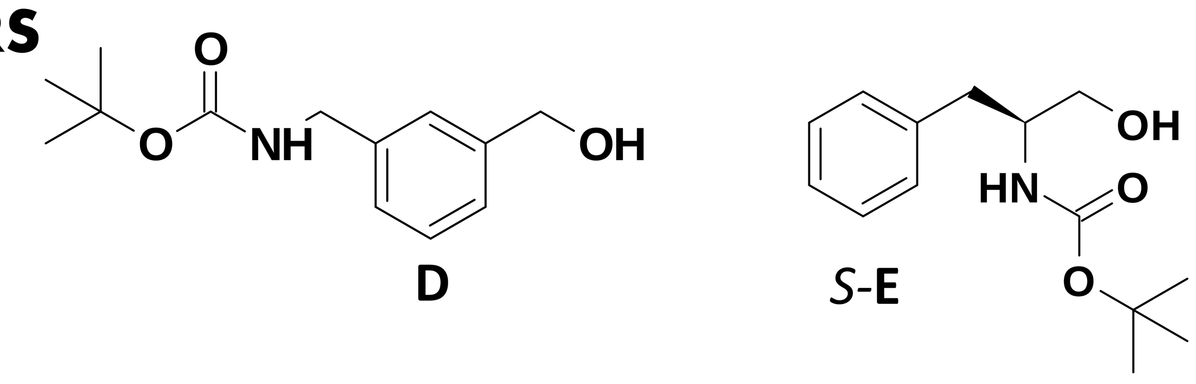
Oligomer	M_{mi}	Purity [%]	Yield [%]	Scale [g]
O1 D-AAAA	641.33	98	72	0.15
O1’ D-AAAA	641.33	99	75	3.80
O2 D-*S*,BAAA	641.33	97	65	0.16
O2’ D-*S*,BAAA	641.33	96	86	1.36
O3 *S*,E-*R*,BAAA	655.34	97	90	4.4
O4 *S*,E-AAAA	**655.34**	**94**	**94**	**50.40**

MONOMERS



A   *S*-B   *R*-B

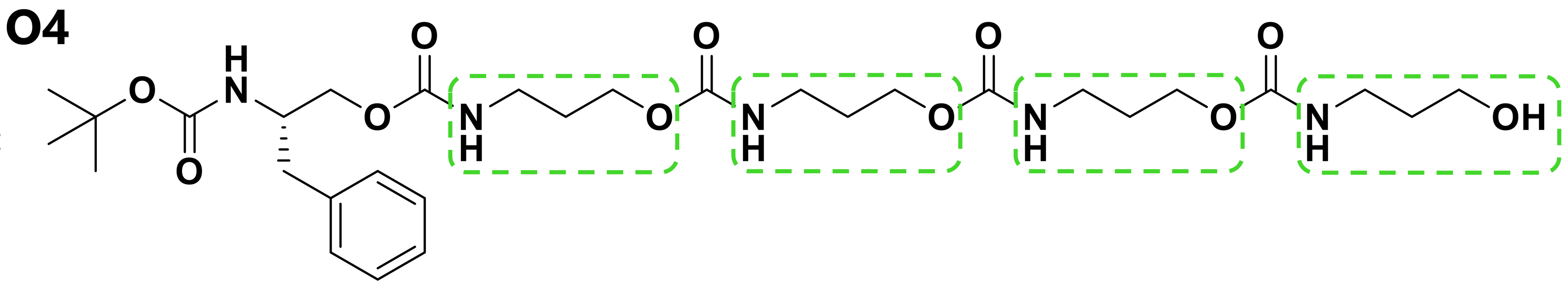
INITIATORS



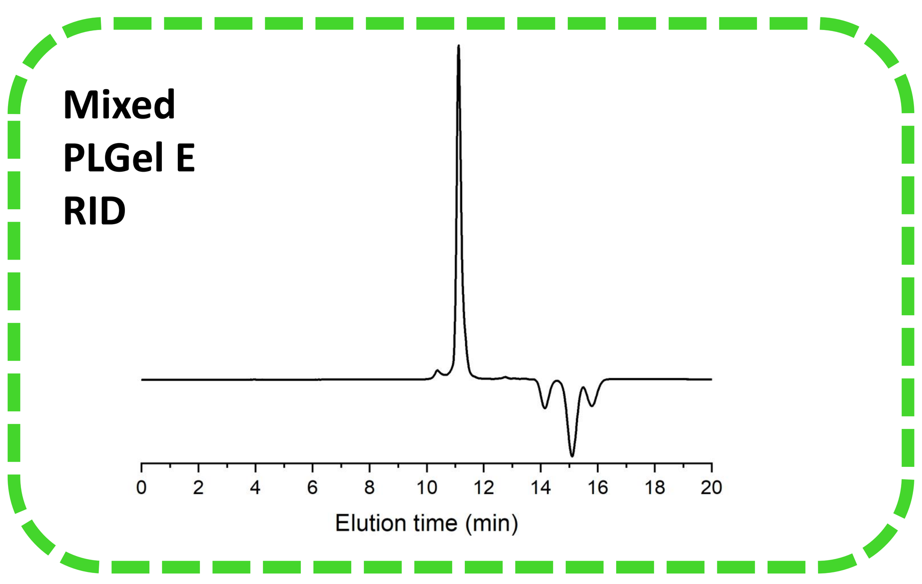
D   *S*-E

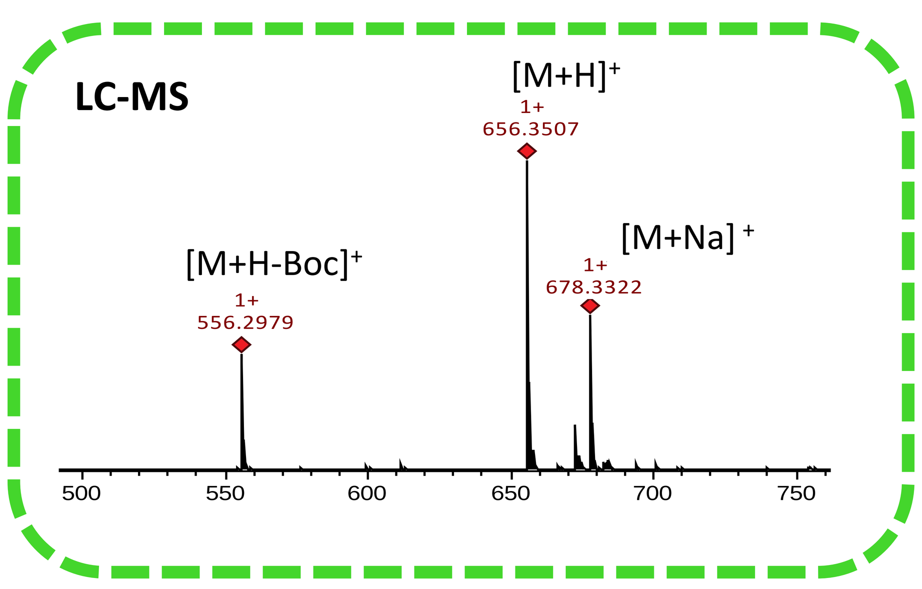
3. CHARACTERIZATION:

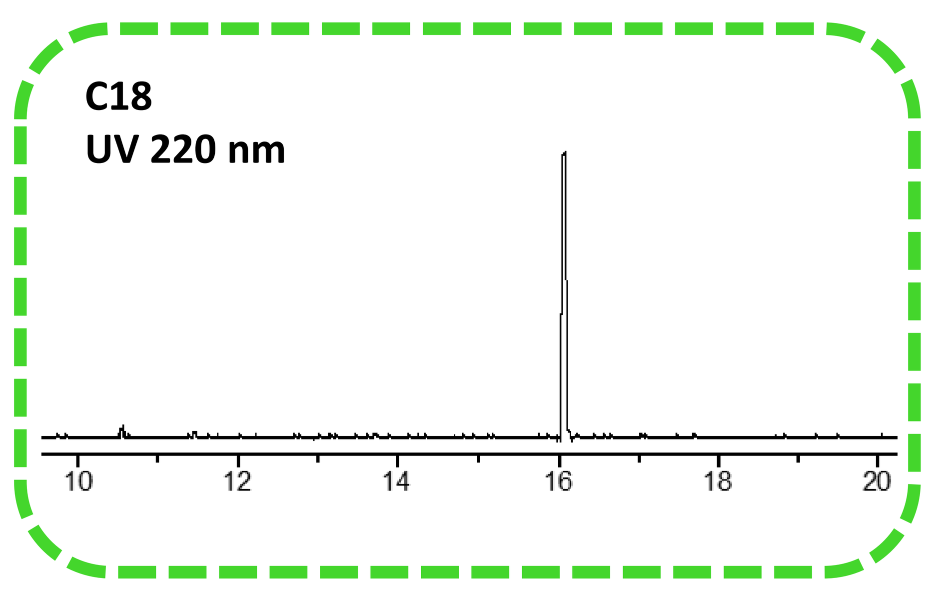
O4



50 g
Y = 94%







4. CONCLUSIONS:

- The one-pot approach for sequence-defined polymers overcomes disadvantages of other methods such as solid-phase and liquid-phase. The most important is scalability (300 times, see oligomer O2 and oligomer O4).
- In the one-pot method there is just one portion of solvent in which a reaction starts so it reduces significantly solvents use.
- Thanks to the reaction is carried out in one vessel there are no yield loss for purification of intermediates.

ACKNOWLEDGEMENT

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[1] E. Laurent, R. Szweda, J.F. Lutz (2022). Synthetic Polymers with Finely Regulated Monomer Sequences: Properties and Emerging Applications. In Macromolecular Engineering (eds N. Hadjichristidis, Y. Gnanou, K. Matyjaszewski and M. Muthukumar).
[2] Aksakal, R., Mertens, C., Soete, M., Badi, N., Du, F., Adv. Sci. 2021, 8, 2004038.
[3] Szweda, R.,Walencik, P., Cwynar, P., Turski, M., no. 2021 PCT/IB2021/057872.