Supplementary Information

Sustainable tailor-made and bio-based high-performance lubricants that combine biorenewability, biodegradability and economic efficiency

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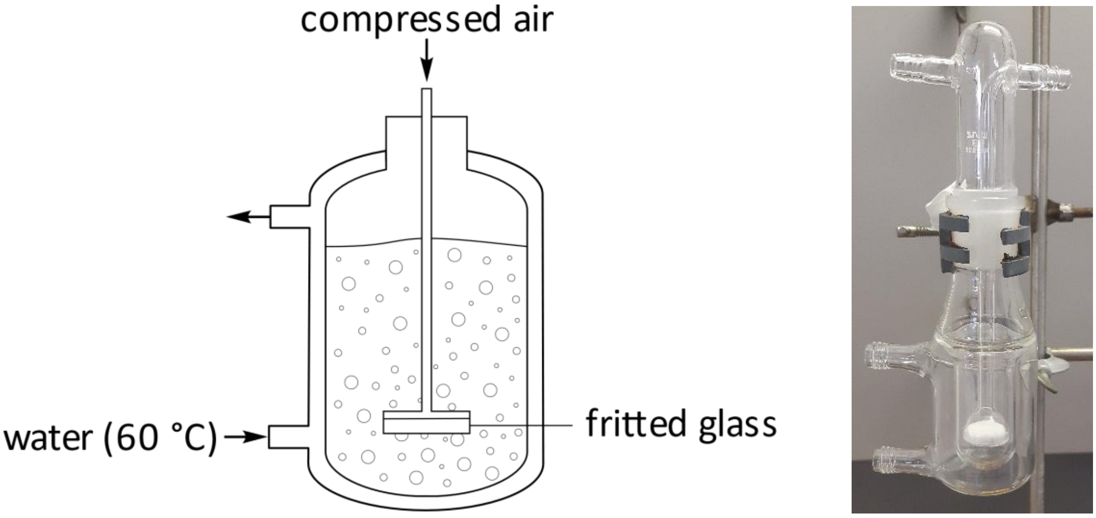
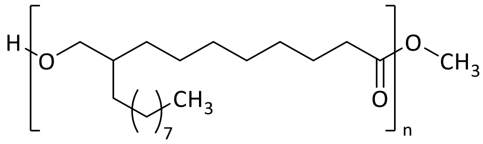
Supplementary Figures



Supplementary Figure 1. Schematic diagram (left) and photo (right) of the designed reactor. All experiments were performed in a double-walled glass reactor heated by a cryostat. Good mixing and expulsion of volatiles was achieved by passing compressed air through the reaction mixture by using a gas wash bottle adapter with a fine-pored glass filter.

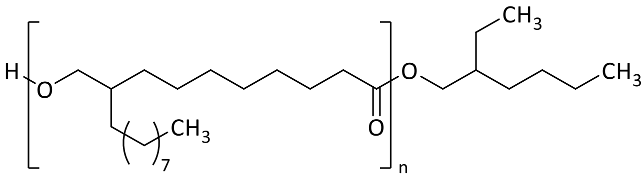
Supplementary Tables

Supplementary Table 1. Chemical-physical properties of oligomers from the oligomerization of hydroxymethylated stearic acid methyl ester.



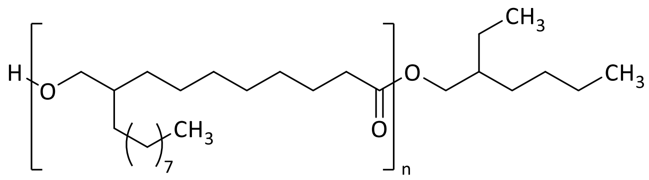
	2 h	4 h	6 h	8 h	24 h
Viscosity at 40 °C [mm^2/s]	94.1	192.2	407.8	459.0	563.9
Viscosity at 100 °C [mm^2/s]	12.7	23.7	46.0	51.4	64.1
Viscosity index	130.7	151.5	171.2	175.4	187.3
Pour point [°C]	−6	−12	−18	−18	−27
Number average molar mass [g/mol]	1048	1562	2290	2370	2459
Oligomerization degree *n*	3.5	5.2	7.7	8.0	8.3

Supplementary Table 2: Chemical-physical properties of oligomers from the oligomerization of hydroxymethylated stearic acid 2-ethylhexyl ester.



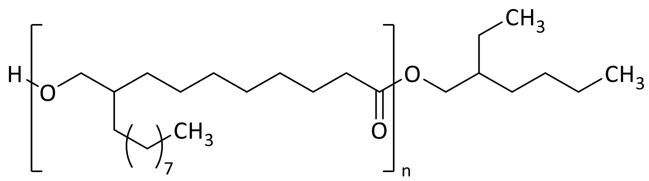
	2 h	4 h	6 h	8 h
Viscosity at 40 °C [mm^2/s]	52.3	56.8	58.1	60.3
Viscosity at 100 °C [mm^2/s]	7.7	8.5	8.6	9.8
Viscosity index	110.5	123.0	121.4	122.1
Pour point [°C]	−24	−27	−27	−27
Number average molar mass [g/mol]	966	854	859	956

Supplementary Table 3: Chemical-physical properties of oligomers from the oligomerization of mixtures of hydroxymethylated stearic acid methyl and 2-ethylhexyl esters.



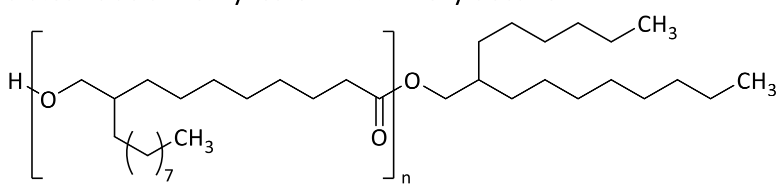
	9:1	7:1	5:1	3:1
Viscosity at 40 °C [mm^2/s]	104.1	105.8	109.0	104.1
Viscosity at 100 °C [mm^2/s]	13.9	14.1	14.6	13.8
Viscosity index	135.0	136.1	138.1	132.8
Pour point [°C]	−9	−15	−15	−15
Number average molar mass [g/mol]	1092	1308	1256	1141

Supplementary Table 4: Chemical-physical properties of oligomers from the oligomerization of hydroxymethylated stearic acid methyl ester with 2-ethylhexanol.



Equivalents of the alcohol	0.05	0.10	0.15	0.20	0.25	0.30
Viscosity at 40 °C [mm^2/s]	127.9	112.4	103.2	96.7	101.7	92.0
Viscosity at 100 °C [mm^2/s]	16.6	14.8	13.7	12.3	13.5	12.4
Viscosity index	139.7	135.2	133.5	131.5	132.4	129.0
Pour point [°C]	−12	−9	−12	−12	−12	−12
Number average molar mass [g/mol]	1261	1172	1136	1106	1151	1097

Supplementary Table 5: Chemical-physical properties of oligomers from the oligomerization of hydroxymethylated stearic acid methyl ester with 2-hexyldecanol.



Equivalents of the alcohol	0.05	0.10	0.15	0.20	0.25	0.30
Viscosity at 40 °C [mm^2/s]	125.3	112.6	110.4	108.9	94.6	78.3
Viscosity at 100 °C [mm^2/s]	16.2	14.8	14.4	14.1	12.4	10.6
Viscosity index	138.1	135.8	132.8	131.1	125.5	119.7
Pour point [°C]	−12	−12	−15	−15	−15	−15
Number average molar mass [g/mol]	1234	1216	1163	1147	1056	958

Supplementary Table 6: Overview of all chemical substrates used, the company where they were purchased and they purity.

Chemical substrate	Company	Purity / %
Hydroxymethylated stearic acid methyl ester	OQ Chemicals	85
Hydroxymethylated stearic acid 2-ethylhexyl ester	OQ Chemicals	88
2-Ethylhexanol	Alfa Aesar	99
2-Hexyldecanol	Sasol Place	96

Supplementary Methods

Calculation of the degree of oligomerization

The degree of oligomerization was calculated according to the following formula:

$$n = \frac{\mathrm{M_n} - \mathrm{M_{end\ group}}}{\mathrm{M_{repetitive\ unit}}}$$

Thereby *n* is the degree of oligomerization, M_n is the number average molar mass, $M_{end\ group}$ is the molar mass of the end group (15 g/mol) and $M_{repetitive\ unit}$ is the molar mass of the repetitive unit (296 g/mol).

OECD 301 F test

OECD 301 F test was performed according to the standard OECD 301 F with Fima OxiTop-C sensor heads (Xylem Analytics Germany Sales GmbH & Co. KG, Weilheim, Germany). For the OECD 301 F test, an inoculum is required. Inoculum is a liquid from an aeration tank of a municipal wastewater treatment plant. This liquid was diluted (100 mL/L nutrient solution) and adjusted to a pH of 7.4. The nutrient solution (164 mL) and the sample (approx. 6 mg) are then placed in a bottle. The bottle is enriched with NaOH and then hermetically sealed with the measuring heads. When the sample is degraded by the bacteria, oxygen is bound and CO_2 is released, which binds to the NaOH. This creates a negative pressure in the bottles, which is detected by the measuring heads. For evaluation, it is calculated how much oxygen would be consumed in the case of complete degradation and this is compared with the oxygen actually consumed. This results in the biodegradability in percent.