Supplementary materials to the article “Scale-up of the downstream process for polyhydroxyalkanoate copolymer P(HB-co-HHx) extraction with nonhalogenated solvents” (Thiele I., Rose J.H., Gutschmann B., Tofaily S., Schöttel J., Widmer T., Neubauer P., Grimm T., Riedel S.L.) published in “Journal of Siberian Federal University. Biology” (DOI: 10.17516/1997-1389-0364)

Приложение к статье “Масштабирование процесса экстракции сополимера П(ГБ-со-ГГ) негалогенированными растворителями” И. Тиле, Я.Х. Роуз, Б. Гутчманн, С. Тофайли, Д. Шеттель, Т. Видмер, П. Нойбауэр, Т. Гримм, С.Л. Ридель

The recovery was performed on different lyophilized cell material (Batch 1, Batch 2, and Batch 3). The batches from different cultivations had different PHA contents of 76.1, 81.1, or 70 % with 16.1, 19.2 or 17.1 mol% HHx content, respectively.

Supplementary Table 1. Overview over recovery conditions, purity, HHx-content and molecular weight characteristics of the PHA recovered from Batch1

Batch 1									
	50 °C				55 °C				
evaporated acetone [%]	50	43.3	43.3	49.8	50.9	50	50	49.7	50
final concentration [2-propanol]	80	77.9	77.9	76.9	81	80	80	81.7	80
Drying	vacuumpot / freezedried	vacuumpot / freezedried	vacuumpot / freezedried	vacuumpot / freezedried	freezedried	freezedried	vacuumpot / freezedried	vacuumpot	vacuumpot
Recovery yield [%]	65	51	71	76	78	68	76	75	77
PHA [%]	98.6 ± 1.6	94.7 ± 2.0	92.1 ± 1.0	96.7 ± 1.1	92.6 ± 0.7	97.38 ± 2.54	89.65 ± 1.1	92.79 ± 2.3	92.09 ± 1.0
HHx [mol%]	17.1 ± 0.3	16.6 ± 0.1	16.0 ± 0.1	13.1 ± 0.03	14.1 ± 0.6	15.2 ± 0.3	16.5 ± 0.1	16.9 ± 0.2	17.4 ± 0.1
M_w [Da] × 10^5	2.07 ± 0.08	1.88 ± 0.02	2.06 ± 0.03	2.02 ± 0.01	2.04 ± 0.04	1.90 ± 0.01	1.99 ±0.00	2.08 ± 0.05	2.09 ± 0.02
M_n [Da] × 10^5	0.93 ± 0.14	0.79 ± 0.01	0.87 ± 0.03	0.86 ± 0.02	0.83 ± 0.01	0.84 ± 0.01	0.89 ± 0.02	0.82 ± 0.03	0.87 ± 0.04
Đ [-]	2.27 ± 0.26	2.39 ± 0.07	2.36 ± 0.04	2.34 ± 0.03	2.45 ± 0.01	2.26 ± 0.03	2.24 ± 0.06	2.54 ± 0.04	2.42 ± 0.08
sample#	B1.1	B1.2	B1.3	B1.4	B1.5	B1.6	B1.7	B1.8	B1.9

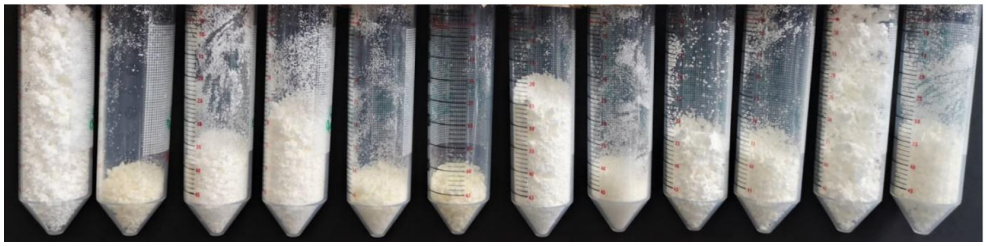
Supplementary Table 2. Overview over recovery conditions, purity, HHx-content and molecular weight characteristics of the PHA recovered from Batch 2

Batch 2												
	30 °C			40 °C				50 °C			58 °C	
evaporated acetone [%]	60.7	59	50	58.8	59.9	39.8	68.3	58.3	58.3	58.3	58.7	47.2
final concentration [2-propanol]	83.6	83.2	80	82.9	86.2	73.7	88	75	75	75	82.8	79.2
Drying	50°C	50°C	50°C	50°C	50°C	50°C	50°C	50°C	50°C	50°C	50°C	50°C
Recovery yield [%]	61	49	66	70	63	58	77	66	69	66	78	68
PHA [%]	94.9 ± 6.6	90.5 ± 1.7	99.5 ± 7.2	87.9 ± 2.6	90.3 ± 3.4	96.2 ± 0.4	94.2 ± 1.5	99.7 ± 1.8	99.3 ± 0.5	96.0 ± 0.6	96.8 ± 7.7	99.2 ± 5.3
HHx [mol%]	19.7 ± 0.5	16.9 ± 0.1	17.2 ± 0.3	18.4 ± 0.2	16.4 ± 0.2	14.9 ± 0.2	17.1 ± 0.4	15.6 ± 0.1	16.2 ± 0.2	15.8 ± 0.1	18.3 ± 0.1	14.2 ± 0.2
M_w [Da] × 10^5	2.68 ± 0.04	2.70 ± 0.04	2.77 ± 0.02	2.75 ± 0.01	2.70 ± 0.05	3.61 ± 1.05	2.70 ± 0.01	2.75 ± 0.02	2.86 ± 0.04	2.79 ± 0.04	2.70 ± 0.01	2.73
M_n [Da] × 10^5	1.12 ± 0.05	1.20 ± 0.01	1.26 ± 0.02	1.14 ± 0.04	1.26 ± 0.02	2.50 ± 1.32	1.06 ± 0.07	1.24 ± 0.02	1.21 ± 0.13	1.26 ± 0.01	1.16 ± 0.04	1.23
Đ [-]	2.39 ± 0.07	2.25 ± 0.01	2.19 ± 0.01	2.42 ± 0.07	2.15 ± 0.06	1.69 ± 0.48	2.56 ± 0.15	2.23 ± 0.02	2.39 ± 0.22	2.22 ± 0.01	2.33 ± 0.08	2.21
sample#	B2.1	B2.2	B2.3	B2.4	B2.5	B2.6	B2.7	B2.8	B2.9	B2.10	B2.11	B2.12

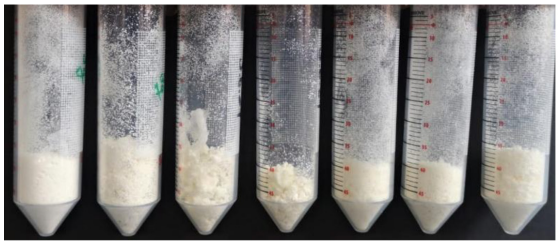
Supplementary Table 3. Overview over recovery conditions, purity, HHx-content and molecular weight characteristics of the PHA recovered from Batch 3

	Batch 3						
	40 °C		50 °C				
evaporated acetone [%]	50.9	57.4	53.2	33.4	58.2	49.9	49.3
final concentration [2-propanol]	80.4	82.5	81	80	80	70	90.2
Drying	50 °C	50 °C	60 °C	60 °C	60 °C	50 °C	50 °C
Recovery yield	67	67	74	74	76	73	78
PHA [%]	95.4 ± 1.3	90.0 ± 3.9	104.3 ± 10.4	94.9 ± 3.2	88.9 ± 0.7	99.9 ± 6.9	102.0 ± 11.8
HHx [mol%]	15.2 ± 0.1	15.3 ± 0.3	14.6 ± 0.1	14.4 ± 0.6	13.7 ± 0.1	13.6 ± 0.3	13.7 ± 0.1
M_w [Da] × 10^5	2.74 ± 0.01	2.84 ± 0.02	n.a.	n.a.	n.a.	n.a.	n.a.
M_n [Da] × 10^5	1.08 ± 0.04	1.11 ± 0.02	n.a.	n.a.	n.a.	n.a.	n.a.
Đ [-]	2.54 ± 0.09	2.55 ± 0.03	n.a.	n.a.	n.a.	n.a.	n.a.
sample#	B3.1	B3.2	B3.3	B3.4	B3.5	B3.6	B3.7

Supplementary Figure 1. Recovered PHA from lyophilized cells from Batch1. B1.1 – B1.9



Supplementary Figure 2. Recovered PHA from lyophilized cells from Batch2. B2.1 – B2.12



Supplementary Figure 3. Recovered PHA from lyophilized cells from Batch3. B3.1 – B3.7