

Supporting Information

Preparation of efficient oligomer-based bulk-heterojunction solar cells with eco-friendly solvents

Duško Popović,^a Ibrahim Ata,^a Johannes Krantz,^a Sebastian Lucas,^a Mika Lindén,^b Elena Mena-Osteritz^a and Peter Bäuerle^{a*}

^aInstitute of Organic Chemistry II and Advanced Materials, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany

^bInstitute of Inorganic Chemistry II, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany

*E-mail: peter.baeuerle@uni-ulm.de

Table S1. Overview of reported oligomer-based BHJSC with the respectively obtained PCEs using various halogen-free solvents.

Solvent	Blend	PCE [%]	Reference
Tetrahydrofuran	SM:PC ₇₁ BM	2.65	[1]
Benzaldehyde/mesitylene (80:20)	N(Ph-2T-DCN-Et)/PC ₇₁ BM	3.75	[2]
2-Methyltetrahydrofuran	X2:PC ₆₁ BC ₈	5.10	[3]
<i>o</i> -Xylene + 1% MN	DPPEZnP-O:PC ₆₁ BM	5.85	[4]
Toluene	SMPV1:PC ₇₁ BM	7.04	[5]
Toluene/CPME (40:60)	SMPV1:PC ₆₁ BM	8.10	[6]
Carbon disulfide	BDTTNTTR: PC ₇₁ BM	10.02	[7]
Carbon disulfide	BDTSTNTTR: PC ₇₁ BM	11.53	[7]

Table S2. Solubility parameters and melting temperatures of co-oligomers **1-3** investigated in this study.

Oligomer	Solubility in chloroform [mg mL ⁻¹]	Solubility in ethyl acetate [mg mL ⁻¹]	Solubility in toluene [mg mL ⁻¹]	Solubility in <i>o</i> -xylene [mg mL ⁻¹]	T _m [°C] ^a
1	15	7	2	>80	181
2	>120 ^b	3	<1	26	183 ^b

3	>80 ^c	3	<1	16	174 ^c
---	------------------	---	----	----	------------------

^aMelting temperatures (T_m) were determined using differential scanning calorimetry. ^bsee ref. 8. ^csee ref. 9.

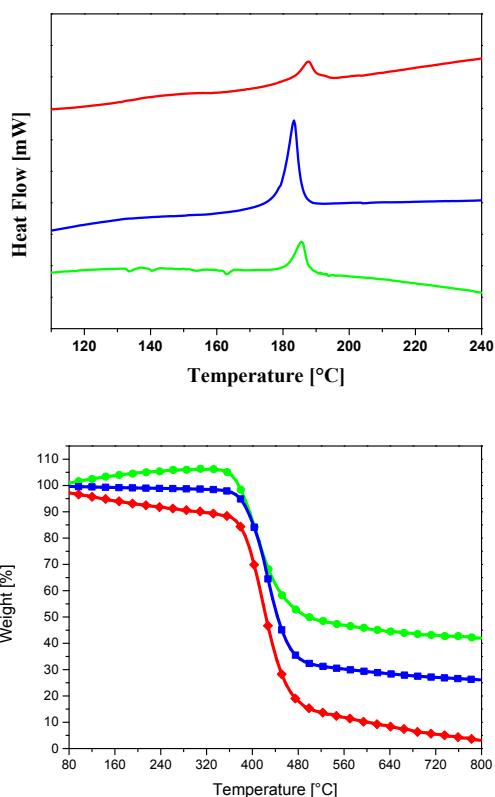


Figure S1. TGA and DSC traces of oligomers **1** (green curve), **2** (blue curve), and **3** (red curve).

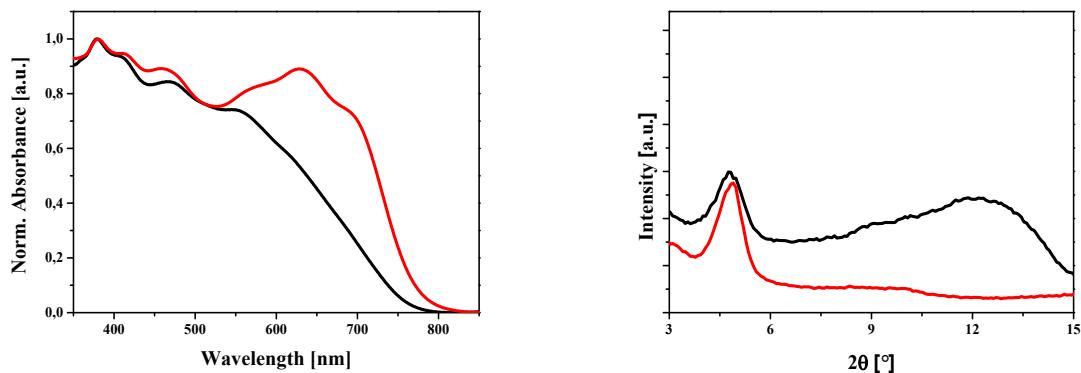


Figure S2. Absorption spectra (left) and GIXRD diffraction patterns (right) of blends containing co-oligomer **2** and PC₇₁BM (1:2) before (black line) and after SVA (red line). The film was deposited by doctor-blading on a PEDOT:PSS coated glass substrate.

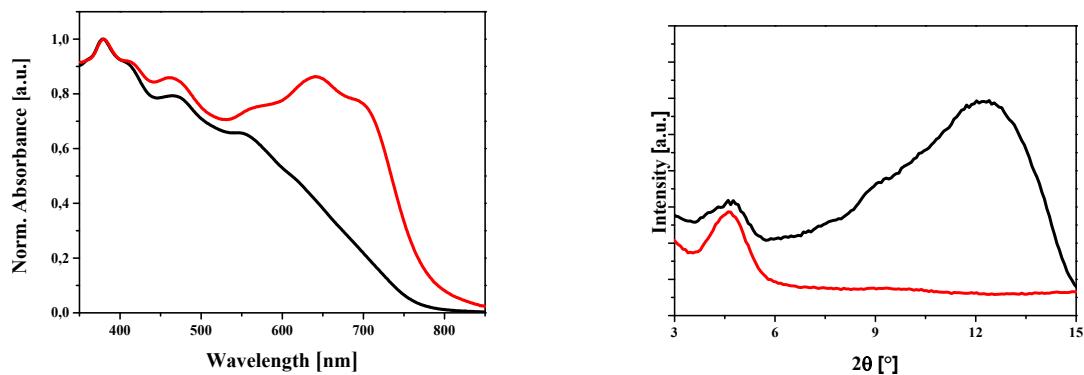


Figure S3. Absorption spectra (left) and GIXRD diffraction patterns (right) of blends containing co-oligomer **3** and PC₇₁BM (1:2) before (black line) and after SVA (red line). The film was deposited by doctor-blading on a PEDOT:PSS coated glass substrate.

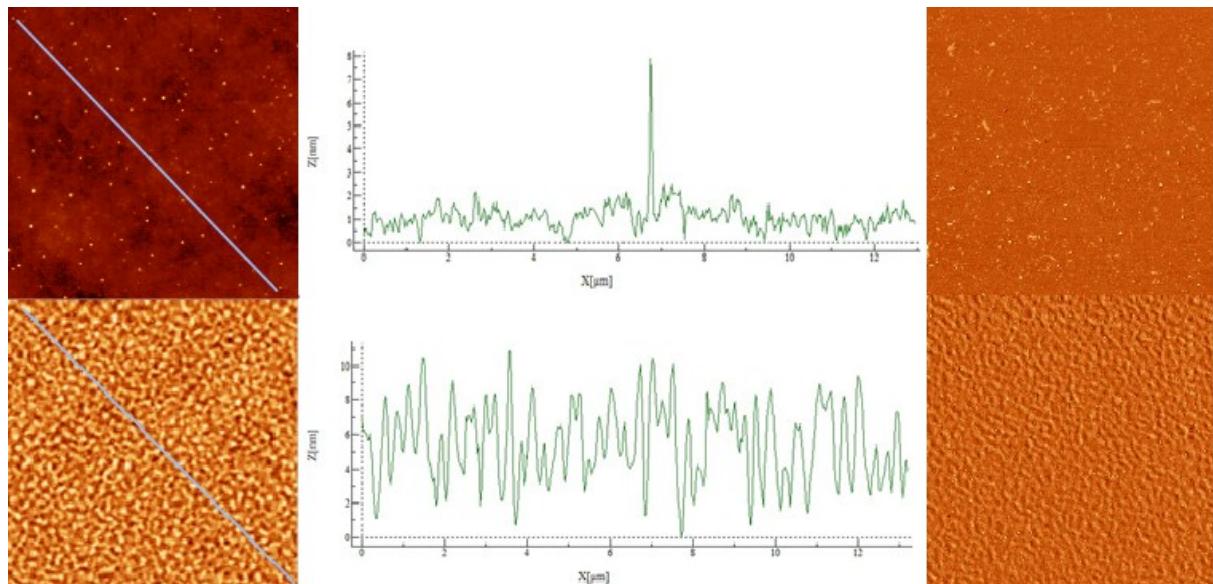


Figure S4. AFM images ($10 \times 10 \mu\text{m}^2$) of the topography ($\Delta z = 10 \text{ nm}$), height profile, and phase ($\Delta\theta = 20^\circ$) of the photoactive blend of **1**:PC₇₁BM deposited by doctor-blading on PEDOT:PSS|glass before (top) and after (bottom) SVA. The average roughness before and after SVA treatment were determined to be 0.55 nm and 1.76 nm, respectively.

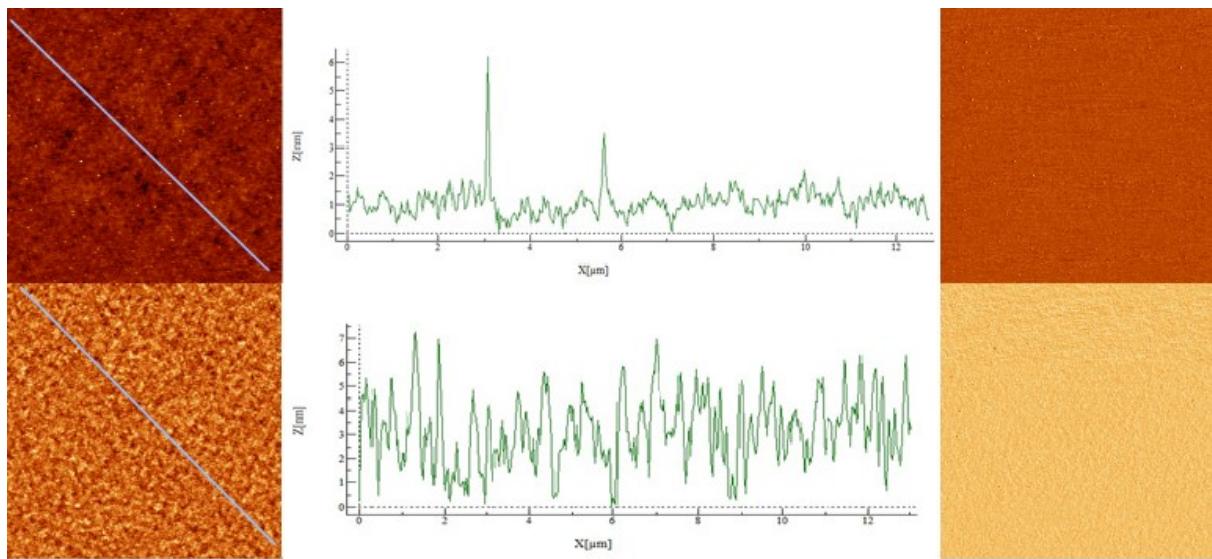


Figure S5. AFM images ($10 \times 10 \mu\text{m}^2$) of the topography ($\Delta z = 10 \text{ nm}$), height profile, and phase ($\Delta\theta = 20^\circ$) of the photoactive blend of **2**:PC₇₁BM deposited by doctor-blading on PEDOT:PSS|glass before (top) and after (bottom) SVA. The average roughness before and after SVA treatment were determined to be 0.31 nm and 1.10 nm, respectively.

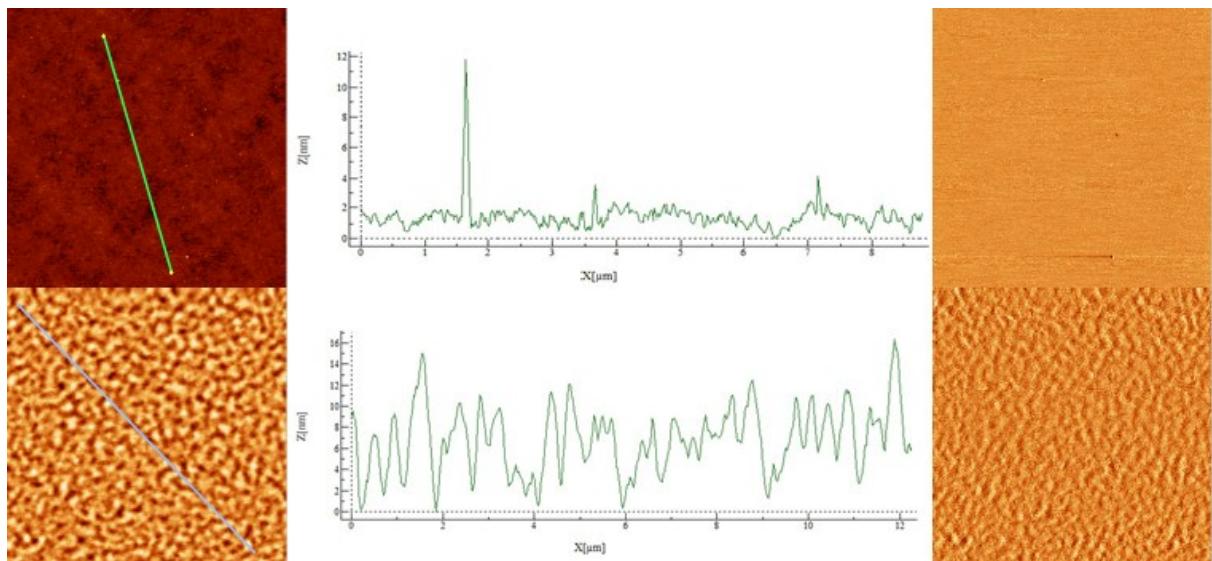


Figure S6. AFM images ($10 \times 10 \mu\text{m}^2$) of the topography ($\Delta z=10 \text{ nm}$), height profile, and phase ($\Delta\theta = 20^\circ$) of the photoactive blend of **3**:PC₇₁BM deposited by doctor-blading on PEDOT:PSS|glass before (top) and after (bottom) SVA. The average roughness before and after SVA treatment were determined to be 0.30 nm and 2.19 nm, respectively.

References

1. M. Singh, R. Kurchania, J. A. Mikroyannidis, S. S. Sharma and G. D. Sharma, *J. Mater. Chem. A*, 2013, **1**, 2297-2306.
2. I. Burgués-Ceballos, F. Machui, J. Min, T. Ameri, M. M. Voigt, Y. N. Luponosov, S. A. Ponomarenko, P. D. Lacharmoise, M. Campoy-Quiles and C. J. Brabec, *Adv. Funct. Mater.*, 2014, **24**, 1449-1457.

3. X. Chen, X. Liu, M. A. Burgers, Y. Huang and G. C. Bazan, *Angew. Chem. Int. Ed.*, 2014, **53**, 14378-14381.
4. L. Xiao, C. Liu, K. Gao, Y. Yan, J. Peng, Y. Cao and X. Peng, *RSC Adv.*, 2015, **5**, 92312-92317.
5. M. E. Farahat, C.-S. Tsao, Y.-C. Huang, S. H. Chang, W. Budiawan, C.-G. Wu and C.-W. Chu, *J. Mater. Chem. A*, 2016, **4**, 7341-7351.
6. M. E. Farahat, P. Perumal, W. Budiawan, Y.-F. Chen, C.-H. Lee and C.-W. Chu, *J. Mater. Chem. A*, 2017, **5**, 571-582.
7. J. Wan, X. Xu, G. Zhang, Y. Li, K. Feng and Q. Peng, *Energy Environ. Sci.*, 2017, **10**, 1739-1745,
8. I. Ata, S. B. Dkhil, M. Pfannmöller, S. Bals, D. Duché, J.-J. Simon, T. Koganezawa, N. Yoshimoto C. Videlot-Ackermann, O. Margeat, J. Ackermann and P. Bäuerle, *Org. Chem. Front.* (submitted 21.3.2017, QO-RES-03-2017-000222)
9. C. D. Wessendorf, G. L. Schulz, A. Mishra. P. Kar, I. Ata, M. Weidelener, M. Urdanpilleta, J. Hanisch, E. Mena-Osteritz, M. Lindén, E. Ahlswede and P. Bäuerle, *Adv. Energy Mater.*, 2014, **4**, 1400266-1400276.