Supplementary Information

for

Poly(butylene 2,4-furanoate), an added member to the class of smart furan-based polyesters for sustainable packaging: structural isomerism as a key to tune the final properties

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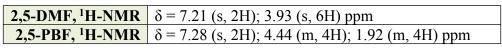
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 35 Figures



Scheme S1. 2,5-PBF. a: as-synthesized; b: purified; c, top: amorphous film; c, bottom: annealed film.

Table S1. Results of the ¹H-NMR analysis on dimethyl 2,5-furandicarboxylate (2,5-DMF) and 2,5-poly(butylene furanoate) (2,5-PBF).



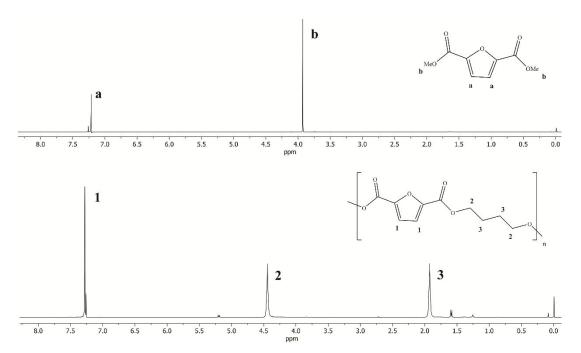


Figure S1. ¹H-NMR spectra of dimethyl 2,5-furandicarboxylate (top) and 2,5-poly(butylene furanoate) (bottom).

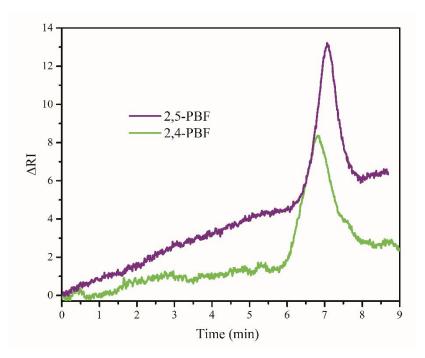


Figure S2. Results of the GPC analysis on 2,4-PBF and 2,5-PBF. ΔRI is the measured difference in refractive index.

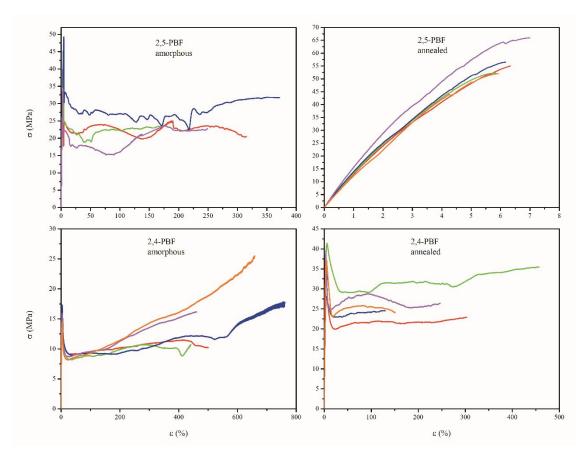


Figure S3. Stress-strain curves of amorphous and annealed 2,5-PBF and 2,4-PBF. Colors are meant to differentiate each curve from the others.

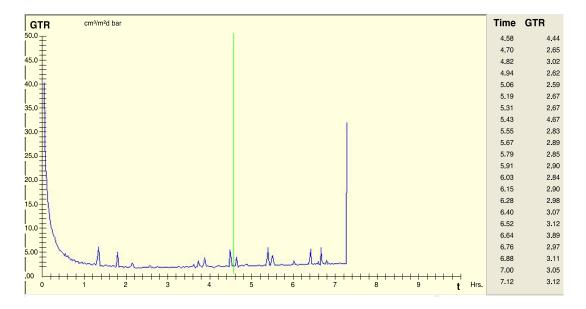


Figure S4. GTR vs. time graph on amorphous 2,5-PBF (O_2 -GTR, 23°C, 0%RH, film sample area of 78.4 cm²). The blue curve represents the evolution of pressure over time at the inferior permeation cell.

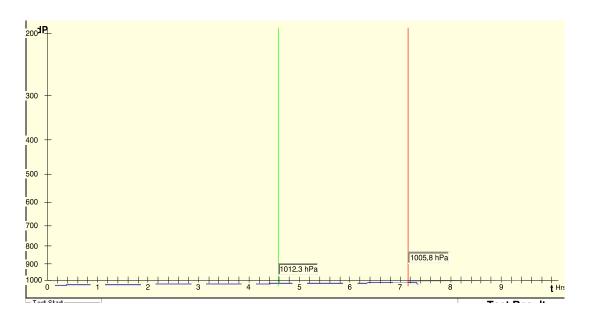


Figure S5. dP vs. time graph on amorphous 2,5-PBF (O₂-GTR, 23°C, 0%RH, film sample area of 78.4 cm²), representing the current pressure values as retrieved by the Instrument. The green and the red vertical lines indicate the range considered for the calculation of the pressure values.

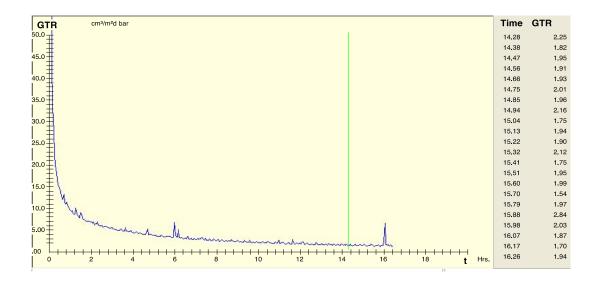


Figure S6. GTR vs. time graph on amorphous 2,5-PBF (CO₂-GTR, 23°C, 0%RH, film sample area of 78.4 cm²). The blue curve represents the evolution of pressure over time at the inferior permeation cell.

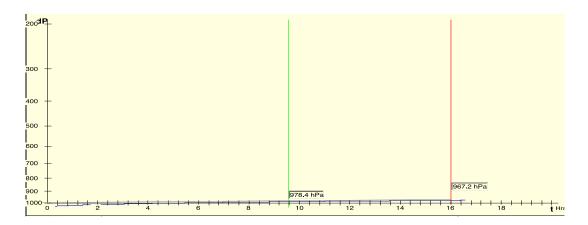


Figure S7. dP vs. time graph on amorphous 2,5-PBF (CO_2 -GTR, 23°C, 0%RH, film sample area of 78.4 cm²), representing the current pressure values as retrieved by the Instrument. The green and the red vertical lines indicate the range considered for the calculation of the pressure values.

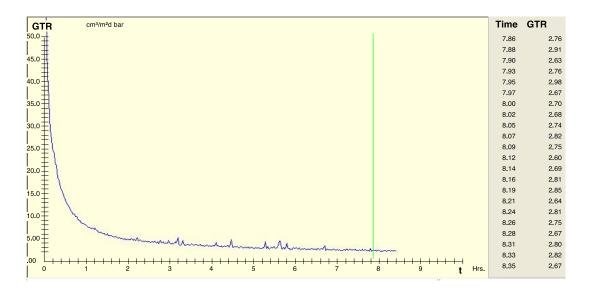


Figure S8. GTR vs. time graph on amorphous 2,5-PBF (O_2 -GTR, 23°C, 85%RH (KCl salt), film sample area of 78.4 cm²). The blue curve represents the evolution of pressure over time at the inferior permeation cell.

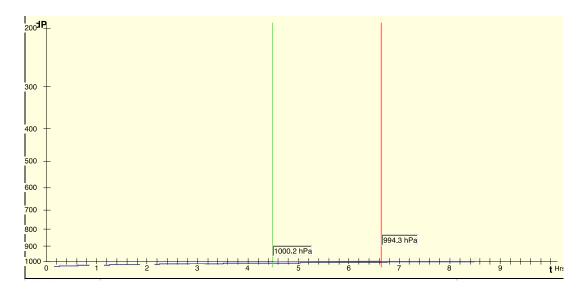


Figure S9. dP vs. time graph on amorphous 2,5-PBF (O_2 -GTR, 23°C, 85%RH (KCl salt), film sample area of 78.4 cm²), representing the current pressure values as retrieved by the Instrument. The green and the red vertical lines indicate the range considered for the calculation of the pressure values.

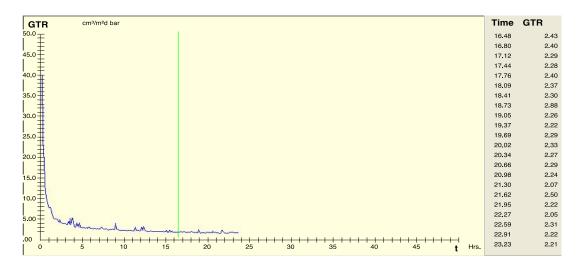


Figure S10. GTR vs. time graph on amorphous 2,5-PBF (CO₂-GTR, 23°C, 85%RH (KCl salt), film sample area of 78.4 cm²). The blue curve represents the evolution of pressure over time at the inferior permeation cell.

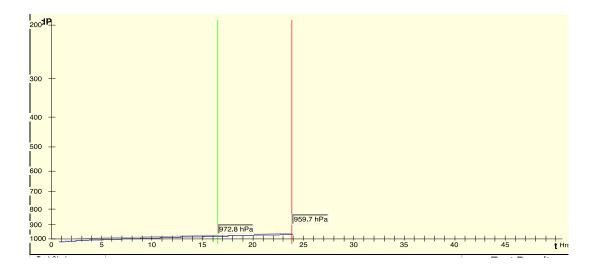


Figure S11. dP vs. time graph on amorphous 2,5-PBF (CO₂-GTR, 23°C, 85%RH (KCl salt), film sample area of 78.4 cm²), representing the current pressure values as retrieved by the Instrument. The green and the red vertical lines indicate the range considered for the calculation of the pressure values.

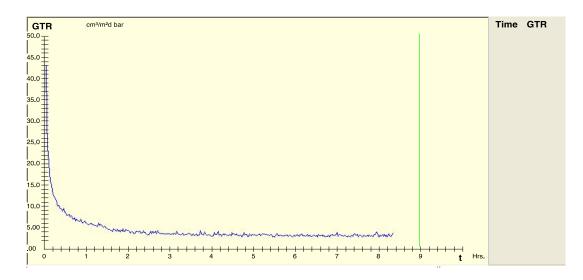


Figure S12. GTR vs. time graph on annealed 2,5-PBF (O_2 -GTR, 23°C, 0%RH, film sample area of 78.4 cm²). The blue curve represents the evolution of pressure over time at the inferior permeation cell.

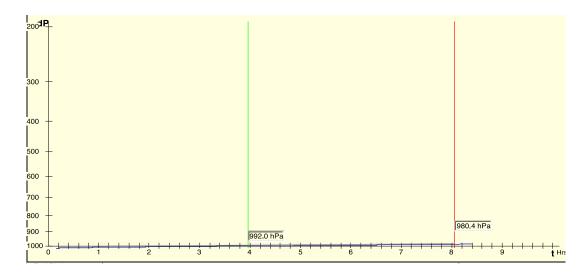


Figure S13. dP vs. time graph on annealed 2,5-PBF (O₂-GTR, 23°C, 0%RH, film sample area of 78.4 cm²), representing the current pressure values as retrieved by the Instrument. The green and the red vertical lines indicate the range considered for the calculation of the pressure values.

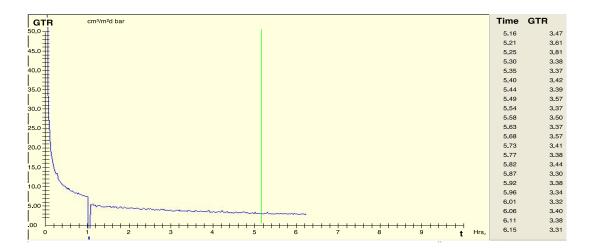


Figure S14. GTR vs. time graph on annealed 2,5-PBF (CO₂-GTR, 23°C, 0%RH, film sample area of 78.4 cm²). The blue curve represents the evolution of pressure over time at the inferior permeation cell.

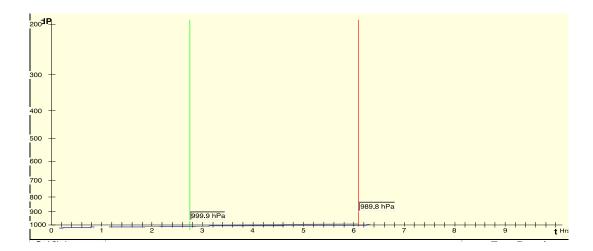


Figure S15. dP vs. time graph on annealed 2,5-PBF (CO₂-GTR, 23°C, 0%RH, film sample area of 78.4 cm²), representing the current pressure values as retrieved by the Instrument. The green and the red vertical lines indicate the range considered for the calculation of the pressure values.

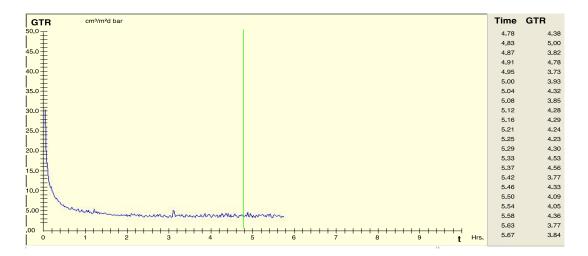


Figure S16. GTR vs. time graph on annealed 2,5-PBF (O_2 -GTR, 23°C, 85%RH (KCl salt), film sample area of 78.4 cm²). The blue curve represents the evolution of pressure over time at the inferior permeation cell.

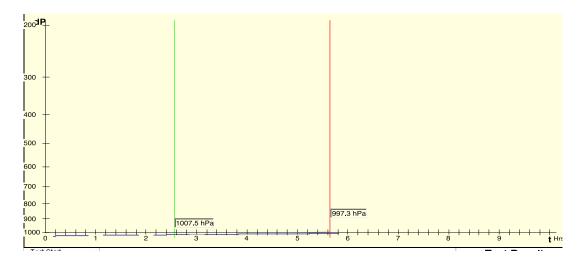


Figure S17. dP vs. time graph on annealed 2,5-PBF (O_2 -GTR, 23°C, 85%RH (KCl salt), film sample area of 78.4 cm²), representing the current pressure values as retrieved by the Instrument. The green and the red vertical lines indicate the range considered for the calculation of the pressure values.

GTR cm³/m²d bar	Time	GTR
50.0 T	11.16	3.54
	11.47	3.31
45.0	11.79	3.46
	12.10	3.51
40.0 —	12.41	3.33
	12.73	3.36
35.0 🛨	13.04	3.35
	13.35	3.34
30.0 🗄	13.66	3.33
	13.98	3.29
25.0 🛓	14.29	3.21
	14.60	3.28
20.0 =	14.92	3.43
	15.23	3.39
15.0 +	15.54	3.14
	15.85	3.35
10.0 #	16.17	3.33
	16.48	3.17
5.00	16.79	3.38
	17.11	3.11
	17.42	3.33
0 2 4 6 8 10 12 14 16 18 t Hrs	17.73	3.57

Figure S18. GTR vs. time graph on annealed 2,5-PBF (CO₂-GTR, 23°C, 85%RH (KCl salt), film sample area of 78.4 cm²). The blue curve represents the evolution of pressure over time at the inferior permeation cell.

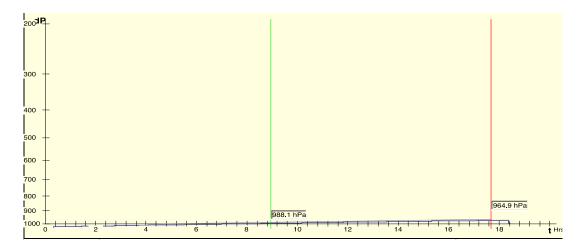


Figure S19. dP vs. time graph on annealed 2,5-PBF (CO₂-GTR, 23°C, 85%RH (KCl salt), film sample area of 78.4 cm²), representing the current pressure values as retrieved by the Instrument. The green and the red vertical lines indicate the range considered for the calculation of the pressure values.

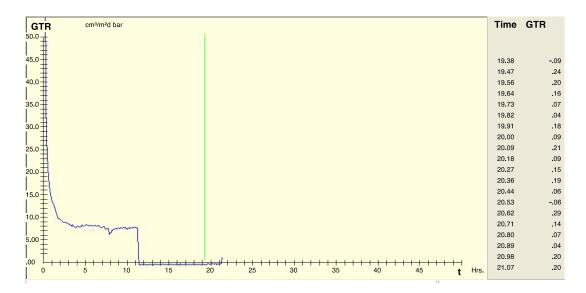


Figure S20. GTR vs. time graph on amorphous 2,4-PBF (O_2 -GTR, 23°C, 0%RH, film sample area of 78.4 cm²). The blue curve represents the evolution of pressure over time at the inferior permeation cell.

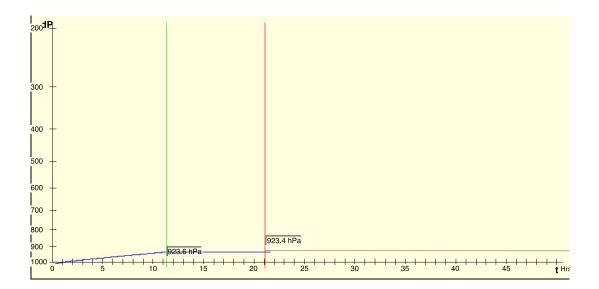


Figure S21. dP vs. time graph on amorphous 2,4-PBF (O_2 -GTR, 23°C, 0%RH, film sample area of 78.4 cm²), representing the current pressure values as retrieved by the Instrument. The green and the red vertical lines indicate the range considered for the calculation of the pressure values.

GTR	cm³/m²d bar	Time	GTR
^{50.0} ∓		18.07	.03
ΙΞ		18.28	06
45.0		18.48	.03
‡		18.69	.02
40.0		18.89	.04
#		19.10	.05
35.0 🛨		19.30	01
±		19.51	01
30.0 <u>±</u>		19.71	02
II		19.92	03
25.0 🕇		20.12	01
ΙΞ		20.33	.03
20.0 🕇		20.53	.02
ΙΞ		20.74	.00
15.0		20.94	.09
ΙΞ		21.14	.01
10.0		21.35	.01
1 1		21.55	.06
5.00		21.76	.02
i Ħ		21.96	.11
.00		22.17	.03
0	5 10 15 20 25 30 35 40 45 <u>t</u> Hrs.	22.37	.09

Figure S22. GTR vs. time graph on amorphous 2,4-PBF (CO_2 -GTR, 23°C, 0%RH, film sample area of 78.4 cm²). The blue curve represents the evolution of pressure over time at the inferior permeation cell.

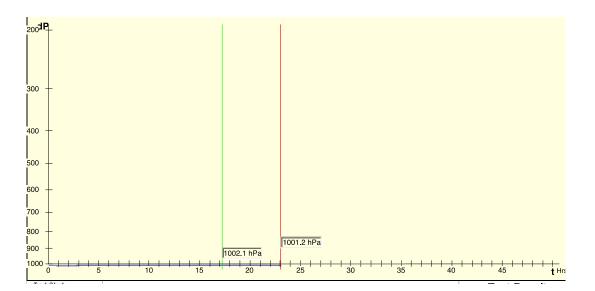


Figure S23. dP vs. time graph on amorphous 2,4-PBF (CO₂-GTR, 23°C, 0%RH, film sample area of 78.4 cm²), representing the current pressure values as retrieved by the Instrument. The green and the red vertical lines indicate the range considered for the calculation of the pressure values.

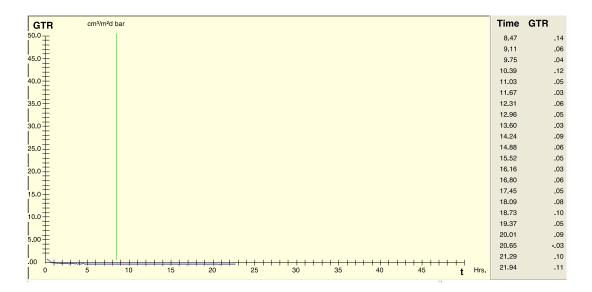


Figure S24. GTR vs. time graph on amorphous 2,4-PBF (O_2 -GTR, 23°C, 85%RH (KCl salt), film sample area of 78.4 cm²). The blue curve represents the evolution of pressure over time at the inferior permeation cell.

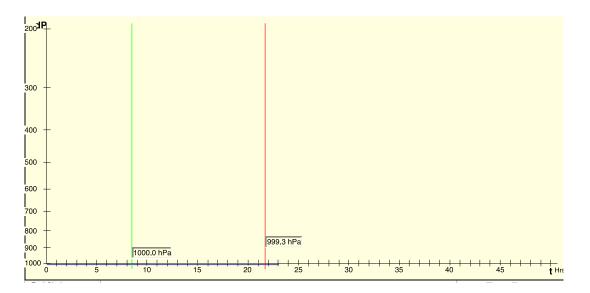


Figure S25. dP vs. time graph on amorphous 2,4-PBF (O_2 -GTR, 23°C, 85%RH (KCl salt), film sample area of 78.4 cm²), representing the current pressure values as retrieved by the Instrument. The green and the red vertical lines indicate the range considered for the calculation of the pressure values.

GTR	cm³/m²d bar	Time	GTR
^{50.0} —		18.81	.05
ΙΞ		19.06	.05
45.0		19.31	.07
‡		19.56	.05
40.0		19.81	.09
=		20.07	.03
35.0		20.32	.05
=		20.57	.04
30.0		20.82	.04
‡		21.08	.09
25.0		21.33	.02
‡		21.58	.05
20.0		21.83	.04
‡		22.08	02
15.0 -		22.34	.09
Ŧ		22.59	.11
10.0 =		22.84	.10
Ŧ		23.09	.11
5.00		23.35	.06
1 #		23.60	.11
.00		23.85	.08
0	5 10 15 20 25 30 35 40 45 t Hrs.	24.10	.07

Figure S26. GTR vs. time graph on amorphous 2,4-PBF (CO₂-GTR, 23°C, 85%RH (KCl salt), film sample area of 78.4 cm²). The blue curve represents the evolution of pressure over time at the inferior permeation cell.

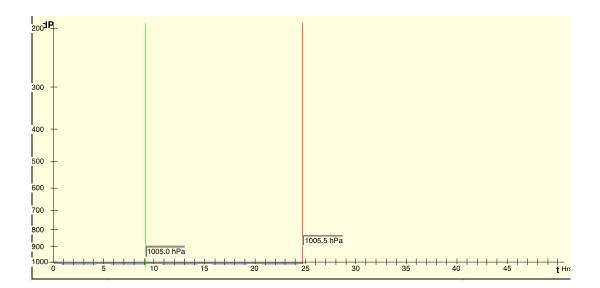


Figure S27. dP vs. time graph on amorphous 2,4-PBF (CO₂-GTR, 23°C, 85%RH (KCl salt), film sample area of 78.4 cm²), representing the current pressure values as retrieved by the Instrument. The green and the red vertical lines indicate the range considered for the calculation of the pressure values.

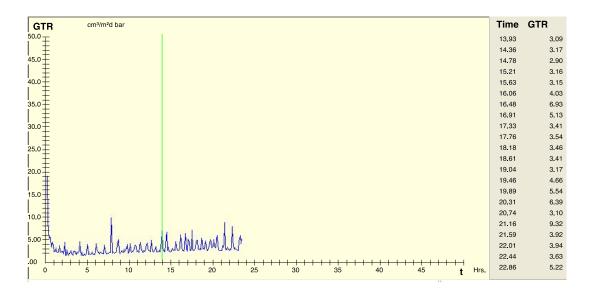


Figure S28. GTR vs. time graph on annealed 2,4-PBF (O_2 -GTR, 23°C, 0%RH, film sample area of 78.4 cm²). The blue curve represents the evolution of pressure over time at the inferior permeation cell.

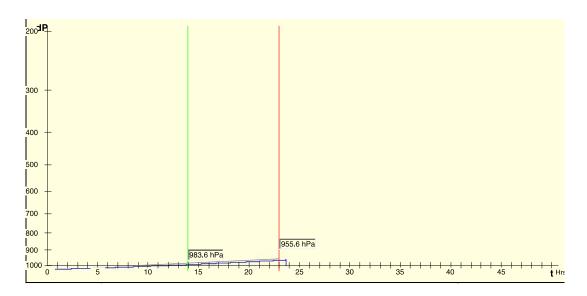


Figure S29. dP vs. time graph on annealed 2,4-PBF (O_2 -GTR, 23°C, 0%RH, film sample area of 78.4 cm²), representing the current pressure values as retrieved by the Instrument. The green and the red vertical lines indicate the range considered for the calculation of the pressure values.

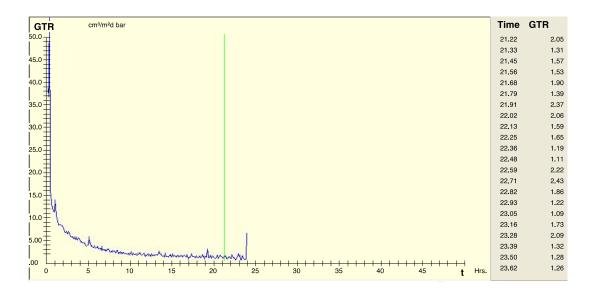


Figure S30. GTR vs. time graph on annealed 2,4-PBF (CO₂-GTR, 23°C, 0%RH, film sample area of 78.4 cm²). The blue curve represents the evolution of pressure over time at the inferior permeation cell.

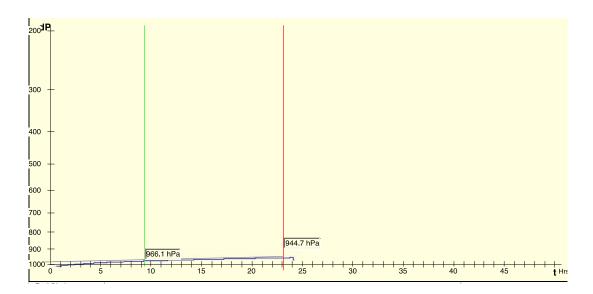


Figure S31. dP vs. time graph on annealed 2,4-PBF (CO₂-GTR, 23°C, 0%RH, film sample area of 78.4 cm²), representing the current pressure values as retrieved by the Instrument. The green and the red vertical lines indicate the range considered for the calculation of the pressure values.

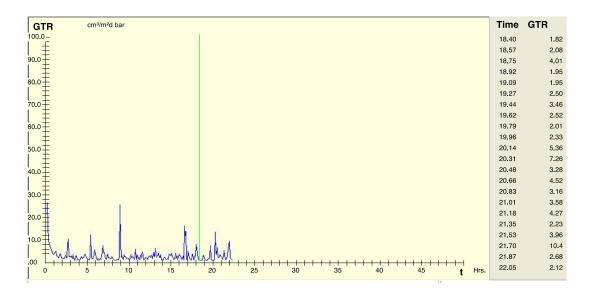


Figure S32. GTR vs. time graph on annealed 2,4-PBF (O_2 -GTR, 23°C, 85%RH (KCl salt), film sample area of 78.4 cm²). The blue curve represents the evolution of pressure over time at the inferior permeation cell.

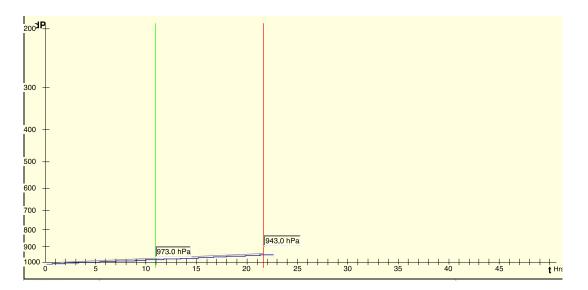


Figure S33. dP vs. time graph on annealed 2,4-PBF (O_2 -GTR, 23°C, 85%RH (KCl salt), film sample area of 78.4 cm²), representing the current pressure values as retrieved by the Instrument. The green and the red vertical lines indicate the range considered for the calculation of the pressure values.

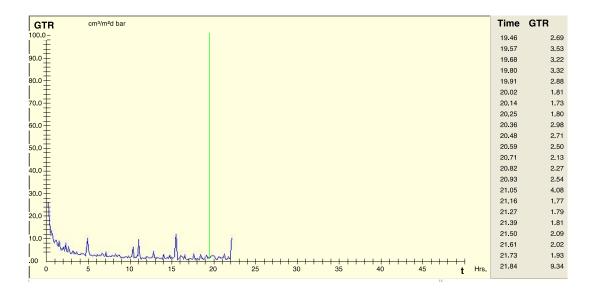


Figure S34. GTR vs. time graph on annealed 2,4-PBF (CO₂-GTR, 23°C, 85%RH (KCl salt), film sample area of 78.4 cm²). The blue curve represents the evolution of pressure over time at the inferior permeation cell.

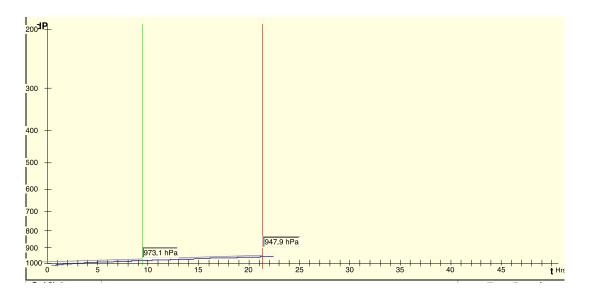


Figure S35. dP vs. time graph on annealed 2,4-PBF (CO₂-GTR, 23°C, 85%RH (KCl salt), film sample area of 78.4 cm²), representing the current pressure values as retrieved by the Instrument. The green and the red vertical lines indicate the range considered for the calculation of the pressure values.