

Supplementary Materials

Removal of Erythromycin from water by ibuprofen driven pre-organized divinyl sulfone cross-linked dextrin

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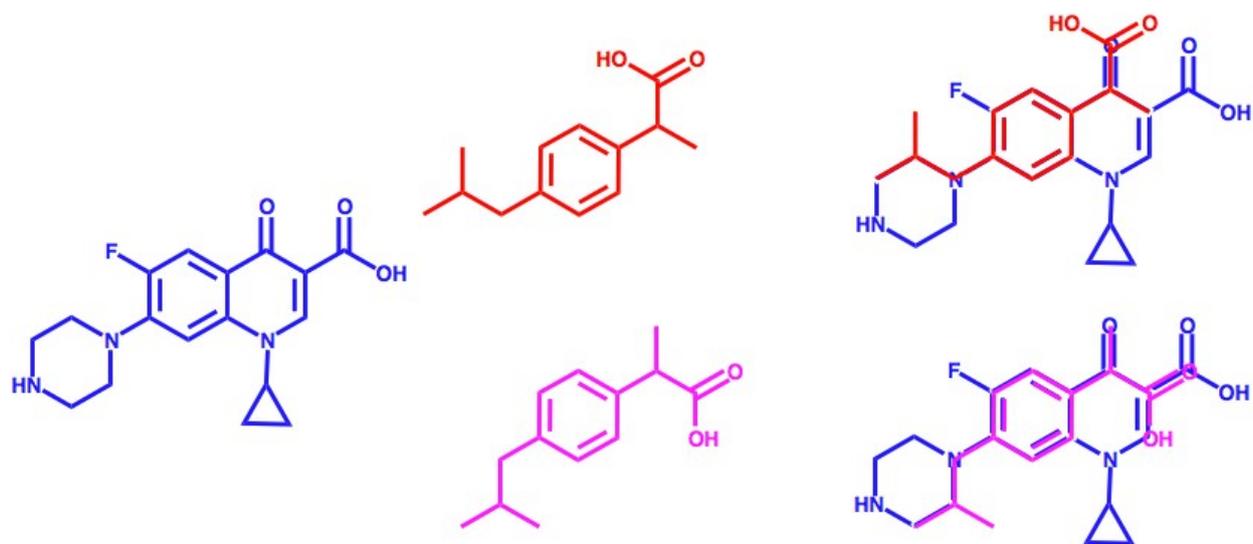


Figure S1. Superimposition of two conformers of ibuprofen (red and magenta) on ciprofloxacin (blue).

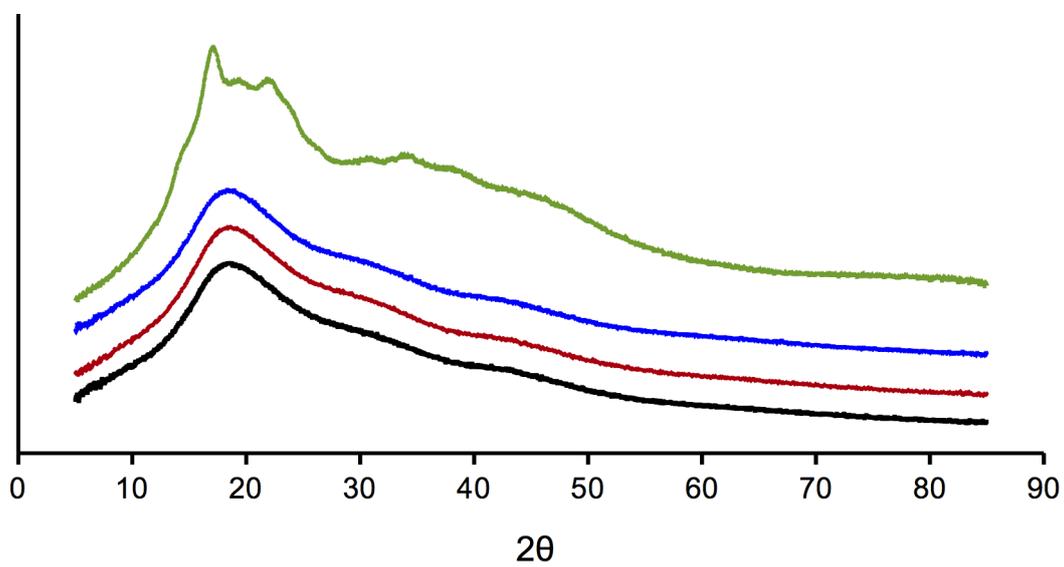


Figure S2. XRPD of the starting material Dx (green) and the polymers **pDx0** (black), **pDx1** (red) and **pDx5** (blue).

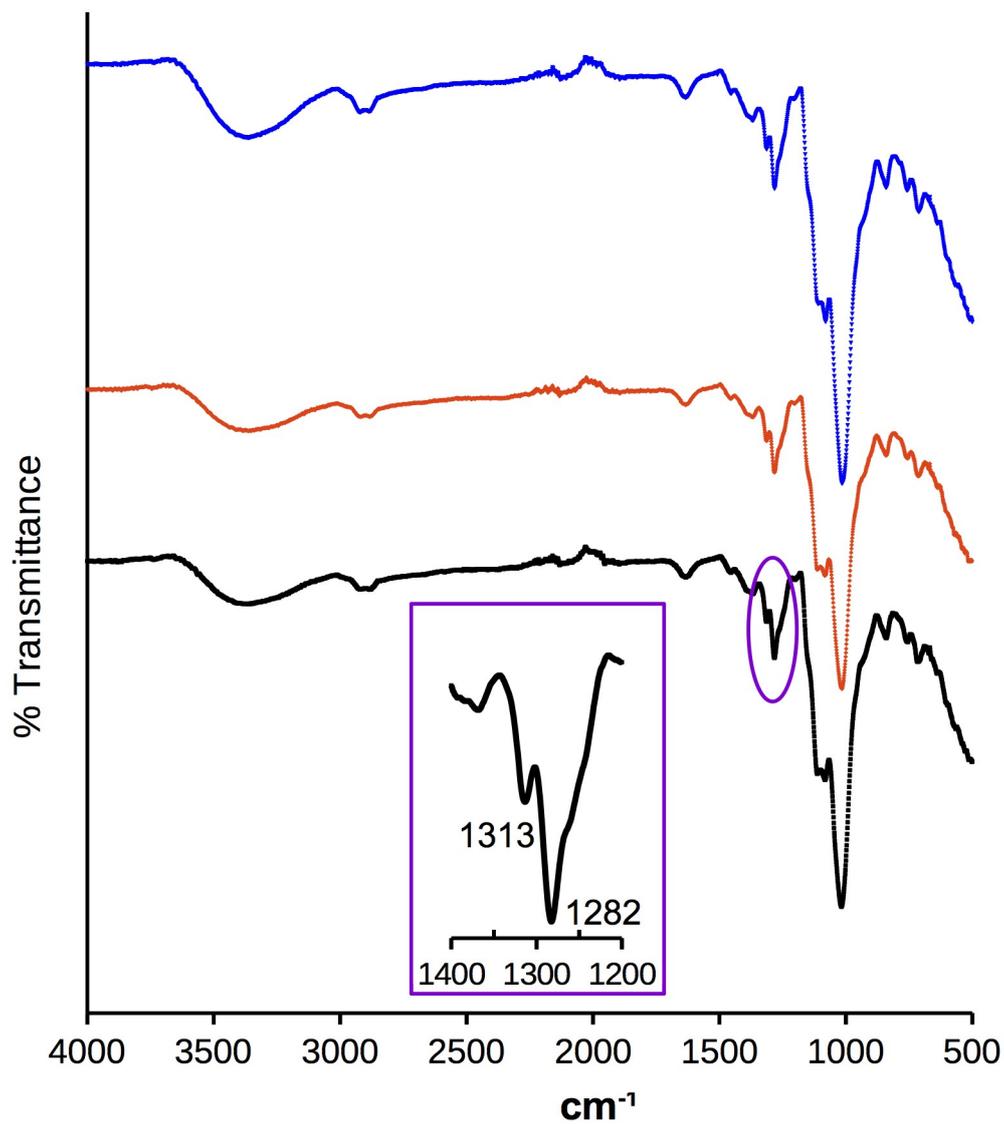


Figure S3. FTIR of **pDx0** (black), **pDx1** (red) and **pDx5** (blue). Insert, detail of the 1400-1200 cm⁻¹ region showing the double signal at 1282 and 1312 that matches with the distinctive signature of the sulfone group.

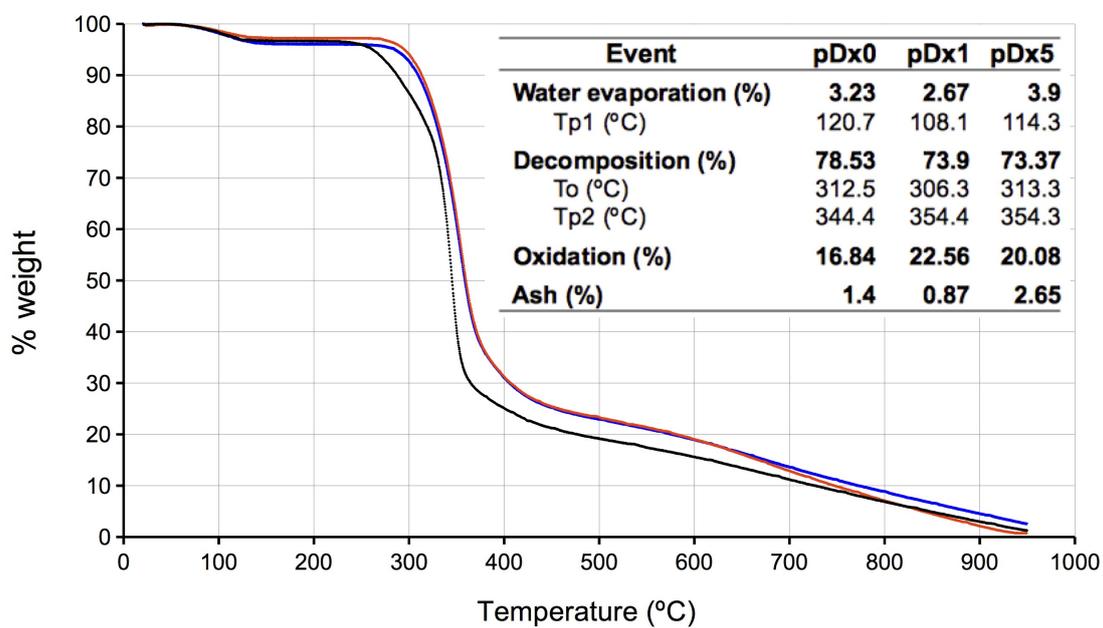


Figure S4. TGA curves of **pDx0** (black), **pDx1** (red) and **pDx5** (blue). Table depicts the significant features, being Tp the first derivative peak and To the onset extrapolated temperature.

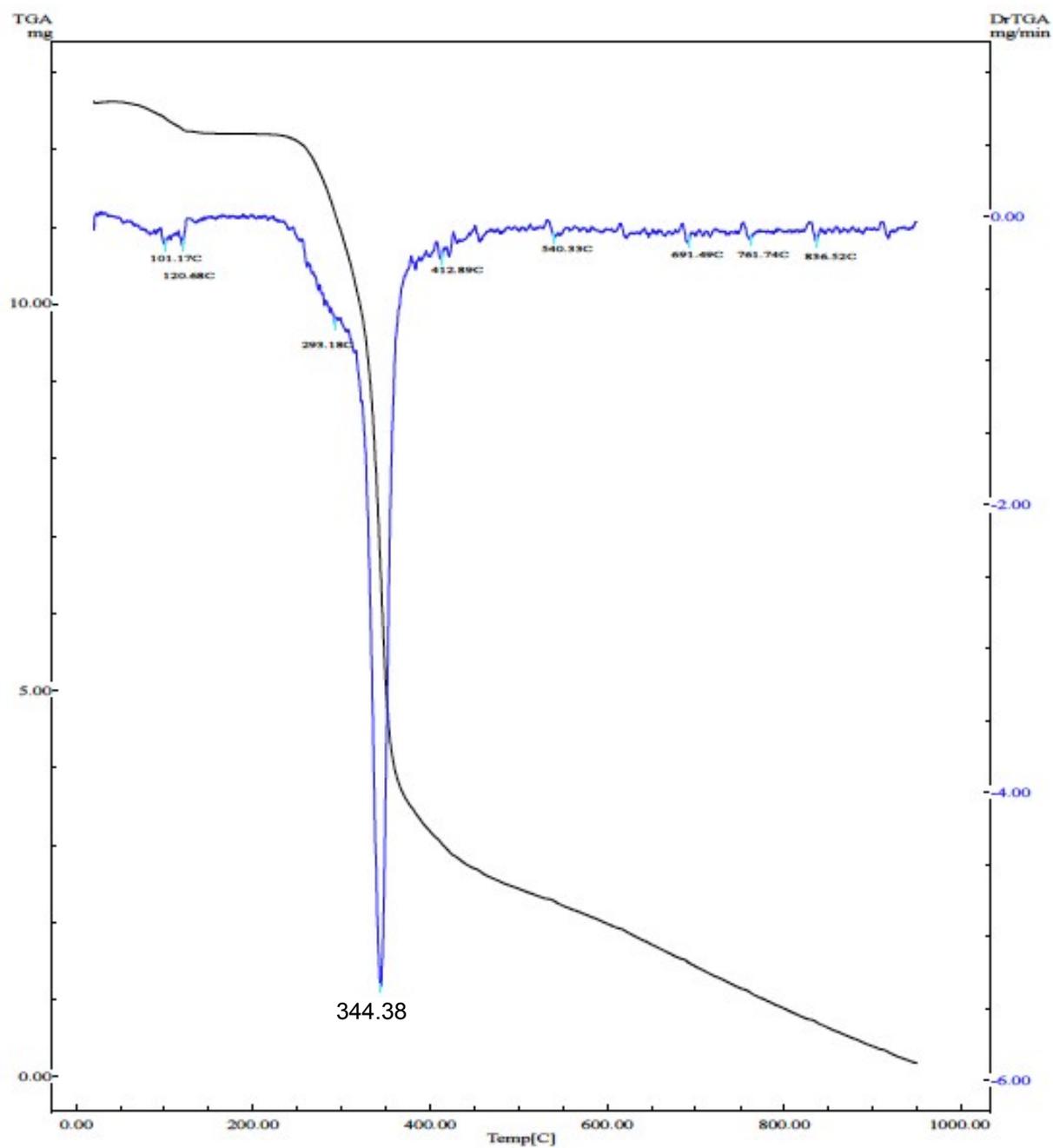


Figure S5. Derivative TGA of **pDx0**. In black is shown the evolution of the mass of the sample as a function of the temperature and in blue the first derivative.

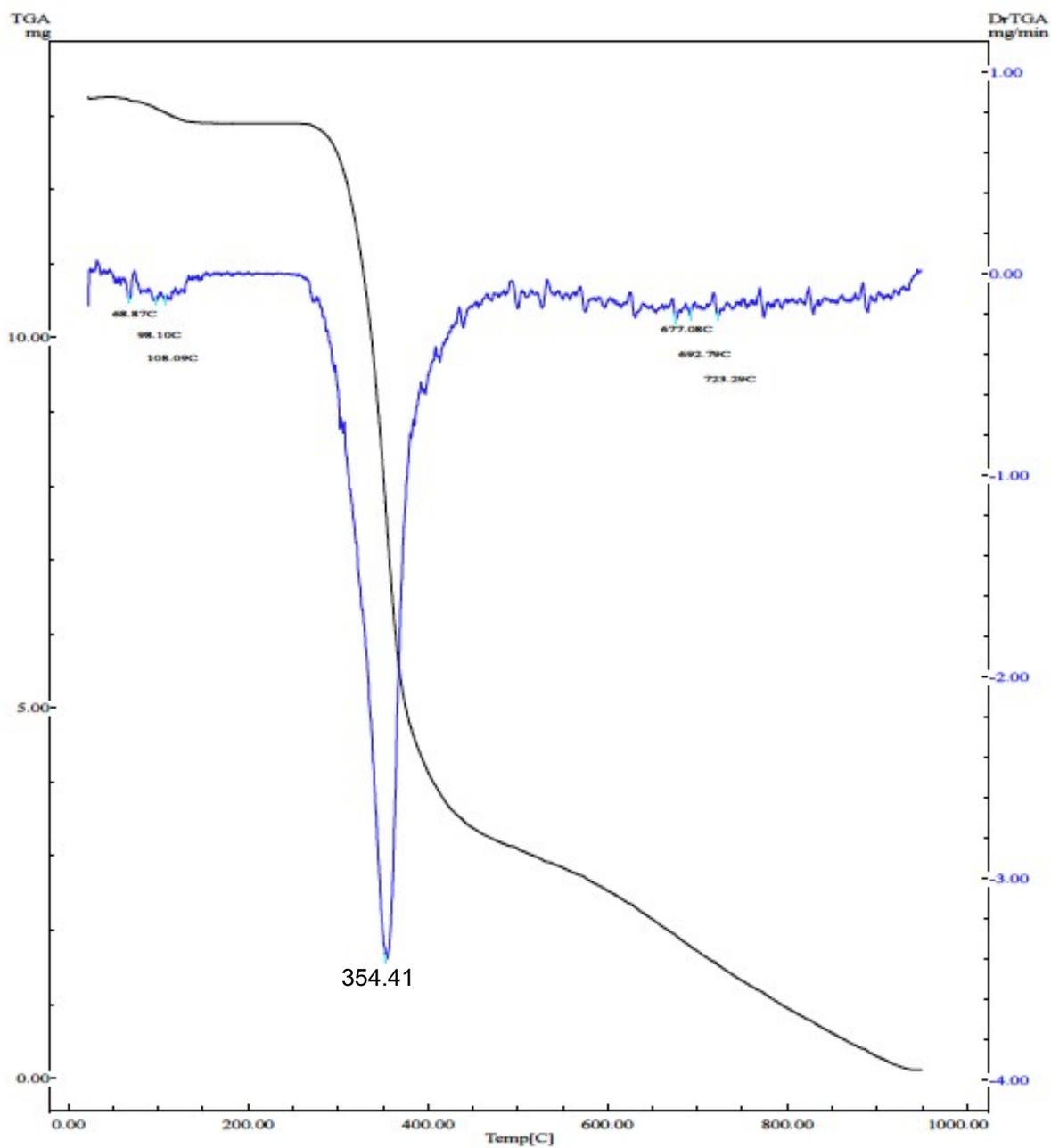


Figure S6. Derivative TGA of **pDx1**. In black is shown the evolution of the mass of the sample as a function of the temperature and in blue the first derivative.

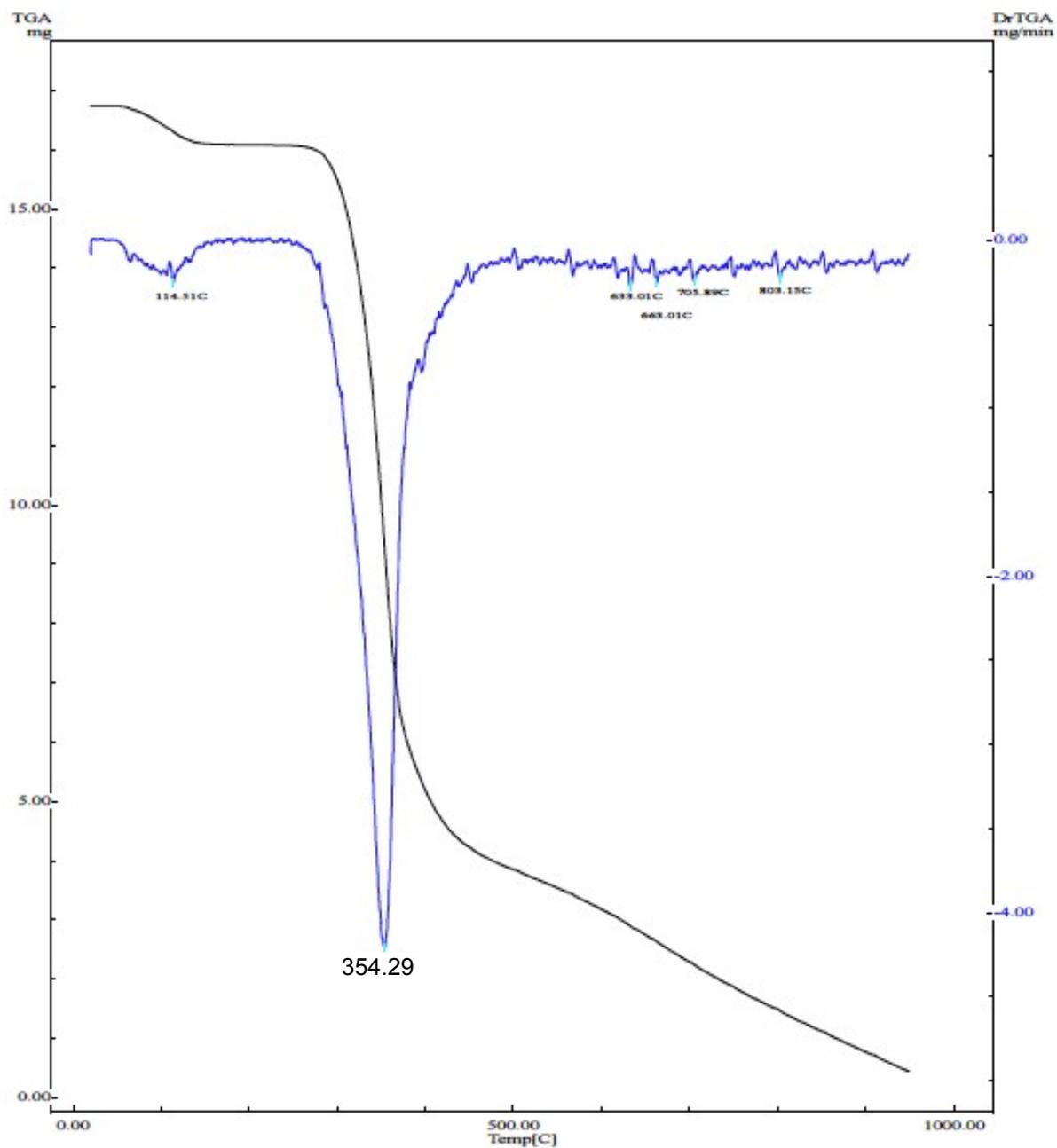
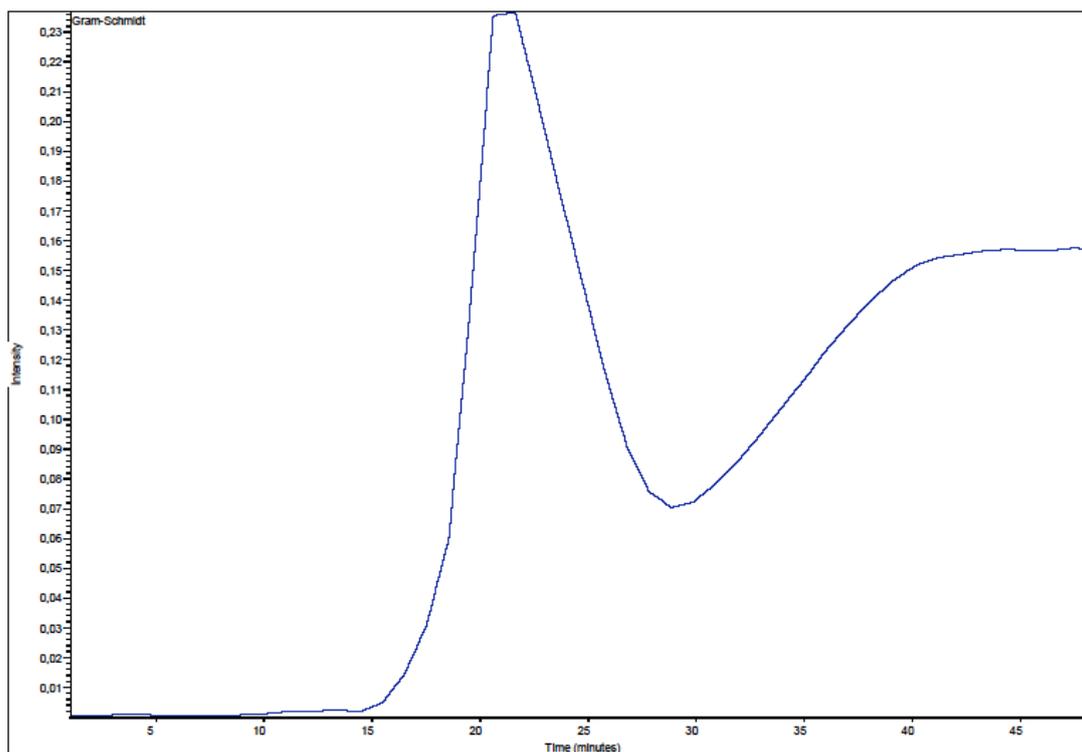


Figure S7. Derivative TGA of **pDx5**. In black is shown the evolution of the mass of the sample as a function of the temperature and in blue the first derivative.

(a)



(b)

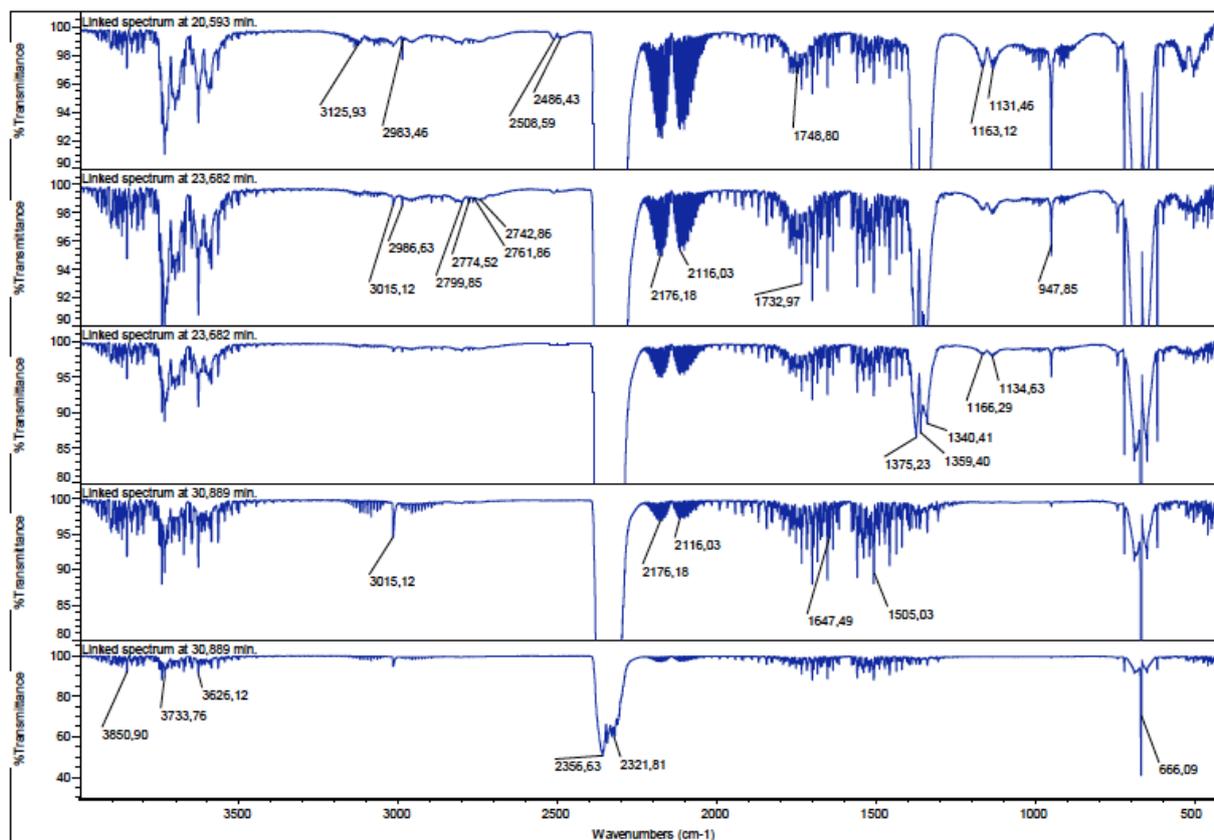
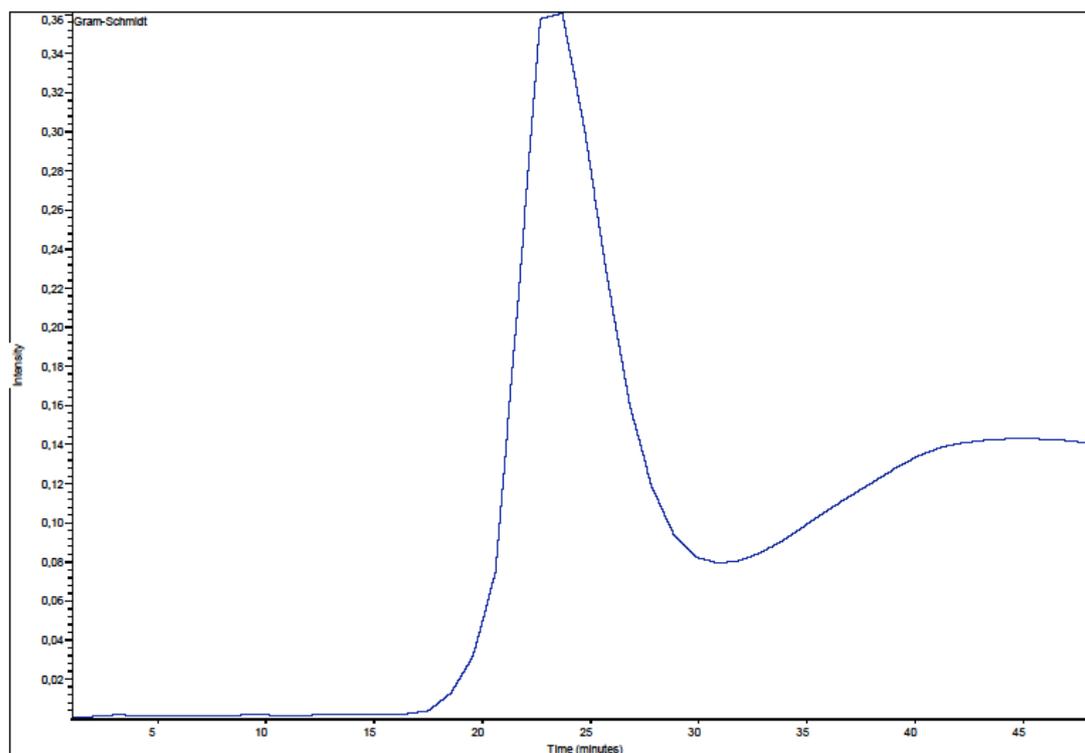


Figure S8. IR-TGA of **pDx0**. (a) Gram-Schmidt. (b) Most representative signals at three single time points 20.6 min, 23.7 min and 34.9 min. The delay between the TG and the FTIR detector is from 4 to 5 min.

(a)



(b)

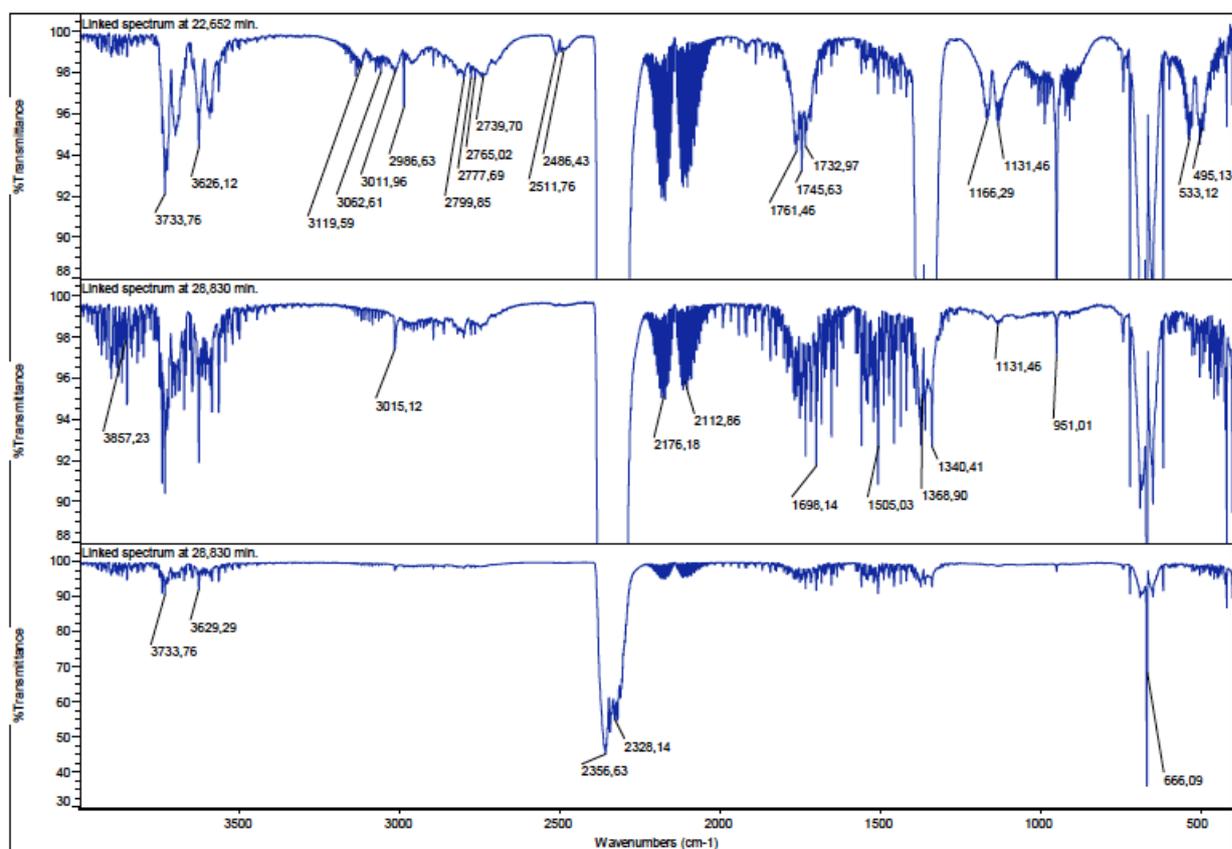
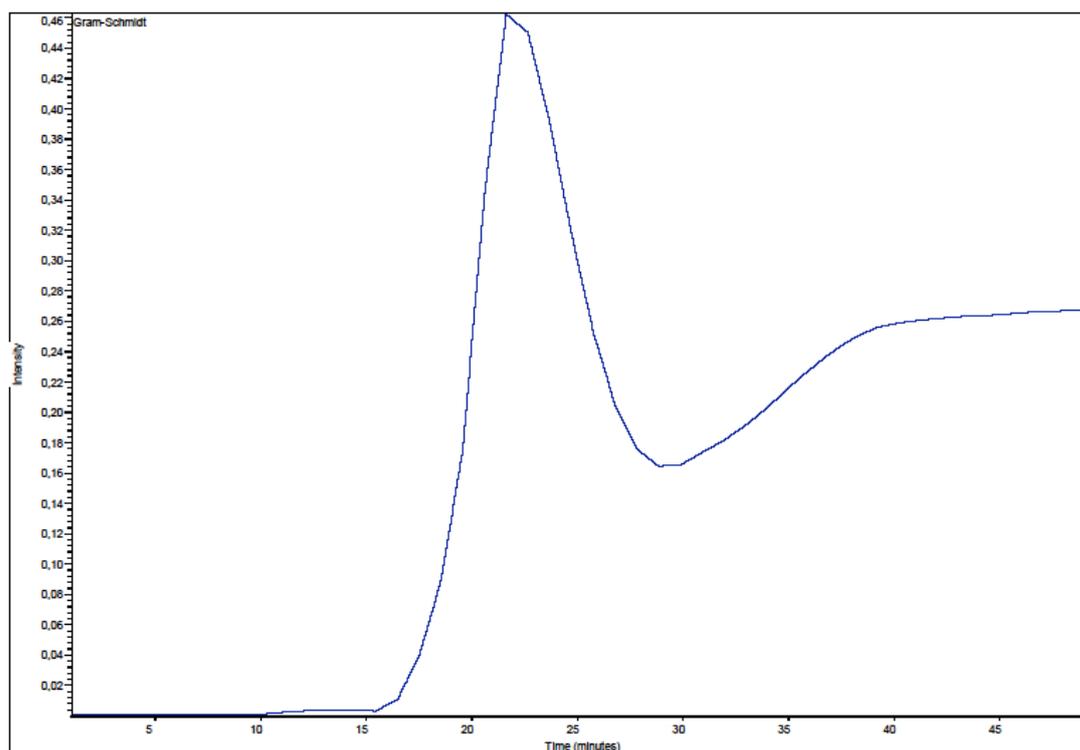


Figure S9. IR-TGA of **pDx1**. (a) Gram-Schmidt. (b) Most representative signals at two single time points 22.6 min and 28.8 min. The delay between the TG and the FTIR detector is from 4 to 5 min.

(a)



(b)

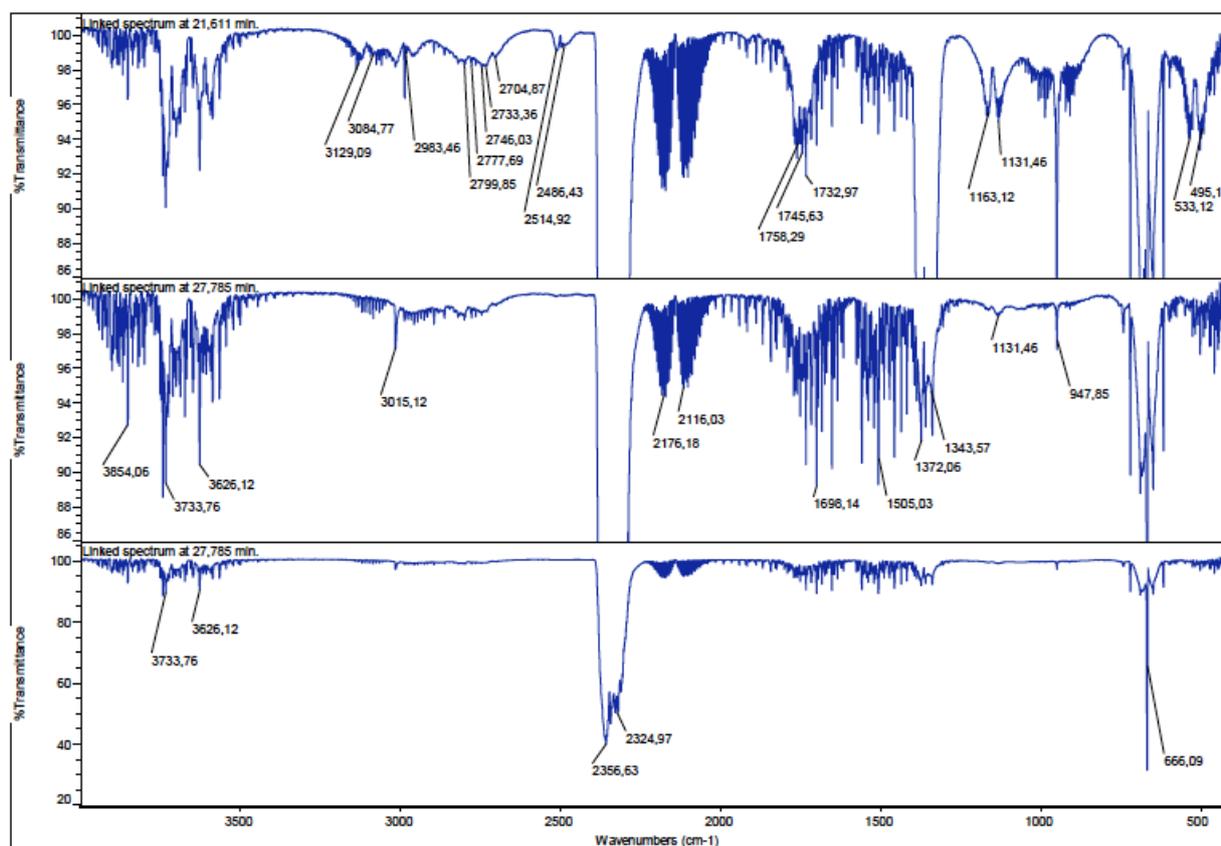


Figure S10. IR-TGA of **pDx5**. (a) Gram-Schmidt. (b) Most representative signals at two single time points 21.6 min and 27.8 min. The delay between the TG and the FTIR detector is from 4 to 5 min.

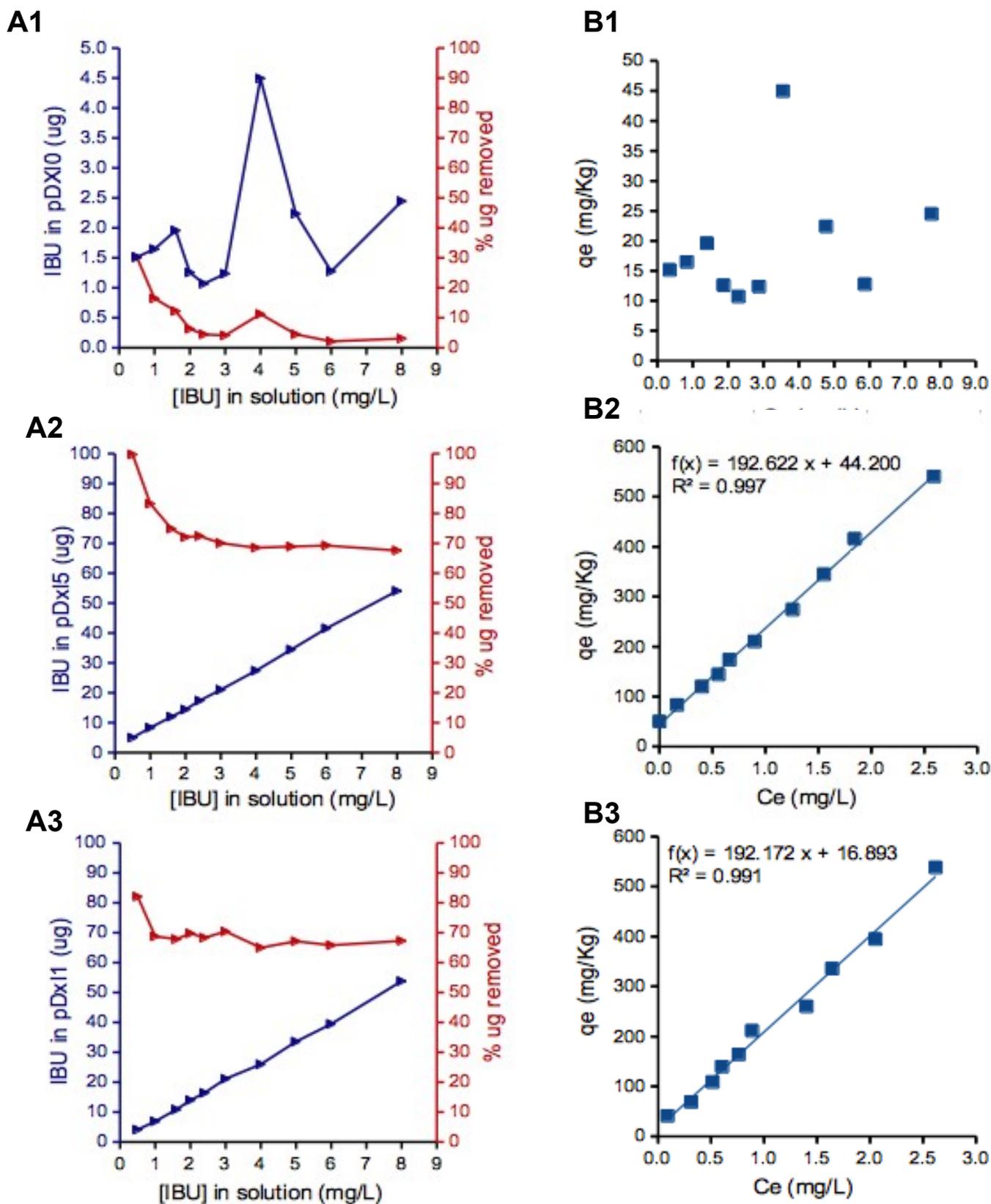


Figure S11. Characterization of the polymers **pDx0** (A1 & B1), **pDx1** (A2 & B2) and **pDx5** (A3 & B3) as scavenger of IBU. A: sorption isotherm showing in blue the amount retained by the polymer and in red the percentage removed from the solution as a function of the initial concentration of IBU. B: estimation of K_d .

Table S1. Elemental analysis of ibuprofen pre-incubated cross-linked polymers. Results are expressed as means \pm SD (n = 3).

	pDx0	pDx1	pDx5
% C	39.84 \pm 0.055	39.85 \pm 0.060	39.91 \pm 0.330
% H	7.35 \pm 0.648	7.39 \pm 0.142	7.62 \pm 0.035
% S	6.21 \pm 0.428	6.31 \pm 0.270	5.85 \pm 0.480

Table S2. Equations of the isotherm model assayed for the fitting of the experimental sorption data as defined by ISOT_calc¹.

Isotherm (# parameters)	Equation (q_e = ...)	Parameter definition²
Temkin (2)	$k_1 \cdot \ln(C_e) + k_2$	k_1 and k_2 are constants of Temkin isotherm and k_1 is related to sorption heat
Freundlich (2)	$K_F \cdot C_e^N$	K_F is adsorption potential N is strength constant associated to heterogeneity (for homogenous systems $N=1$)
Langmuir (2)	$S_T \frac{K_L \cdot C_e}{1 + K_L \cdot C_e}$	S_T is maximum adsorption capacity K_L is affinity constant
Redlich-Peterson (3)	$S_T \frac{k \cdot C_e}{(1 + C_e)^N}$	S_T is maximum adsorption capacity k is related to constants of Redlich-Peterson model N ranges from 0 to 1
Vieth-Sladek (3)	$K_D \cdot C_e + \frac{S_T \cdot b \cdot C_e}{1 + b \cdot C_e}$	K_D and b are Vieth-Sladek constants S_T is the maximum adsorption capacity
2-sites Langmuir (4)	$\frac{S_{T1} \cdot k_1 \cdot C_e}{1 + k_1 \cdot C_e} + \frac{S_{T2} \cdot k_2 \cdot C_e}{1 + k_2 \cdot C_e}$	S_{T1} and S_{T2} are the maximum adsorption capacity for sites 1 and 2 K_1 and K_2 are affinity constant for sites 1 and 2

- 1 José L. Beltrán, Joseph J. Pignatello, and Marc Teixidó, "ISOT_Calc: A Versatile Tool for Parameter Estimation in Sorption Isotherms," *Computers & Geosciences*, 2016, 94: 11–17, doi:10.1016/j.cageo.2016.04.008.
- 2 Mahdiah Mozaffari Majd et al., "Adsorption Isotherm Models: A Comprehensive and Systematic Review (2010–2020)," *Science of The Total Environment*, 2022, 812, 151334, doi:10.1016/j.scitotenv.2021.151334.