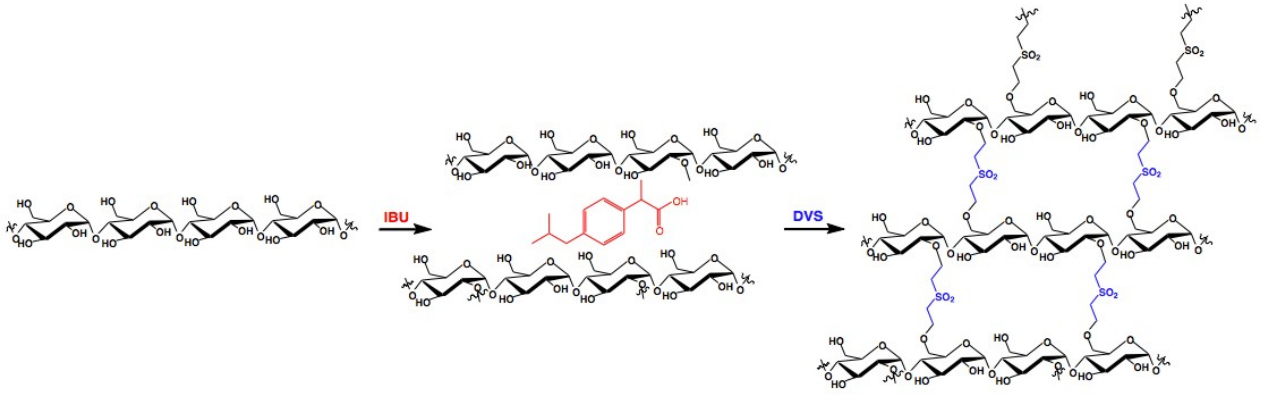
# Supplementary Materials

## Removal of Erythromycin from Water by Ibuprofen-Driven Pre-Organized Divinyl Sulfone Cross-Linked Dextrin

**Mariano Ortega-Muñoz [1,2,3], Sarah Alvarado [1,†], Alicia Megia-Fernandez [1,2,3], Fernando Hernandez-Mateo [1,2,3], Francisco Javier Lopez-Jaramillo [1,2,3,*] and Francisco Santoyo-Gonzalez [1,2,3,*]**

1 Department of Organic Chemistry, Faculty of Sciences, University of Granada, 18073 Granada, Spain
2 Unit of Excellence in Chemistry Applied to Biomedicine and the Environment, University of Granada, 18073 Granada, Spain
3 Biotechnology Institute, University of Granada, 18071 Granada, Spain
* Correspondence: fjljara@ugr.es (F.J.L.-J.); fsantoyo@ugr.es (F.S.-G.)
† Current address: Institute for Advanced Chemistry of Catalonia, CSIC, 08034 Barcelona, Spain.




**Scheme S1.** Synthesis of the ibuprofen (IBU) driven preorganized divinyl sulfone (DVS) cross-linked dextrin

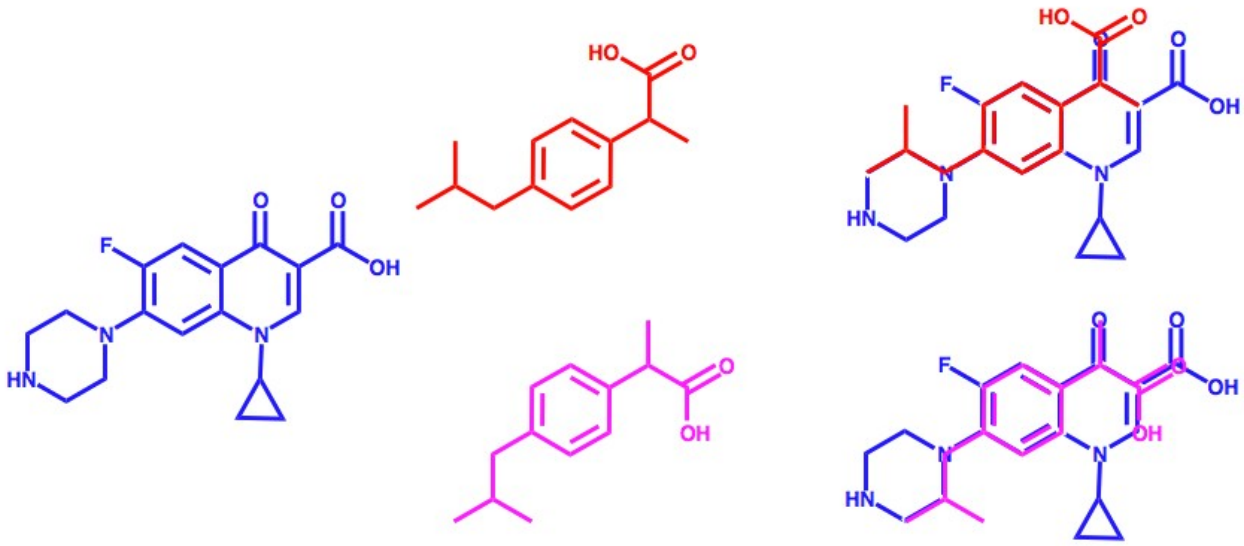



**Figure S1.** Superimposition of two conformers of ibuprofen (red and magenta) on ciprofloxacin (blue).

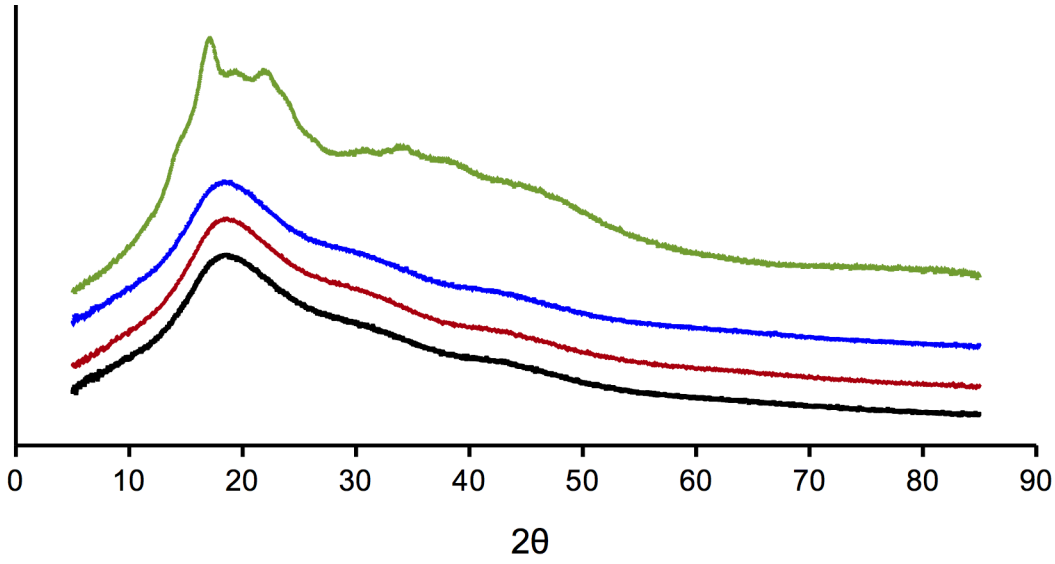



**Figure S2.** XRPD of the starting material Dx (green) and the polymers **pDx0** (black), **pDx1** (red) and **pDx5** (blue).

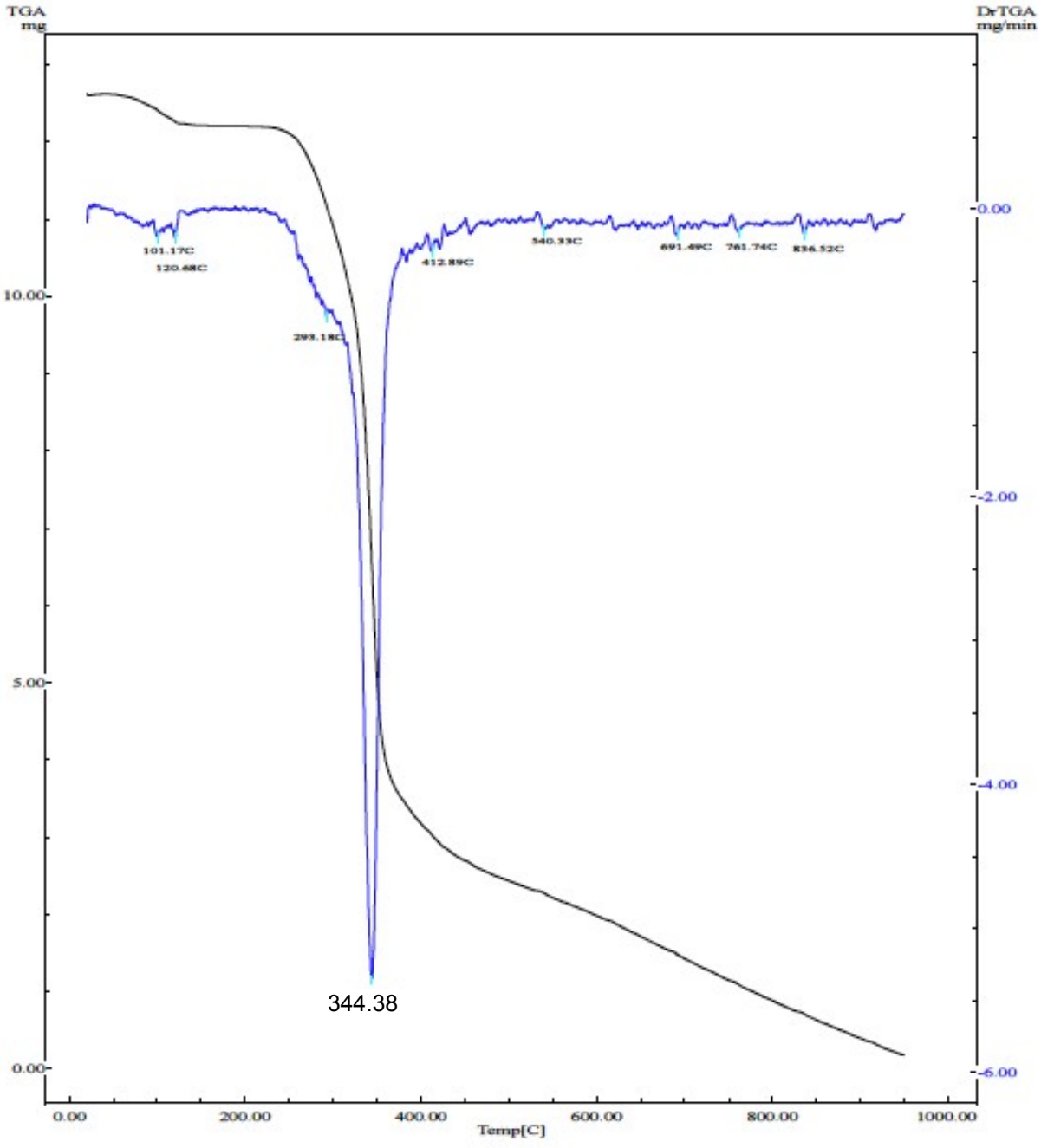



**Figure S3.** Derivative TGA of **pDx0**. In black is shown the evolution of the mass of the sample as a function of the temperature and in blue the first derivative.

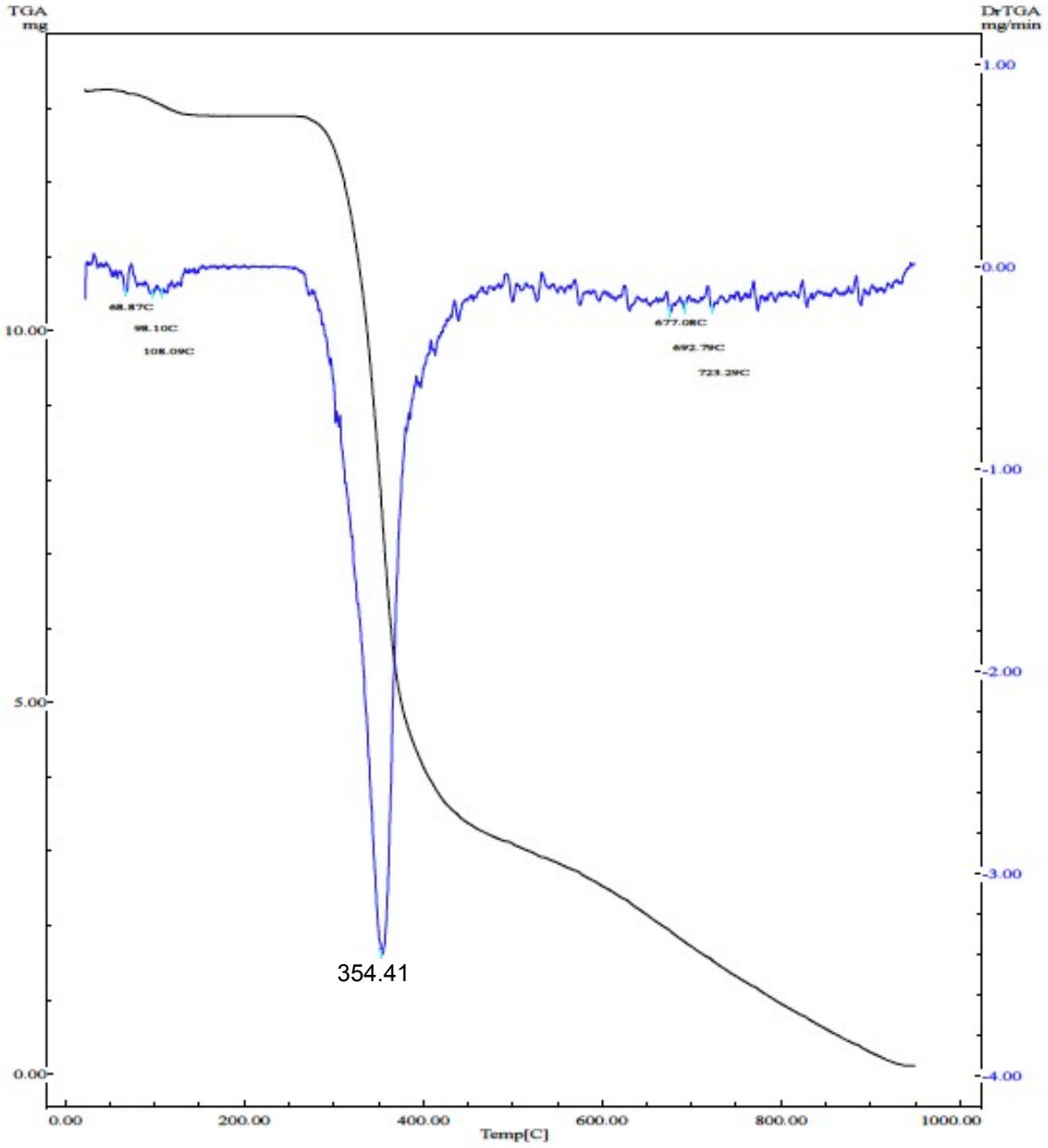



**Figure S4.** Derivative TGA of **pDx1**. In black is shown the evolution of the mass of the sample as a function of the temperature and in blue the first derivative.

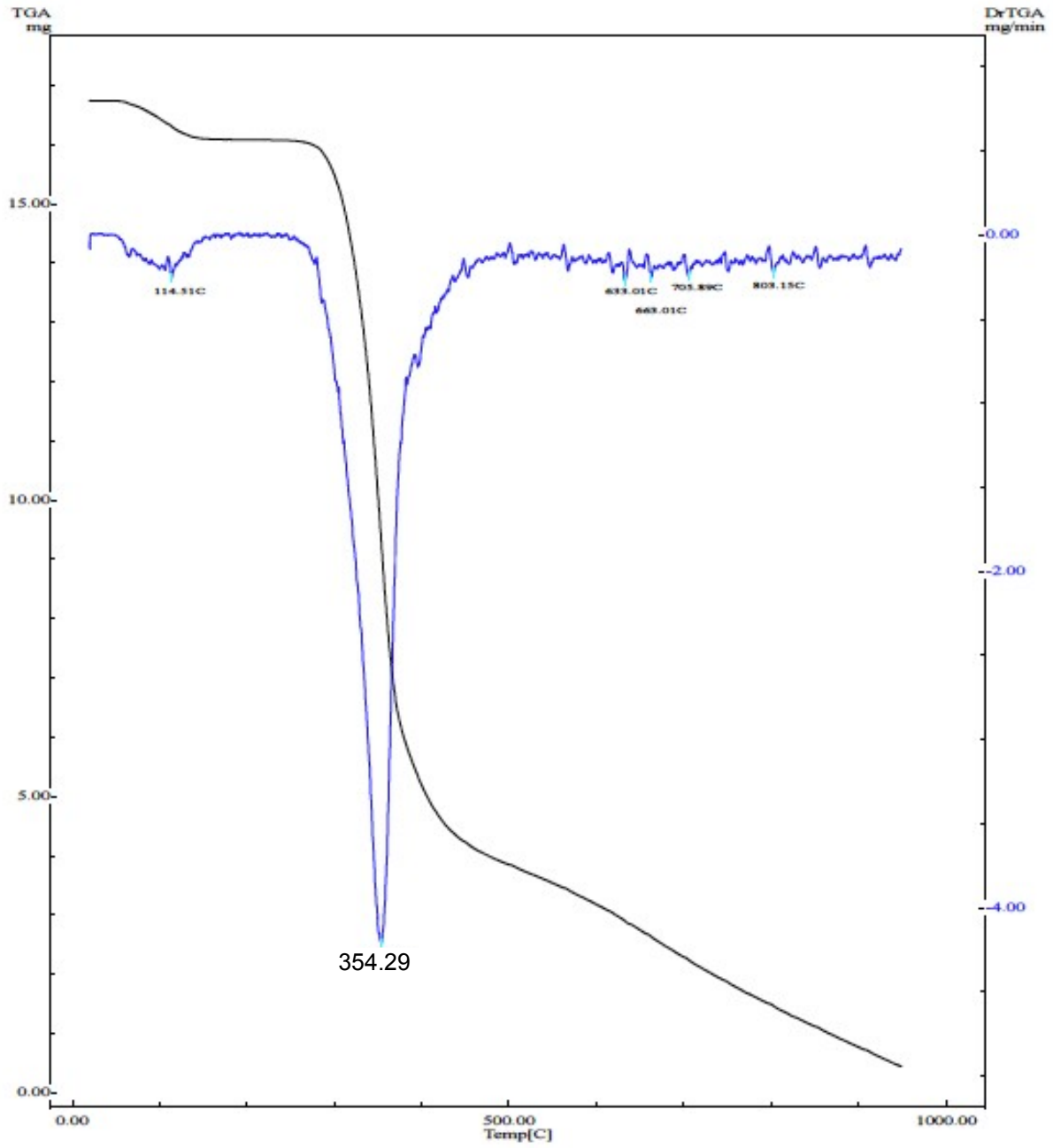
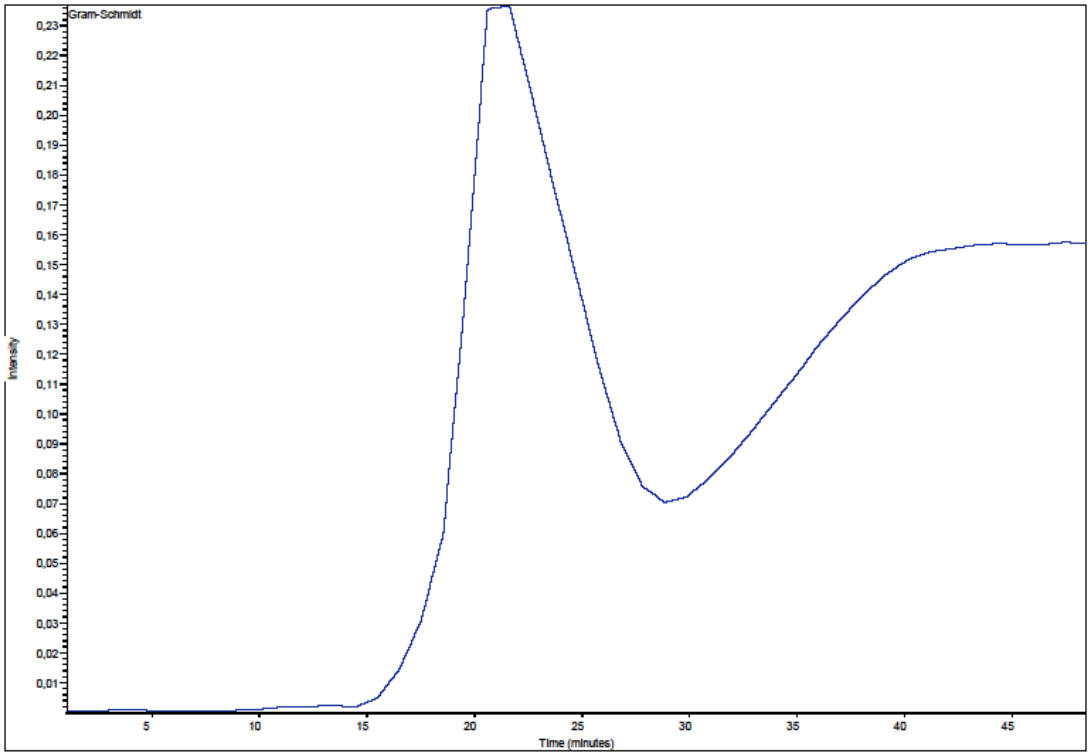



**Figure S5.** Derivative TGA of **pDx5**. In black is shown the evolution of the mass of the sample as a function of the temperature and in blue the first derivative.

(a)




(b)

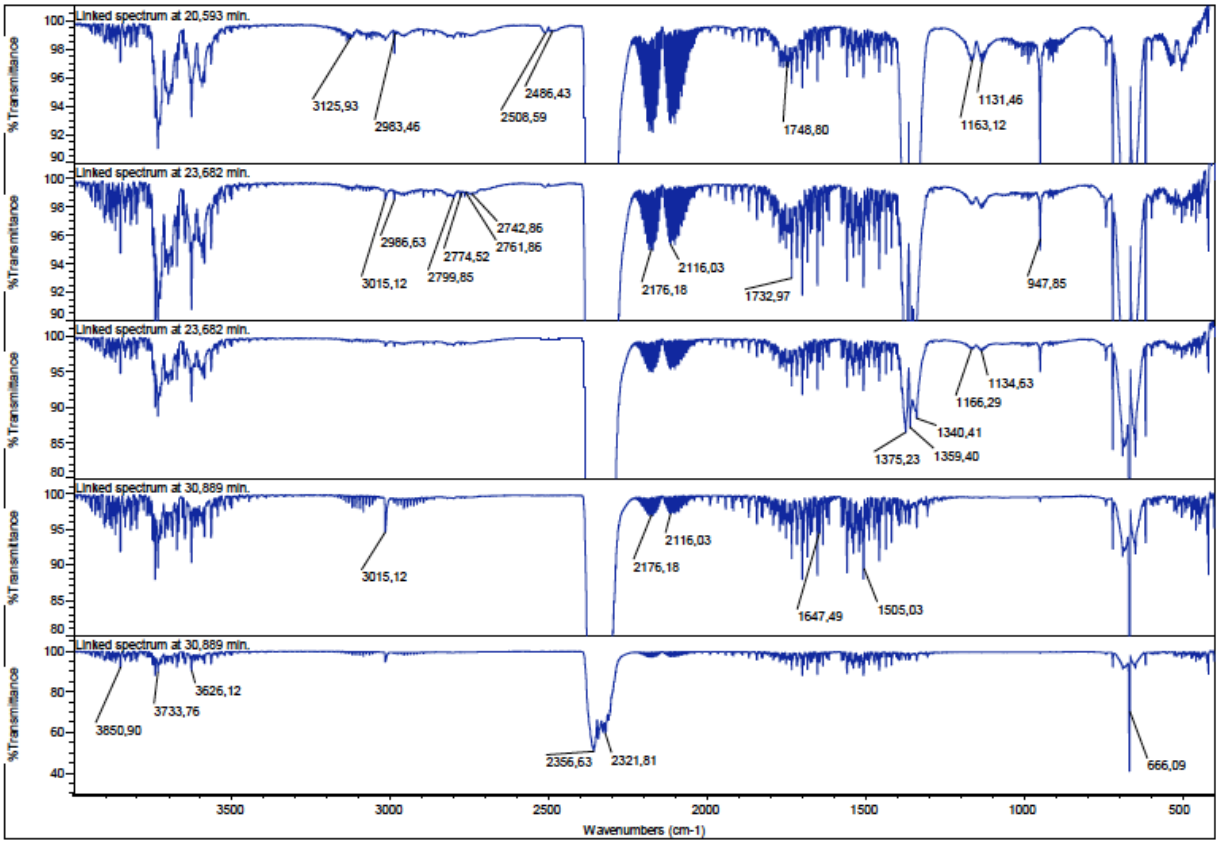
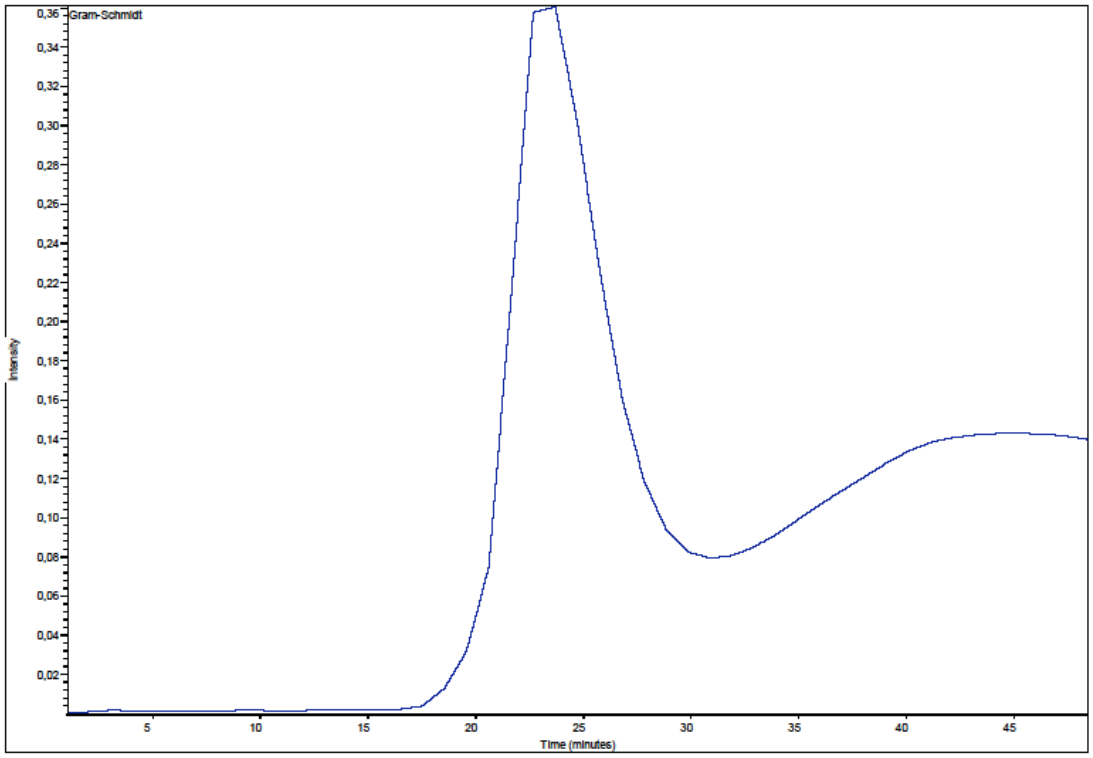



**Figure S6.** IR−TGA of **pDx0**. (a) Gram−Schmidt. (b) Most representative signals at three single time points 20.6 min, 23.7 min and 34.9 min. The delay between the TG and the FTIR detector is from 4 to 5 min.

(a)




(b)

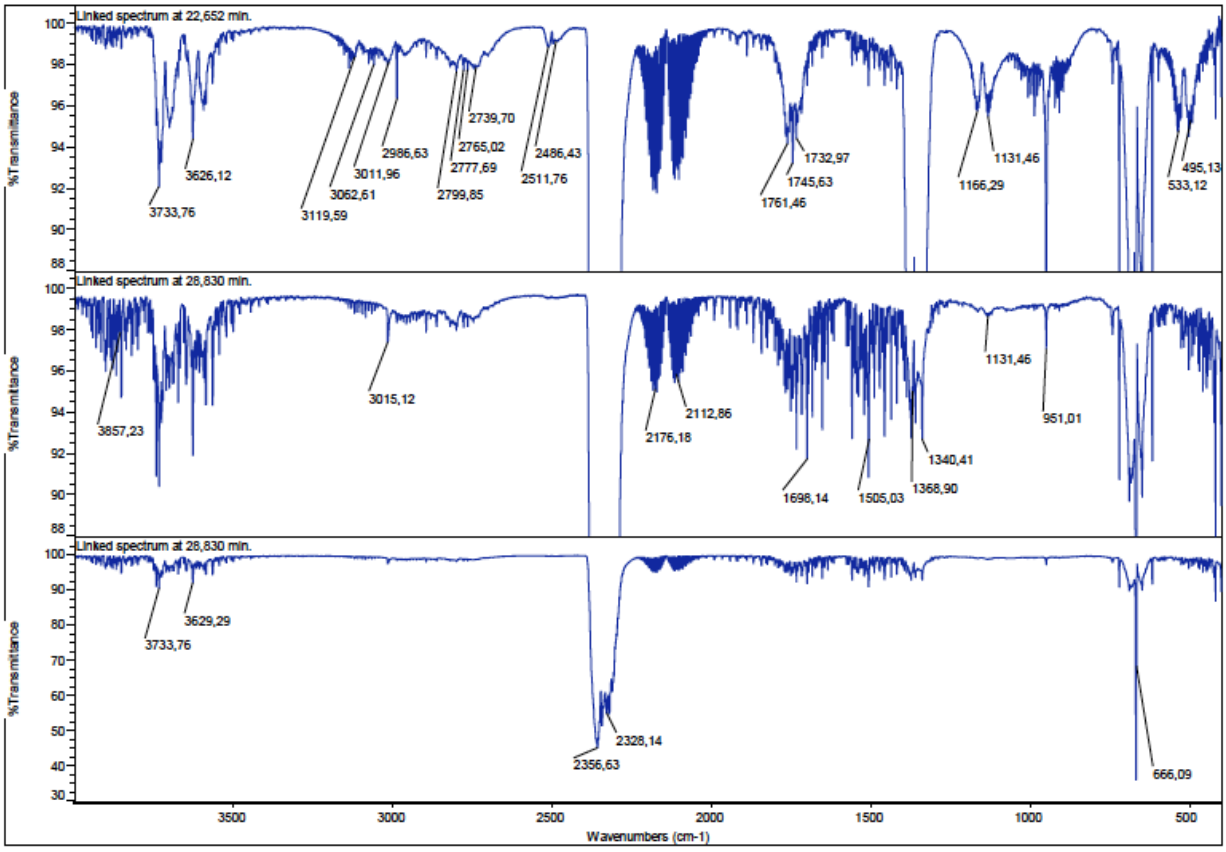
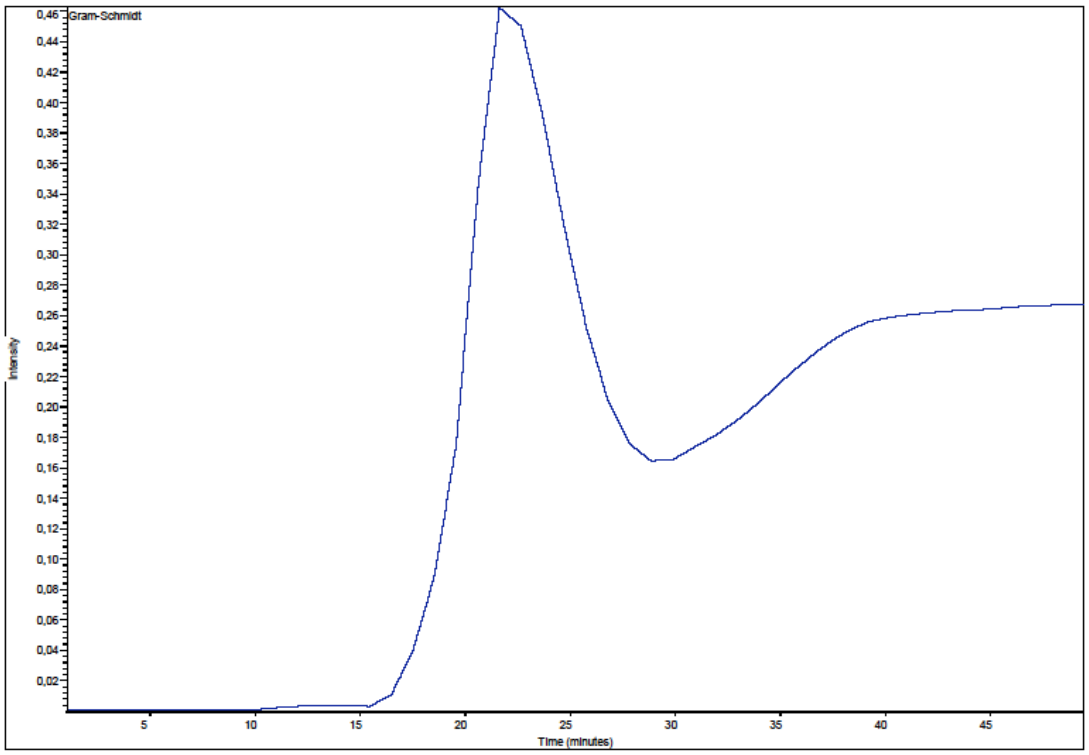



**Figure S7.** IR−TGA of **pDx1**. (a) Gram−Schmidt. (b) Most representative signals at two single time points 22.6 min and 28.8 min. The delay between the TG and the FTIR detector is from 4 to 5 min.

(a)




(b)

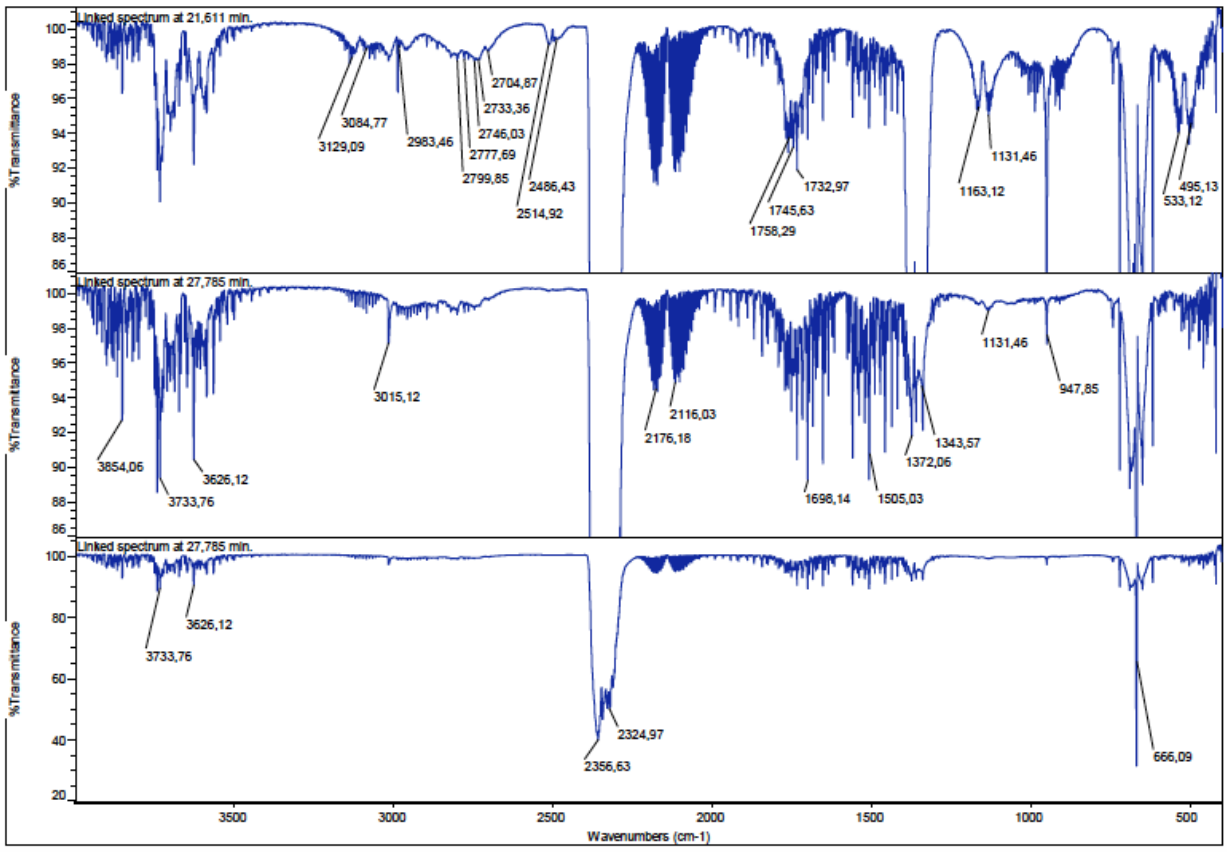



**Figure S8.** IR−TGA of **pDx5**. (a) Gram−Schmidt. (b) Most representative signals at two single time points 21.6 min and 27.8 min. The delay between the TG and the FTIR detector is from 4 to 5 min.

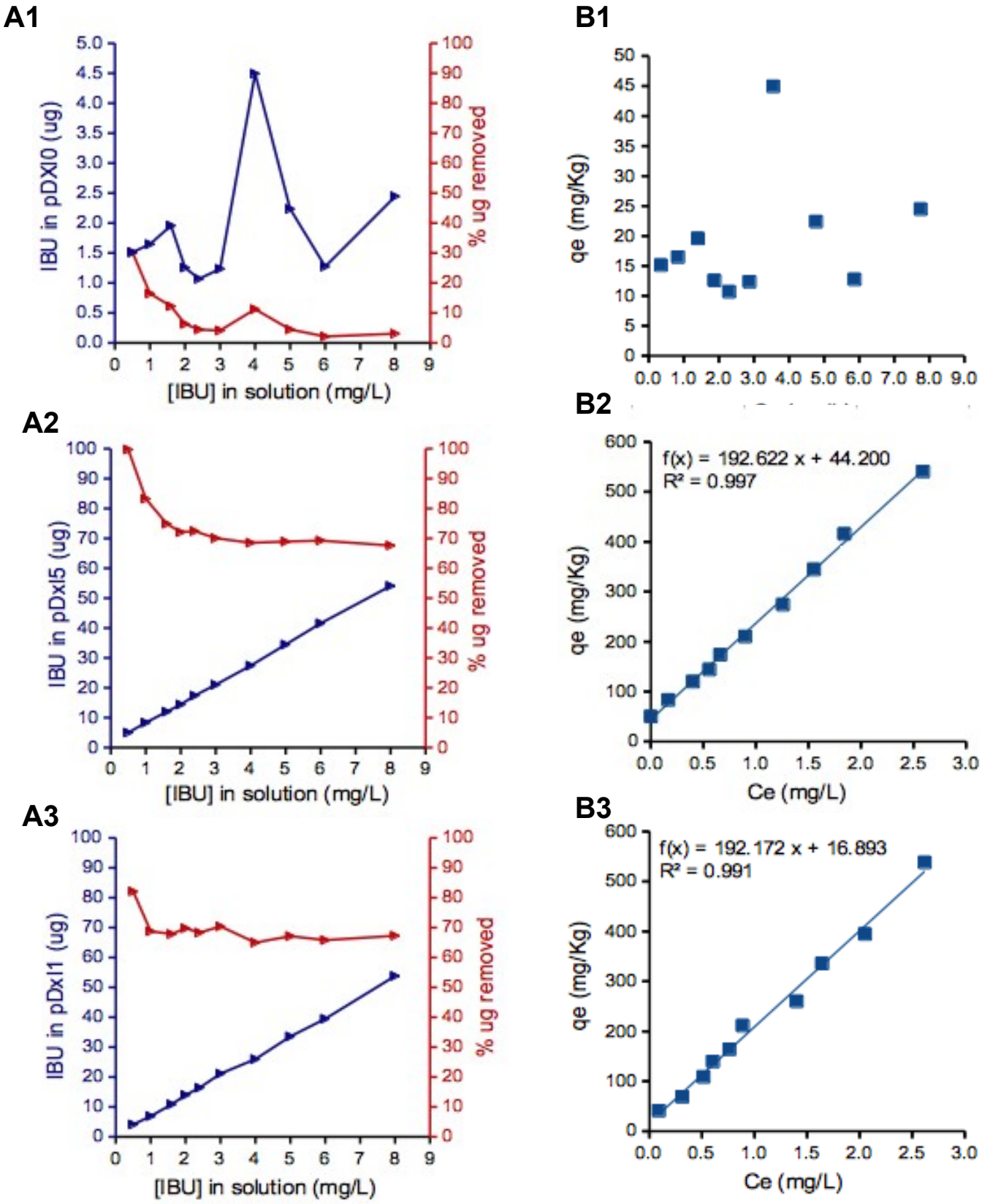



**Figure S9.** Characterization of the polymers **pDx0** (A1 & B1), **pDx1** (A2 & B2) and **pDx5** (A3 & B3) as scavenger of IBU. A: sorption isotherm showing in blue the amount retained by the polymer and in red the percentage removed from the solution as a function of the initial concentration of IBU. B: estimation of Kd.

**Table S1. Mass/volume of reagents used for the synthesis of the polymers**

| Reagent | Mass (g) | Volume (mL) | Resulting pH |
|---|---|---|---|
| Ibuprofen | 0.206 / 1.03 | | |
| Water | | 200 | |
| 0.83 M $Na_2CO_3$ | | 13 | 9.5 |
| | 5.5 hour s of gentle stirring | | |
| DVS | 5.7 | 5 | |
| Water | | 100 | |
| | 30 min of gentle stirring | | |
| 0.83 M $Na_2CO_3$ | | 187 | 12 |
| | 16 hours of gentle stirring | | |

**Table S2**. Equations of the isotherm model assayed for the fitting of the experimental sorption data as defined by ISOT_calc[1].

| **Isotherm (# parameters)** | **Equation ($q_e$ = ...)** | **Parameter definition[2]** |
|---|---|---|
| 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<br>$N$ 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<br>$K_L$ is affinity constant |
| Redlich-Peterson (3) | $S_T \frac{k \cdot C_e}{(1 + C_e)^N}$ | $S_T$ is maximum adsorption capacity<br>$k$ is related to constants of Redlich-Peterson model<br>$N$ 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<br>$S_T$ 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<br>$K_1$ 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 Mahdieh 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.

**Table S3**. Elemental analysis of ibuprofen pre-incubated cross−linked polymers. Results are expressed as means ± SD (n = 3).

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