Supplementary Information

The Role of Water in the Confinement of Ibuprofen in SBA-15

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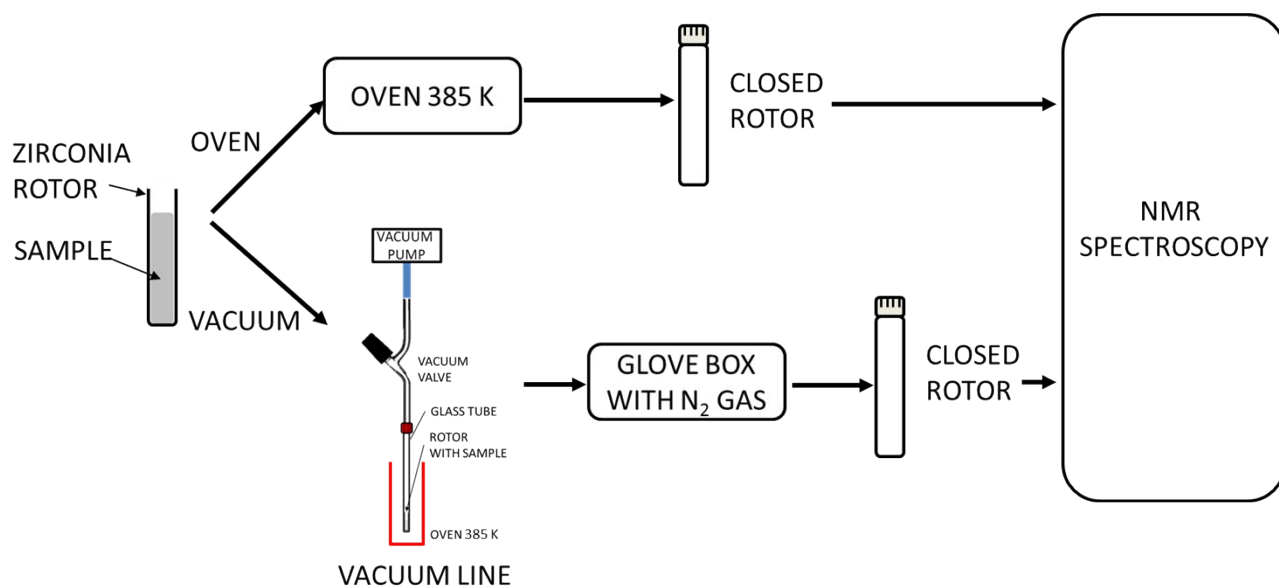
Figure S1. Scheme of experimental procedures and instrumentation for dehydration of samples used in the study.
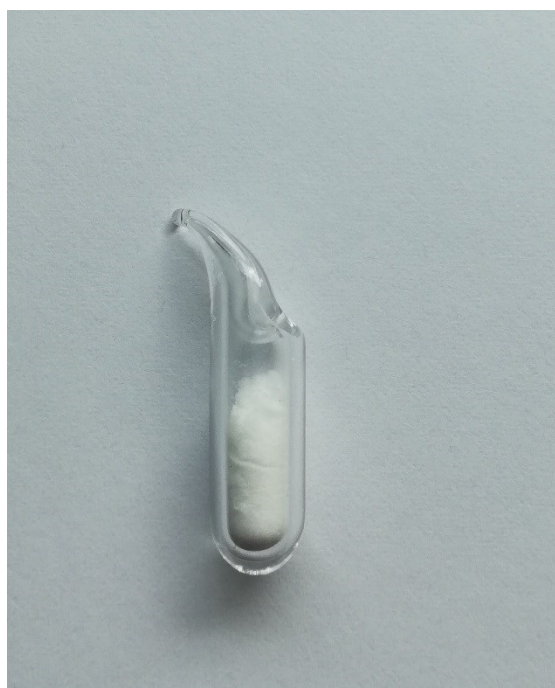

Figure S2. Degassed sample using vacuum treatment used for release studies. After degassing in room temperature for 20 hours, the glass tube with the sample was sealed with gas burner. The sealed tube was immersed in SBF solution and crushed with wooden rod to open the tube and start the release procedure.
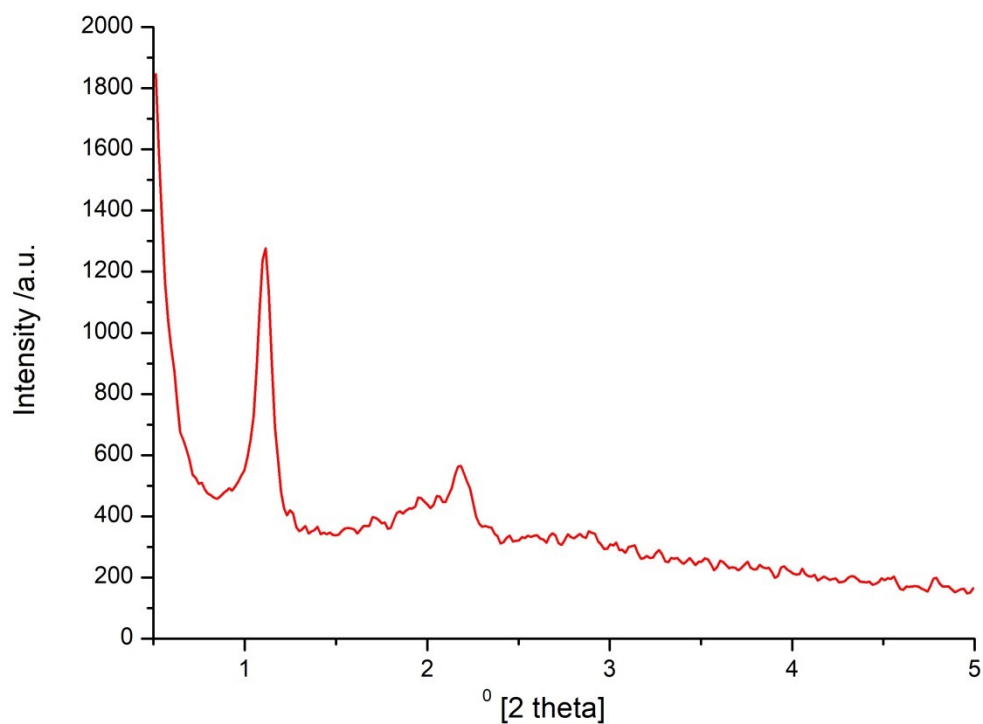
Figure S3. XRD pattern of SBA-15(33) sample after calcination in 673 K for 18 hours. Reflexes at ca. 2 [° 2 Theta] are visible again, which confirms, that hexagonal structure is preserved in the sample under study.
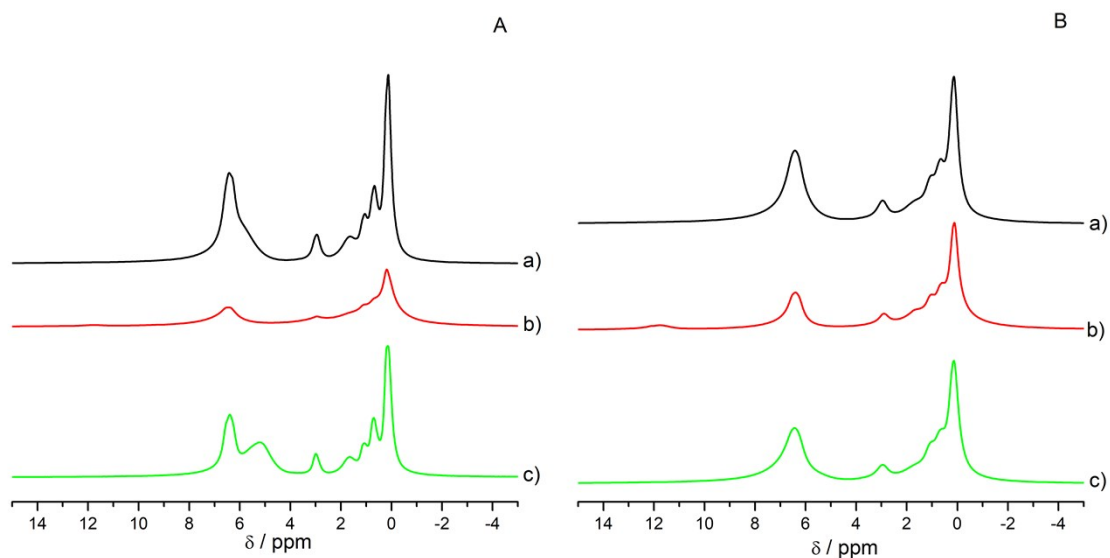

Figure S4. 1H MAS NMR spectra of samples SBA-15 IBU(25) (A) and SBA-15 IBU(33) (B) a) before the thermal treatment, b) after the thermal treatment in a dehydrated state, c) after the contact with atmospheric humidity.
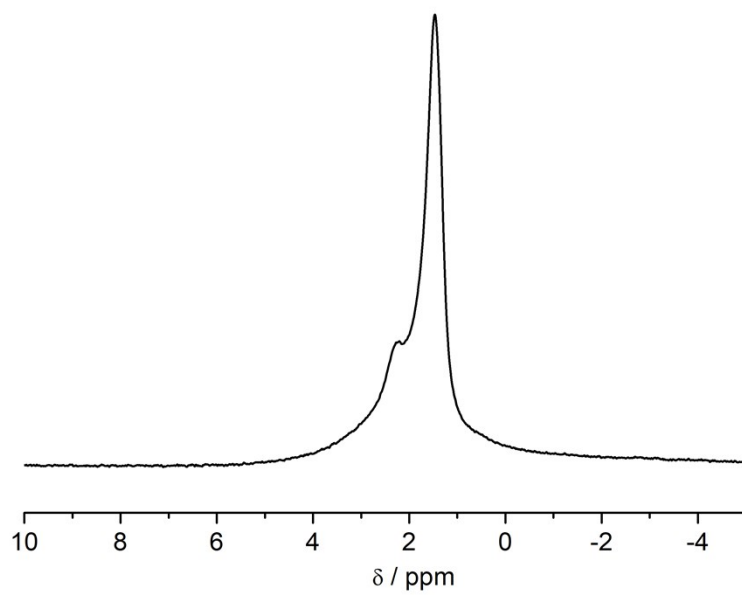
Figure S5. ^{1}H MAS NMR spectrum of SBA-15 in degassed state (after degassing in 573K for 20 hours).
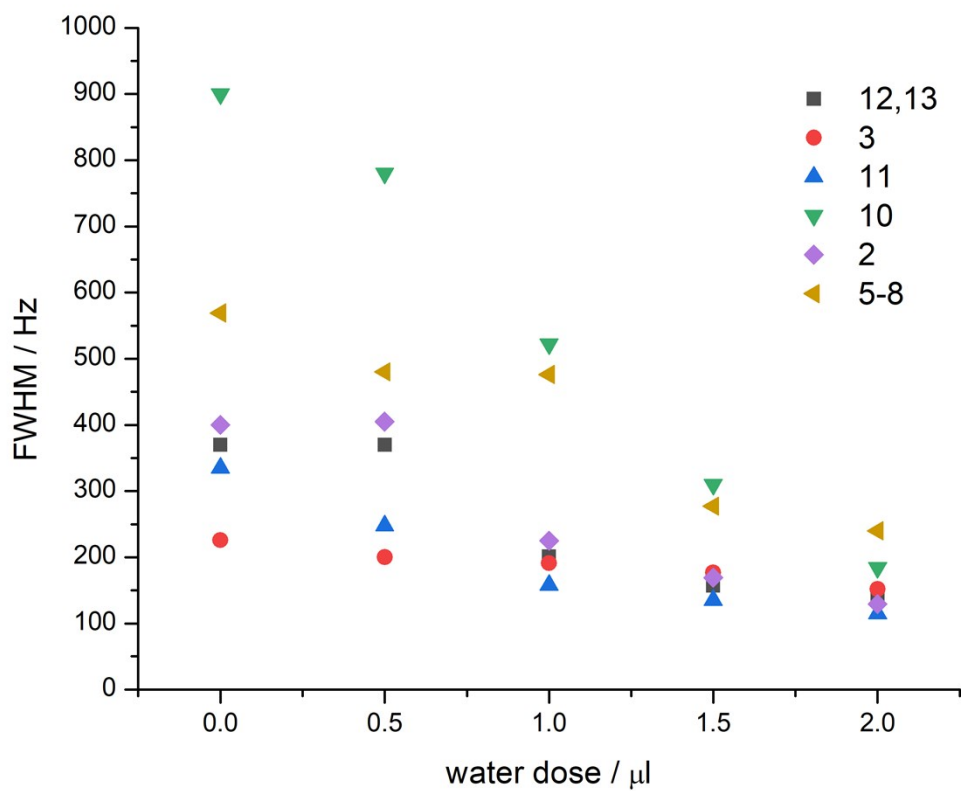
Figure S6. FWHM (full width at half maximum) values of peaks from deconvolutions of ^{1}H spectra of sample SBA-15 IBU(17)vac with varying content of water added to the sample. The numbers corresponds to atoms labeling from Figure 5 in the main text. Proton 10 show the highest decrease in FWHM with increasing water content.
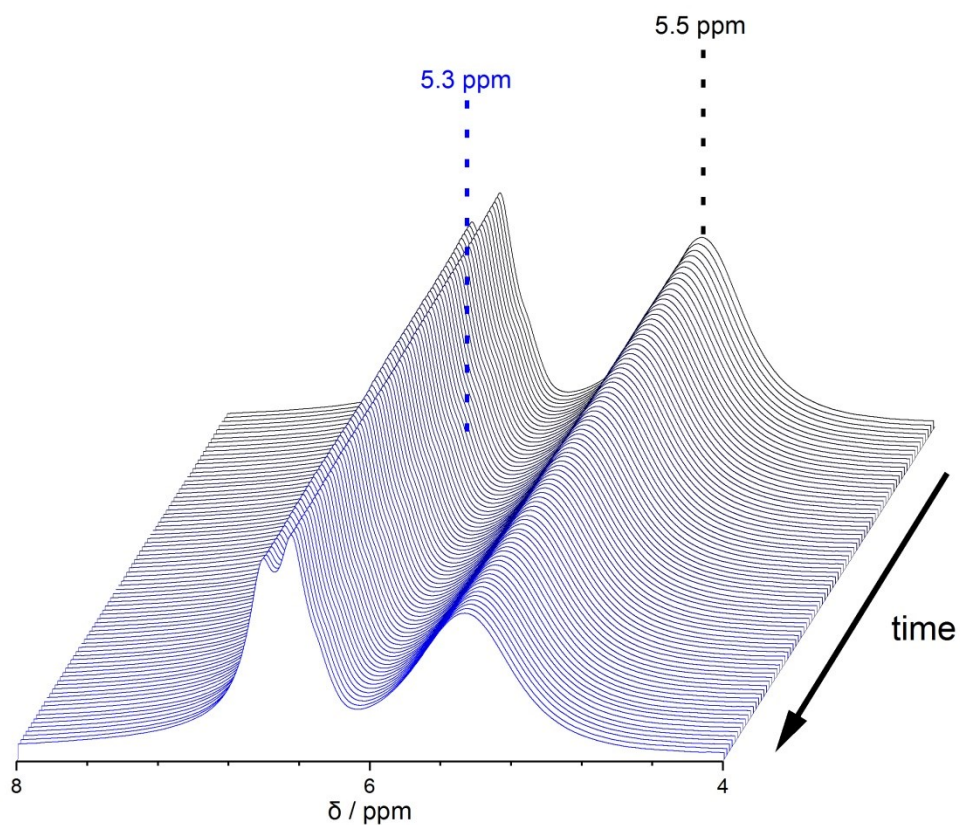
Figure S7. ^{1}H MAS NMR spectra of the sample SBA-15-IBU(17) vac during a constant rotation for 90 minutes. The shift of the peak from 5.5 ppm to 5.3 ppm is observed.
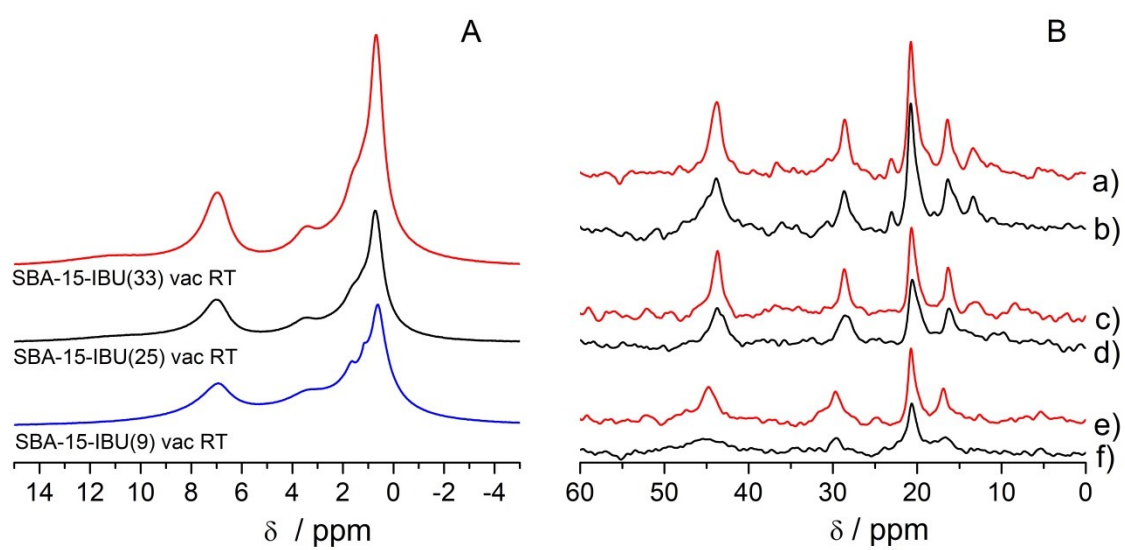

Figure S8. ^{1}H MAS NMR (A), and 13C HPDEC MAS NMR spectra (B) of samples SBA-15-IBU(33) (a), SBA-15-IBU(33) vac RT (b), SBA-15-IBU(25) (c), SBA-15-IBU(25) vac RT (d), SBA-15-IBU(9) (e), SBA-15-IBU(9) vac RT (f) used for release studies.

Table S1. Parameters obtained from the fit of the mathematical models to the release data of the samples under study.

Model	Value	SBA-15-IBU(9)	SBA-15-IBU(9) vac RT	SBA-15-IBU(25)	SBA-15-IBU(25) vac RT	SBA-15-IBU(33)	SBA-15-IBU(33) vac RT
Korsmeyer-Peppas[a]	k [min^{-1}]	0.89	0.97	0.93	0.85	0.78	0.66
	n	0.008	0.005	0.015	0.023	0.045	0.087
	R^2	0.81	0.88	0.57	0.47	0.95	0.84
Gallagher-Corrigan[b]	k_1 [min^{-1}]	3.35	1.86	2.83	2.15	2.50	1.24
	R^2	0.91	0.64	0.57	0.88	0.99	0.99

[a] $F = k \cdot t^n$, [b]
$$F = F_{tmax} \cdot \left(1 - e^{-k_1 \cdot t}\right) + (F_{tmax} - F_B) \cdot \left(\frac{e^{k_2 \cdot t - k_2 \cdot t_{2max}}}{1 + e^{k_2 \cdot t - k_2 \cdot t_{2max}}}\right)$$
, where k – rate constant, F – release fraction, F_{tmax} – maximum fraction released, F_B – fraction of the drug released during the burst effect, k_1 – the first order kinetic constant, k_2 – kinetic constant of the second stage of the release, t_{2max} – time to maximum release rate