

## **3D-printed system optimizing dissolution of hyperpolarized gaseous species for micro-sized NMR**

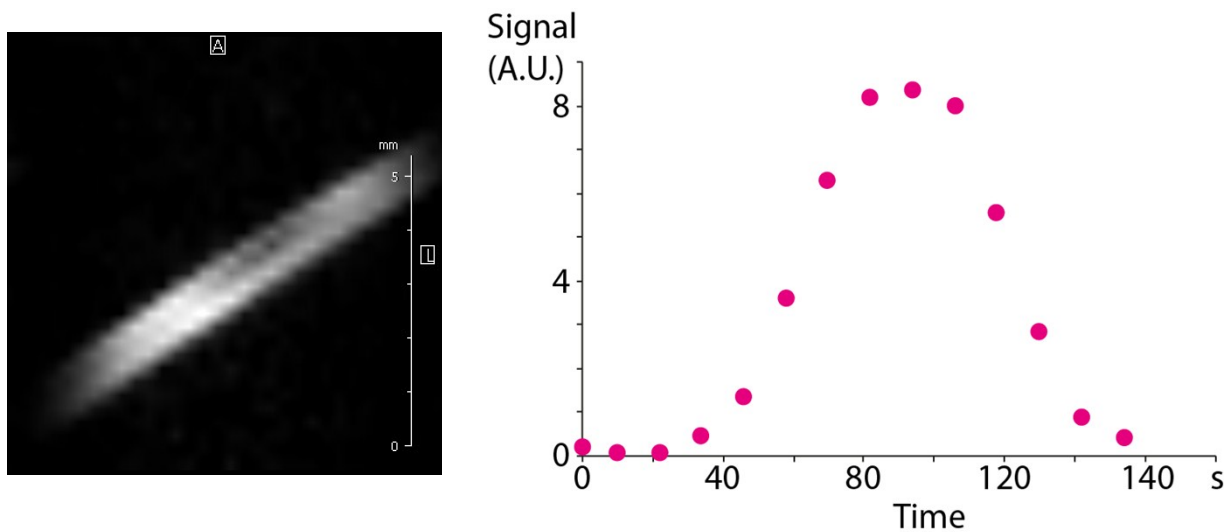
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### Electronic Supplementary Information

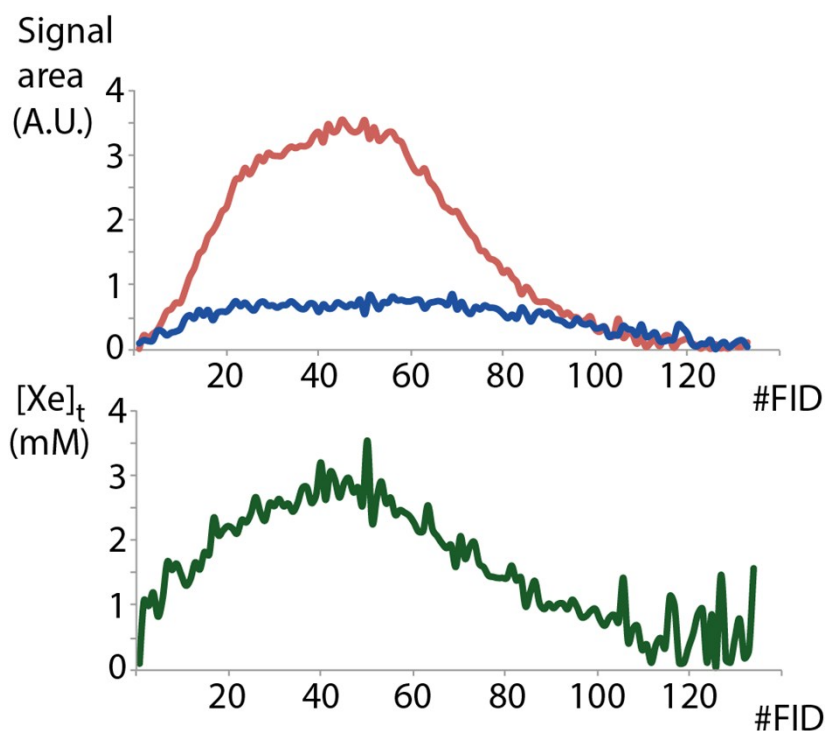
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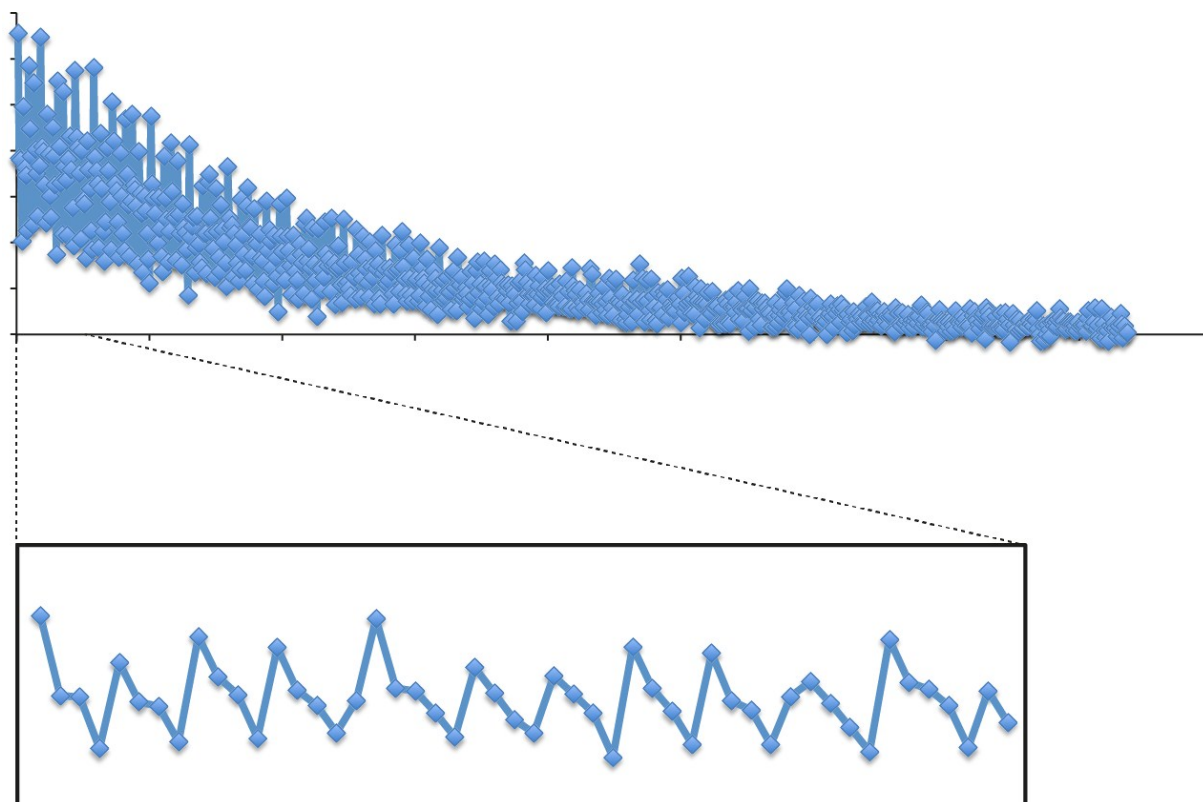
- Figure S1:  $^{129}\text{Xe}$  MR images recorded during the operation of the bubble pump
  - Figure S2: Time evolution of the xenon signals for the experiment of Figure 3.
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**Figure S1.** Left:  $^{129}\text{Xe}$  MR image recorded during the operation of the bubble pump with a FLASH sequence. Experiment time for one image: 1024 ms ; 64 x 64 points ; repetition time : 16ms; echo time : 6ms. Right: normalized intensity.



**Figure S2.** Top: Areas of the signals of dissolved xenon (in red) and of xenon in cryptophane (in blue) according to the FID number, in the experiment of Fig. 3 of the main text. Bottom : Evolution of the estimated xenon concentration, extracted from the previous signal areas.

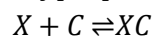


**Figure S3.** Details of the time evolution of the dissolved xenon signal in the experiment of Fig. 4 of the main text, showing the oscillatory character attributable to flow discontinuities.

#### S4. Estimation of the instantaneous concentration of dissolved xenon

When working with highly hyperpolarized species, the drawback is that it is impossible to directly derive the number of molecules from the signal areas, but the advantage is that a  $90^\circ$  rf pulse totally destroys the magnetization.

The in-out exchange of xenon  $X$  with cryptophane  $C$  can be written as:



$$\text{Binding constant } K = \frac{[XC]}{[X][C]}$$

The use of a water solution of cryptophane of known concentration  $[C]_t$ , for which the binding constant with xenon  $K$  is also known enables one to extract the instantaneous concentration of dissolved xenon  $[X]_t$  simply by the measurement of the ratio  $r$  of the area of the two peaks.

$$r = \frac{[X]}{[XC]}$$

$$[X]_t = [X] + [XC] = (r + 1)[XC] = (r + 1)([C]_t - [C])$$

Now  $[C] = \frac{1}{rK}$ ; thus  $[X]_t = (r + 1)([C]_t - \frac{1}{rK})$ .