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# Supplementary Information: Quantifying Apatite Formation and Cation Leaching from Mesoporous Bioactive Glasses in Vitro: A SEM, Solid-State NMR and Powder XRD Study

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**Table S1.** Textural parameters obtained by $N_2$ adsorption porosimetry of the samples deriving from S58 and S85 before and after immersion in TRIS and/or SBF solutions.[a]

| Sample | $S_{BET}$ ($m^2 \cdot g^{-1}$)[b] | $V_P$ ($cm^3 \cdot g^{-1}$)[c] | $D_P$ (nm)[d] |
|---|---|---|---|
| **S58** | 195 | 0.46 | 9.45 |
| **S58-7d$_{20}$** | 90 | 0.29 | 15.15 |
| **S85** | 427 | 0.61 | 5.73 |
| ***sbf*8h$_{20}$** | 366 | 0.56 | 5.61 |
| ***sbf*16h$_{20}$** | 378 | 0.55 | 5.53 |
| ***tris*8h$_{20}$** | 410 | 0.57 | 5.57 |
| ***tris*16h$_{20}$** | 393 | 0.56 | 5.71 |
| ***tris*8h$_3$** | 421 | 0.61 | 5.93 |
| ***tris*16h$_3$** | 428 | 0.61 | 6.01 |

[a]The textural properties of each specimen were obtained by nitrogen adsorption/desorption analyses at −196 ºC on a Micromeritics ASAP 2020 instrument (Micromeritics Co., Norcross, USA). Before each measurement, 50 mg of each sample was degassed under vacuum (<0.3 kPa) at 200ºC during 24 h.

[b]Surface area determined using the Brunauer–Emmett–Teller (BET) method [Brunauer, S.; Emmett, P.H.; Teller, E. *J. Am. Chem. Soc.*, 1938 **60**, 309].

[c]Total total pore volume calculated from the amount of $N_2$ adsorbed at a relative pressure of $P/P_0$= 0.98 according to [Gregg, S.J.; Sing, K.S.W. Adsorption, "Surface Area and Porosity", 2nd ed.; Academic Press, New York, **1982**].

[d]Average mesopore diameter, obtained from the adsorption branch of the isotherm by means of the Barrett–Joyner–Halenda (BJH) method [Barrett, E.P.; Joyner, L.G.; Halenda, P.H. *J. Am. Chem. Soc.* 1951, **73**, 373].

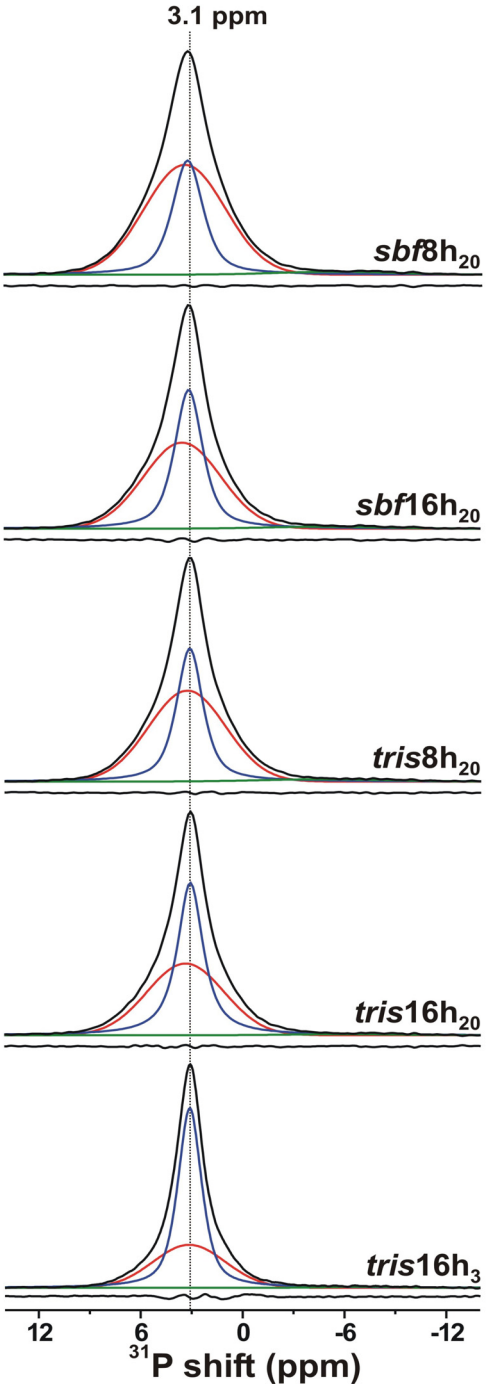


**Figure S1.** Experimental $^{31}$P MAS NMR spectra (black traces) and their deconvolutions into peaks stemming from ACP (red) and H(C)A (blue) contributions. The iterative fitting employed a Gaussian peakshape for ACP and a 65/35 % mixed Lorentzian/Gaussian shape for H(C)A. The curve beneath each spectrum represents the deviation between the experimental and best-fit spectra. The barely visible green peak stems from a minor population of **P**–O–Si moieties of the S85 MBG: see (E. Leonova, I. Izquierdo-Barba, D. Arcos, A. Lopez-Noriega, N. Hedin, M. Vallet-Regí and M. Edén, *J. Phys. Chem. C*, 2008, **112**, 5552) and Fig. 1(a). Their population diminishes rapidly when the MBG is subjected to the SBF/TRIS solutions, and amounts to <2.5% of the total integrated intensity throughout: the relative fractions of the ACP and H(C)A components (listed in Table 1) were renormalized to a unity sum.

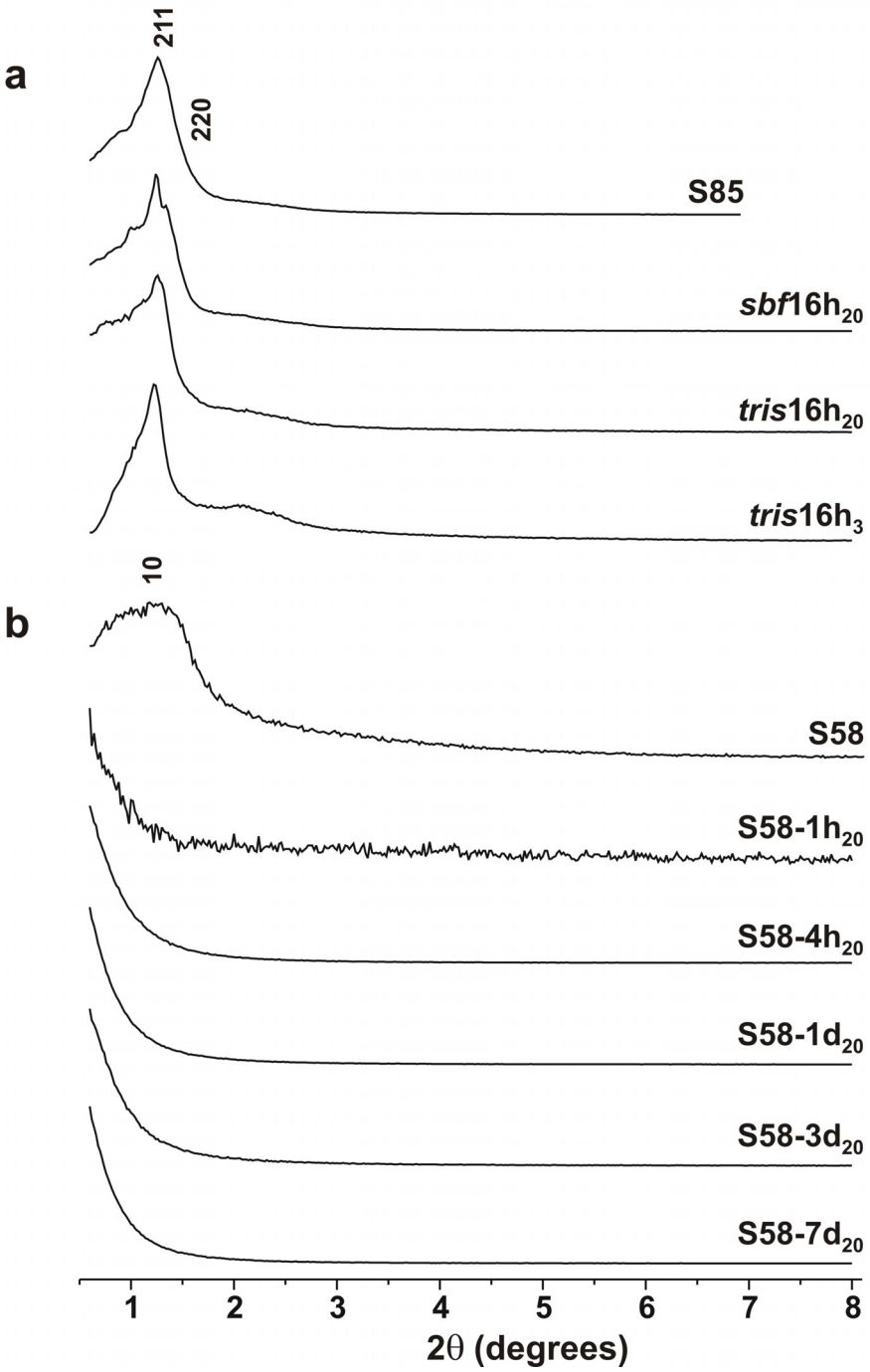


**Figure S2.** Small angle PXRD patterns recorded from the as-indicated specimens of (a) S85 and (b) S58 before and after immersion in SBF and/or TRIS solutions. The PXRD patterns of the pristine S85 and S58 MBGs are characteristic of 3D bicontinuous cubic and 2D hexagonal mesoporous arrangements, respectively, as indicated by the indexed diffraction maxima. After *in vitro* exposure, the S58 MBG structure degrades rapidly, whereas the mesoporous arrangement of the S85 structure remains intact. The diffraction patterns were collected over a 2θ range between 0.6º and 8º, with a step size of 0.02º and a counting time of 0.5 s per step, using a Philips X'Pert diffractometer (Cu $K_\alpha$ radiation; λ=1.5406 Å).

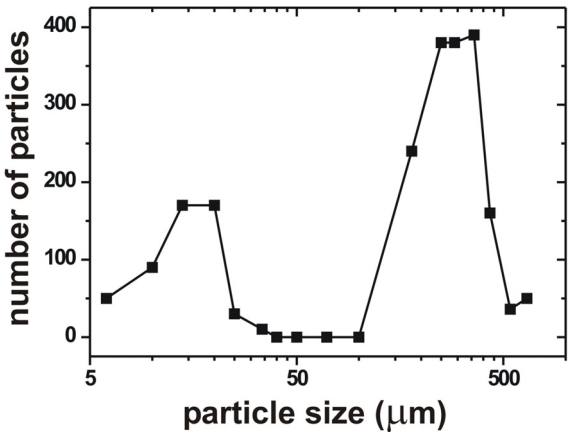


**Figure S3.** Distribution of particle sizes of the pristine S85 sample prior to SBF/TRIS immersion.