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# Supporting information

## Supramolecular Association of 2D Aluminosiloxane Aquagel Building Blocks to 3D Porous Cages and its Efficacy for Topical and Injectable Delivery of Fluconazole, an Antifungal Drug

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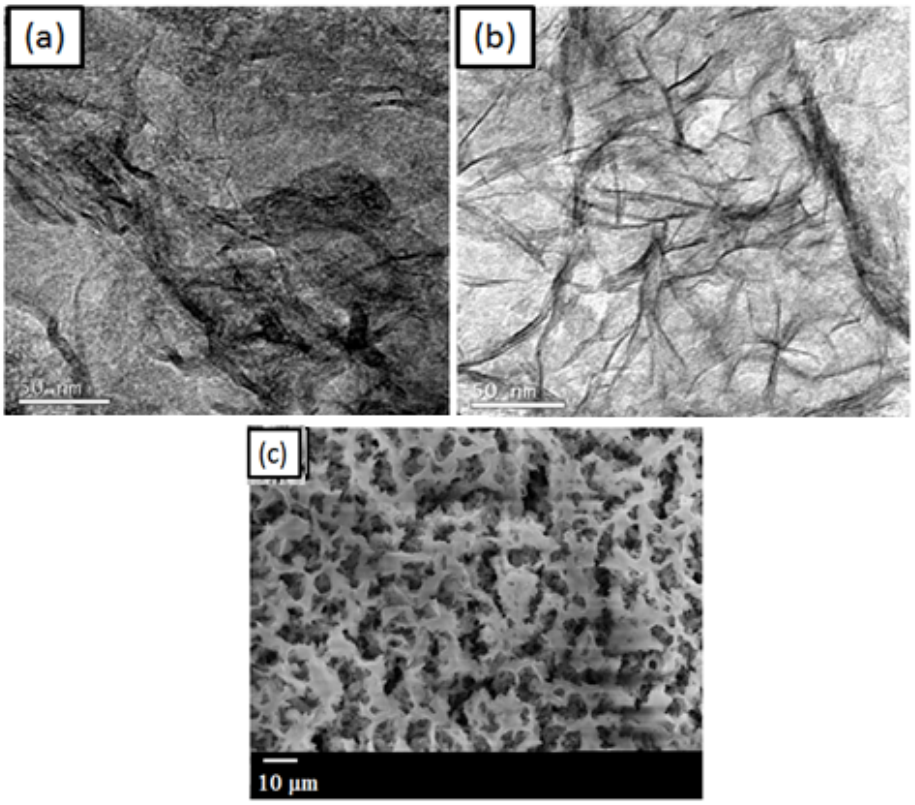

Figure S1. (a-b) TEM and (c) SEM images of the ALS aquagel.

Table S1. Yield stress and hysteresis loop area values obtained in flow mode of rheological experiment.

| Serial no: | $H_2O$/Al | Al/APTMS | Yield stress (Pa) | Hysteresis loop area ( Pa/s) |
|---|---|---|---|---|
| **1** | **60** | **0.2** | **85.5±15** | **1685** |
| **2** | **70** | **0.2** | **49.6±15** | **885** |
| **3** | **80** | **0.2** | **39.5±15** | **578** |
| 4 | 90 | 0.2 | 15.5±15 | 198 |
| 5 | 100 | 0.2 | 6.0±15 | 9 |
| 6 | **80** | **0.1** | **45.5±15** | **736** |
| 7 | **80** | **0.2** | **33.4±15** | **646** |
| 8 | **80** | **0.4** | **25.7±15** | **619** |
| 9 | **80** | **0.6** | **21.3±15** | **452** |
| 10 | **80** | **0.8** | **16.1±15** | **378** |

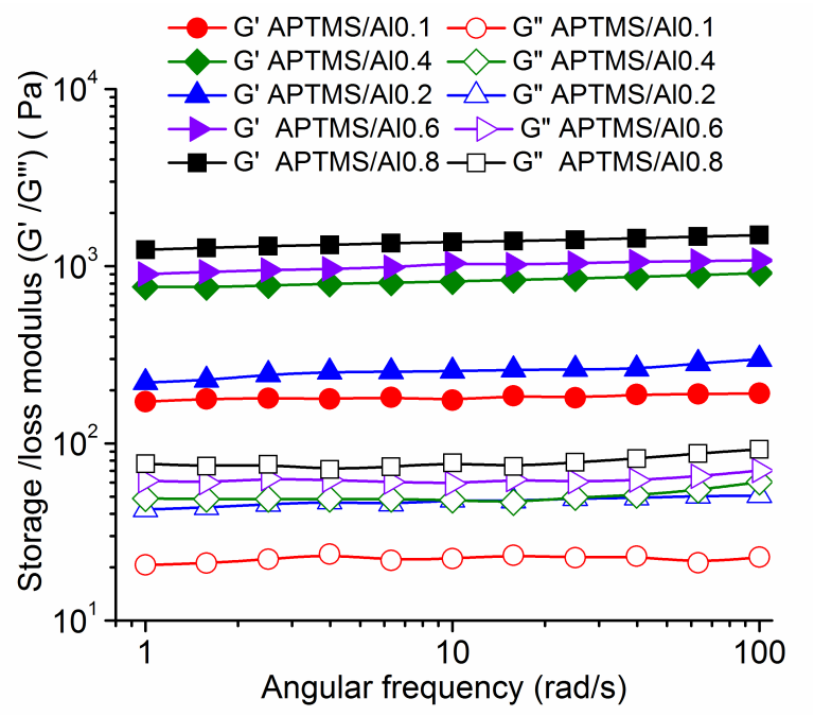


Figure S2. Angular frequency sweep experiments of ALS aquagel prepared with different APTMS concentrations for fixed 0.1% strain.

Table S2. The values of storage modulus (G') and loss modulus (G'') at a fixed strain of 0.1% for ALS aquagel.

| Serial no: | $H_2O$/Al | Al/APTMS | Storage modulus (G') (Pa) | Loss Modulus (G") (Pa) |
|---|---|---|---|---|
| 1 | 80 | 0.1 | 1201±10 | 95±10 |
| 2 | 80 | 0.2 | 978±10 | 62±10 |
| 3 | 80 | 0.4 | 797±10 | 48±10 |
| 4 | 80 | 0.6 | 250±10 | 42±10 |
| 5 | 80 | 0.8 | 40±10 | 25±10 |

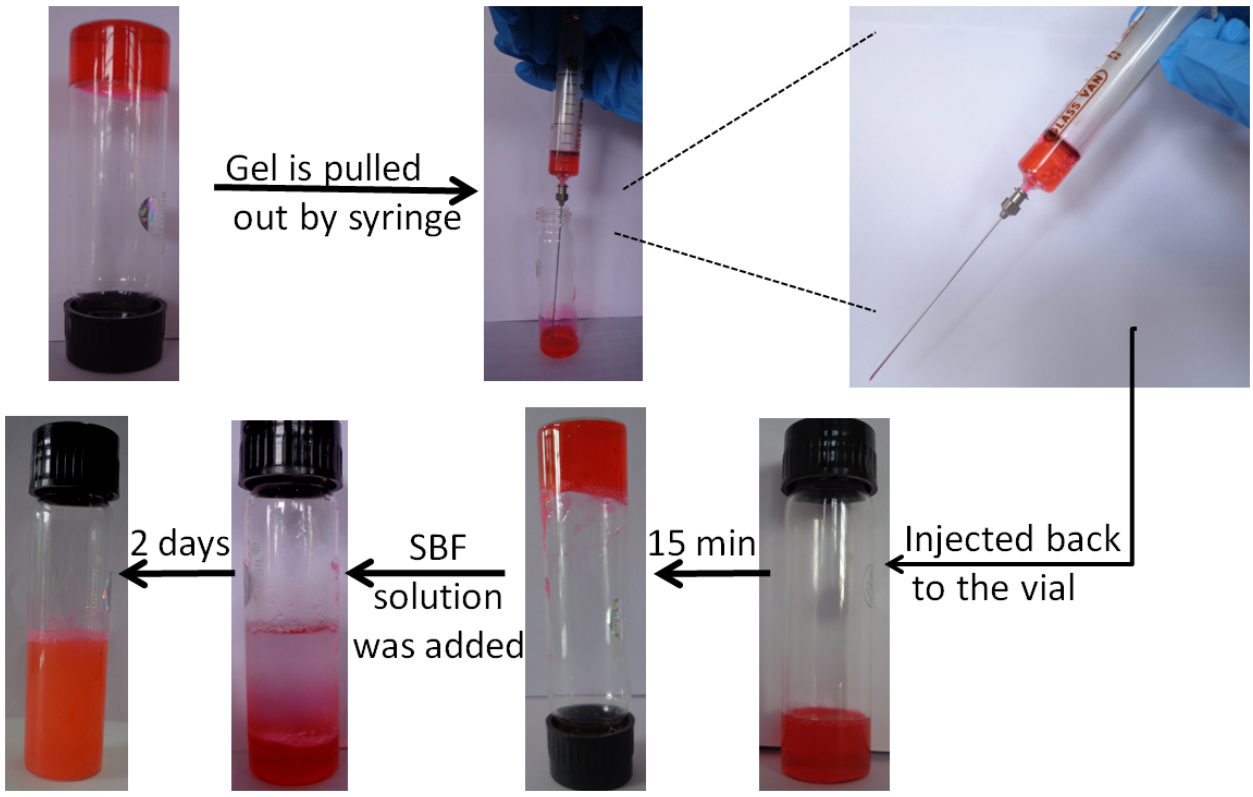


Figure S3. Demonstration of the injectable nature of the ALS aquagel and its release phenomenon using rhodamine B dye.

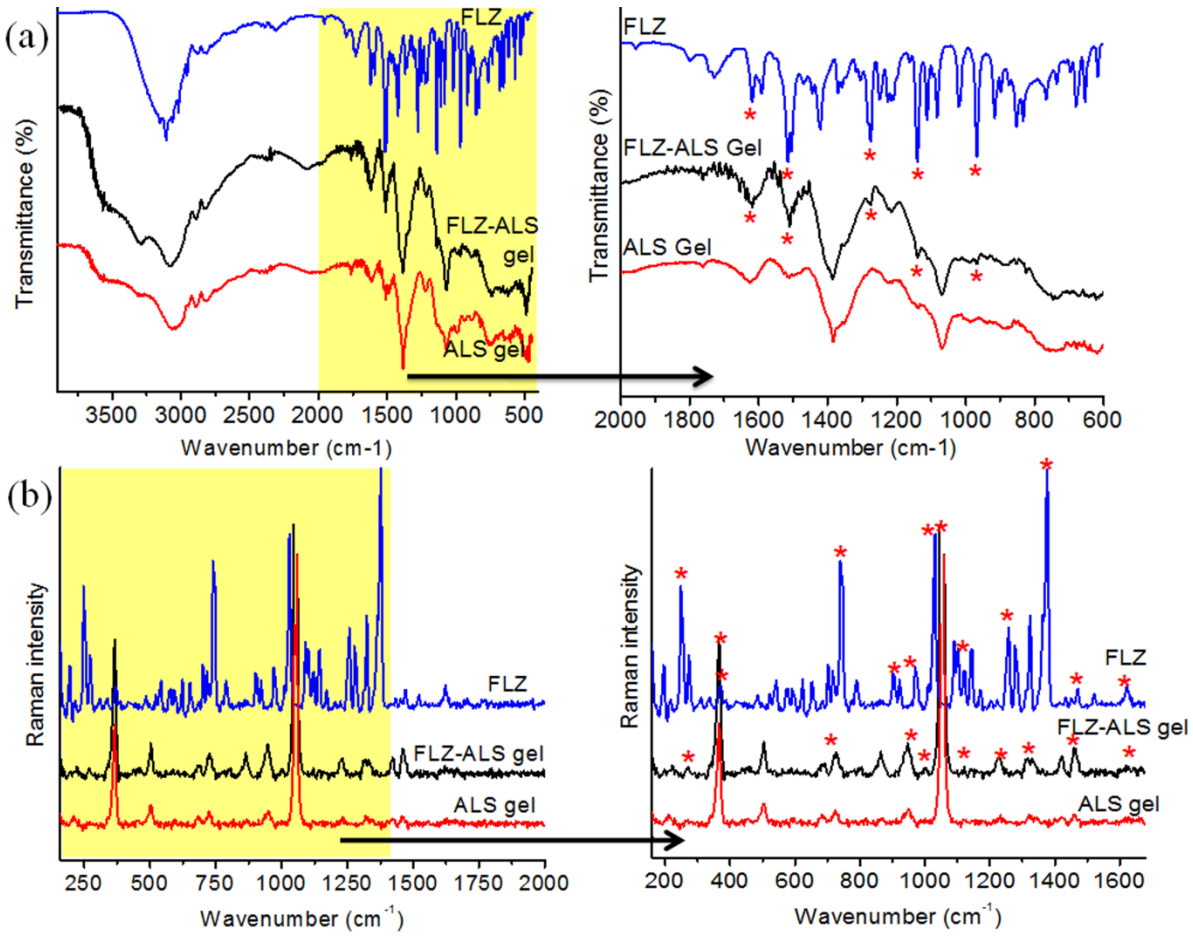


Figure S4. FTIR (a) and Raman (b) spectra of ALS aquagel, FLZ-ALS aquagel and pure FLZ drug. Marked by the asterisks are structure-sensitive bands of FLZ in FLZ-ALS aquagel.

Table S3. Wavenumber ($cm^{-1}$) of observed bands in infrared and Raman spectra of FLZ[1].

| Assignments | Raman | FTIR |
|---|---|---|
| H-bonded OH stretching | **--** | **3022** |
| C=C stretching aromatic ring | **1618** | **1620** |
| C=C stretching aromatic ring | **1376** | -- |
| Triazole ring stretching /C =C stretching aromatic ring | **1471** | **1467** |
| C =C stretching aromatic ring/ ring stretching of triazole group | **1376** | - |
| C-F stretching of 2, 4 difluoro-benzyl group/OH deformation | **1255** | **1274** |
| β-C-H triazole ring | 1217 | 1223 |
| Triazole ring breathing | **1135** | 1143 |
| C-OH str./CH deformation of 2, 4 difluorobenzyl group | 1086 | 1081 |
| β-CH aromatic ring/C-(OH) stretching of propane backbone | **1027** | 1019 |
| β-CH aromatic ring | **969** | **968** |
| Triazole ring deformation | **903** | 919 |
| γ-CH aromatic ring | **745** | 738 |
| Skeletal and ring deformation | **243,367** | - |

1. Cyr, T. D.; Dawson, B. A.; Neville, G. A.; Shurvell, H. F., Spectral characterization of fluconazole. *J. Pharm. Biomed. Anal.* **1996,** *14*, 247-255.

Table S4. Kinetic models used for analysis of drug release data from ALS aquagels

| Model name | Equation | Parameters definition |
|---|---|---|
| Zero order | $F = Q + kt$ | F amount of drug release at time t, Q is the initial amount of drug in the solution (most times Q=0) and k is the zero order release constant |
| First order | $F = 100\ (1- e^{(-kt)})$ | F amount of drug release at time t, and k is the first order kinetic constant |
| Higuchi | $F = k(t)^{1/2}$ | F amount of drug release at time t, k is the rate constant |
| Korsmeyer-Peppas | $F = kt^n$ | F is the amount of drug release, *n* is the value release exponent, and k is the release constant |

Table S5. Properties of the Kinetic Model Parameters for Drug-Release Studies at pH 7.4.

| Drug formulations | Kinetic models and related parameters | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | First Order | | Korsmeyer-Peppas | | | Higuchi | | Zero Order |
| | $R^2$ | k | $R^2$ | k | n | $R^2$ | k | $R^2$ |
| FLZ-ALS0.2 | 0.9576 | 0.0744 | 0.9681 | 14.1727 | 0.556 | 0.9952 | 13.2271 | 0.97716 |
| FLZ-ALS0.4 | 0.9356 | 0.0744 | 0.9591 | 12.1447 | 0.596 | 0.9832 | 12.2371 | 0.98984 |
| FLZ-ALS0.6 | 0.8947 | 0.0744 | 0.9421 | 11.7949 | 0.636 | 0.9898 | 11.6511 | 0.98783 |
| Flucos gel | 0.9165 | 0.0744 | 0.9011 | 13.678 | 0.686 | 0.9767 | 11.6971 | 0.96934 |

**S1. Procedures for H9c2 cell culture**: H9c2 cell lines (immortalized ventricular myoblasts from rat embryo) were purchased from ATCC. They were maintained in cell culture flasks containing Dulbeccos Modified Eagle's Medium (DMEM) with 10% fetal bovine serum (FBS), antibiotics (100 U/ml Penicillin and 100µg/ml streptomycin) and amphotericin (0.25µg/ml) at 37 $^{o}$C with 5% $CO_2$ in air and 99% humidity. Medium renewal was carried out every 2-3 days. Passaging of cells was carried out on 70% confluency. The confluent cells in cell culture flasks were treated with 0.25% trypsin and 0.02% EDTA in phosphate buffered saline (PBS) and placed at 37 ˚C in $CO_2$ incubator for 1 minute allowing the cells to detach from the surface. After the detached cells were viewed under phase contrast microscope, the trypsin present in the flask was inactivated using DMEM containing 10% FBS. The cells were then centrifuged at 3000 rpm for 2 min and the pellet (cells) formed was resuspended in 10% FBS supplemented medium and plated at a concentration of $1x10^5$ cells in cell culture flasks (for the purpose of maintenance) or seeded at appropriate densities in well plates for experiments to be carried out.