Article

Spatial-Temporal Heterogeneity in Large Three-Dimensional Nanofibrillar Cellulose Hydrogel for Human Pluripotent Stem Cell Culture

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FTIR for cellulose

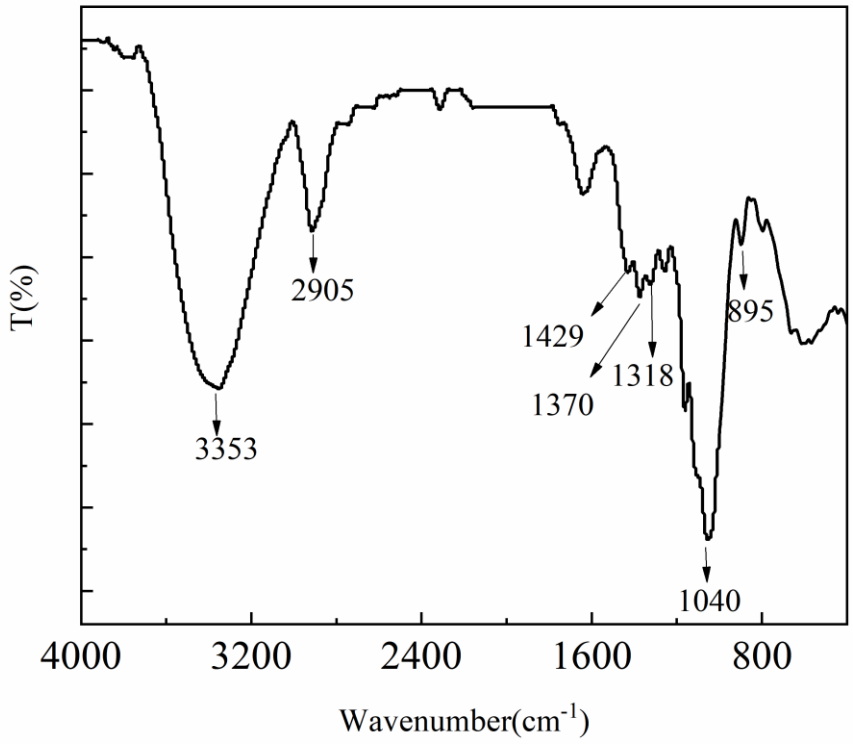

Figure S1. FTIR for cellulose.

Cell morphology in hydrogel with different thickness

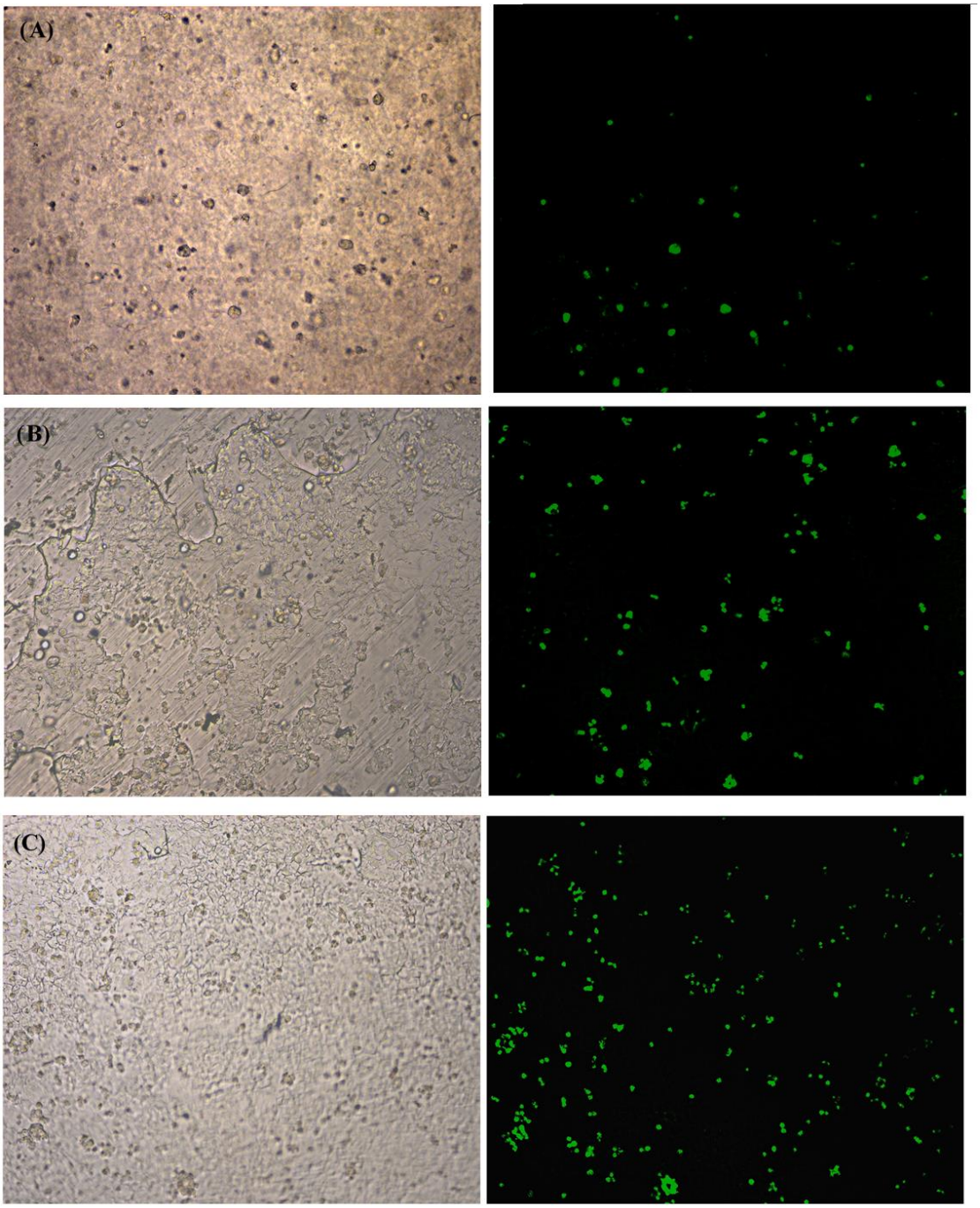

Figure S2. Cell morphology at day1 (A) 2mm (B) 3.5 mm (C) 5mm.

Cell viability after 1 day of culture

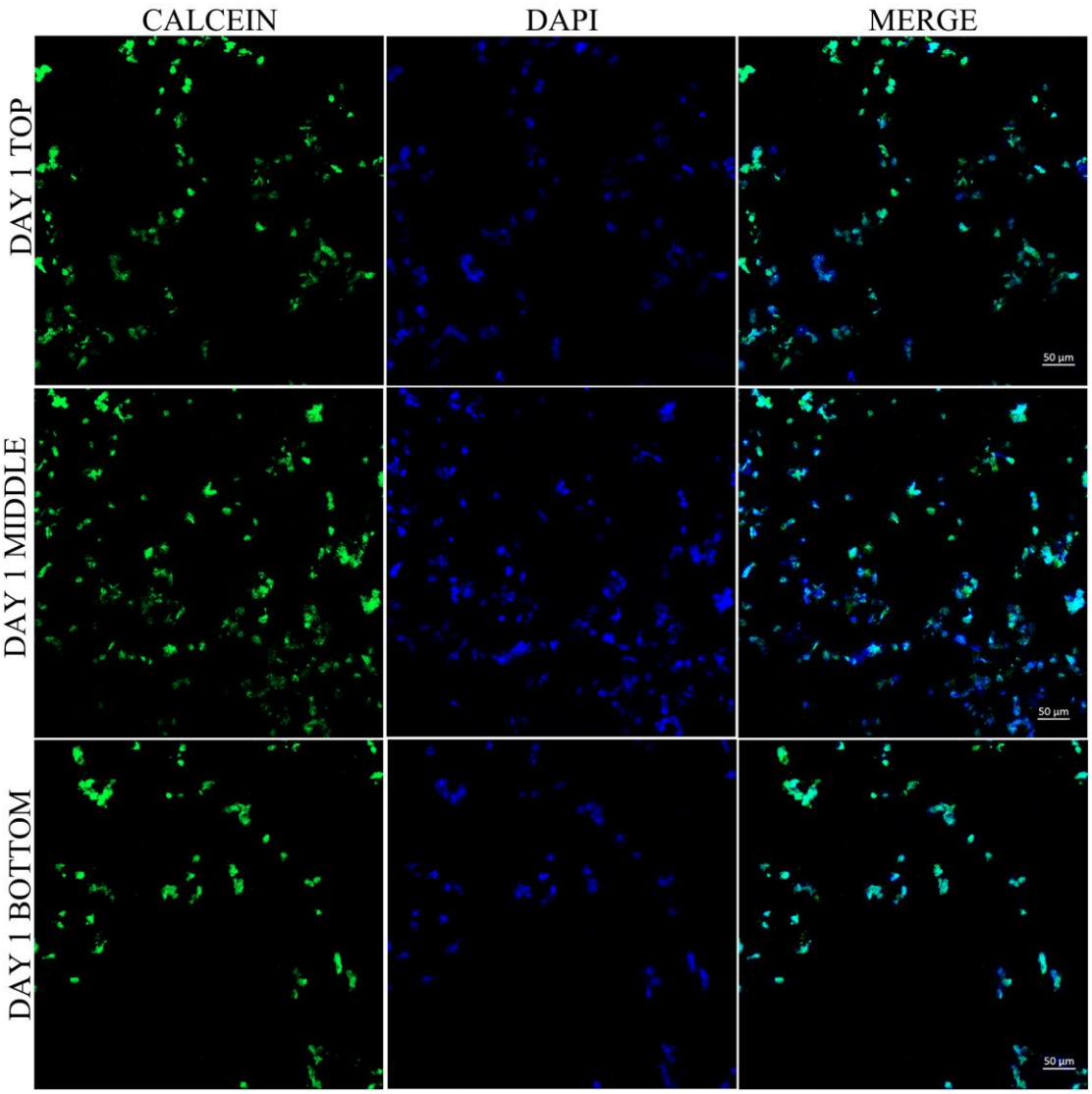

Figure S3. Cell viability at different locations after 1 day of culture.

Cell viability after 3 day of culture

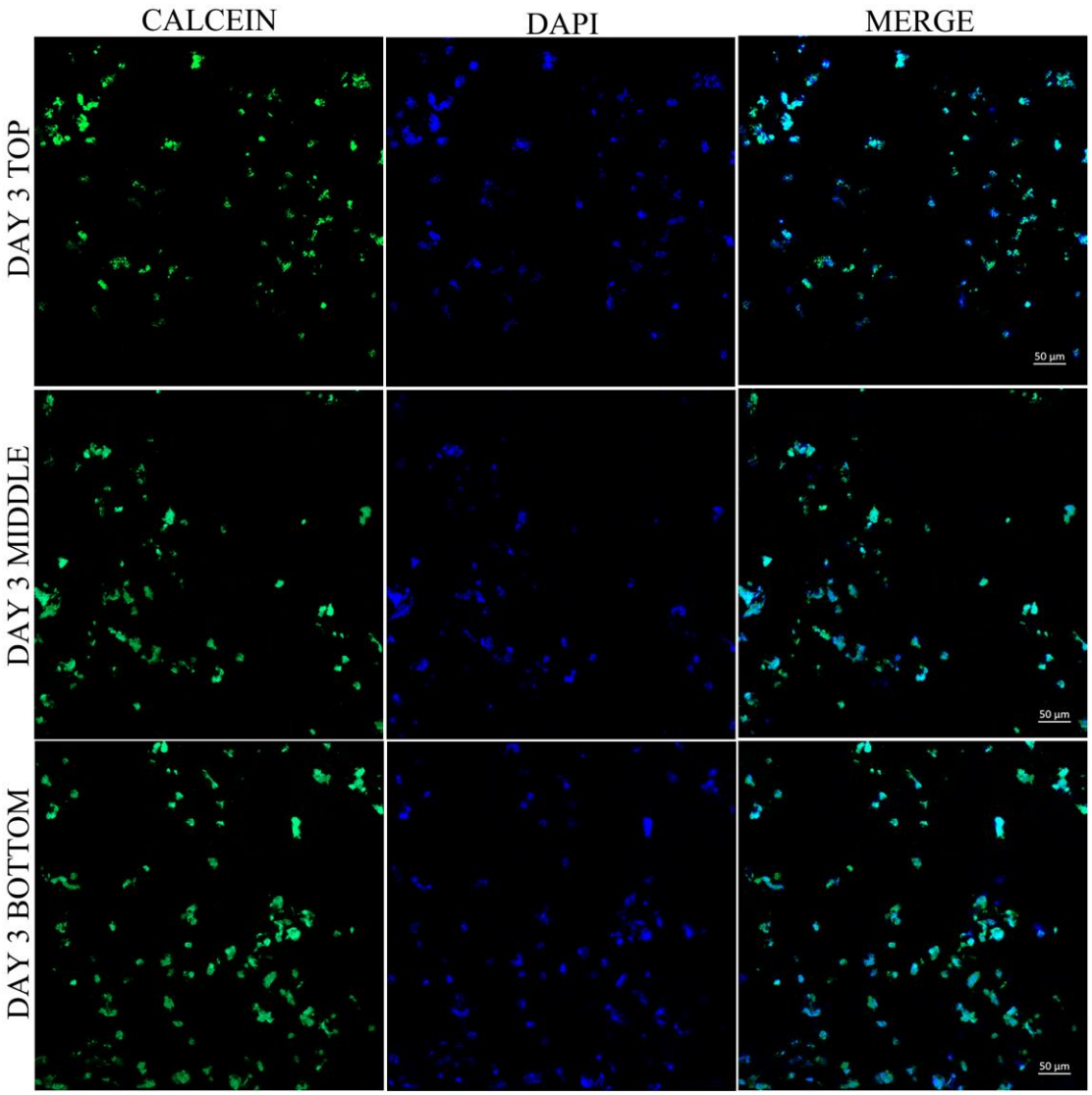

Figure S4. Cell viability after 3 days of culture.

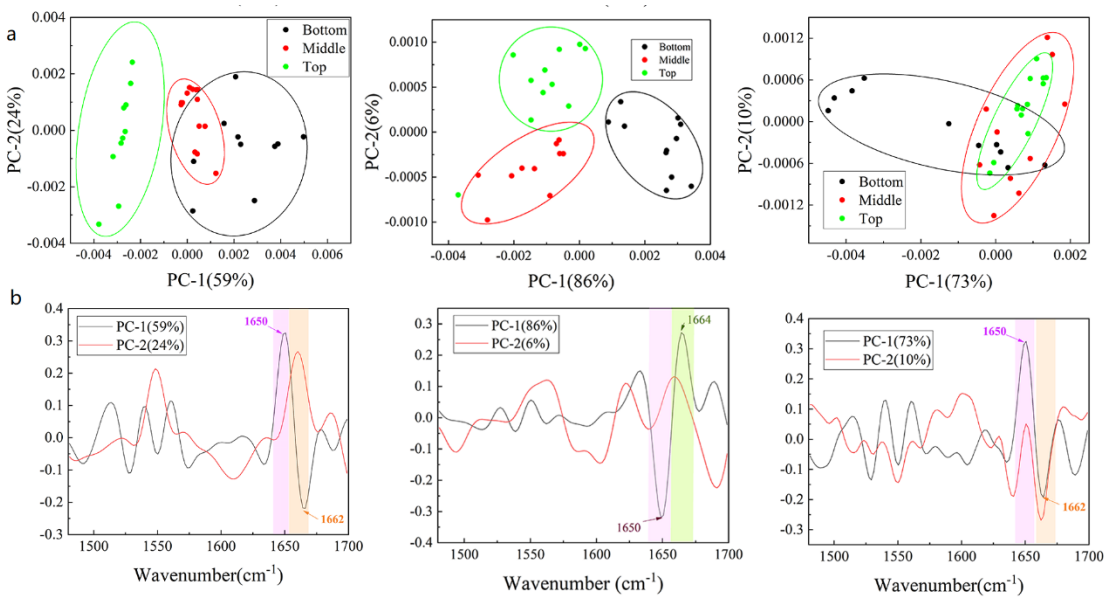

Figure S5. Score and loading plots of PCA at the different zones (left day 1, middle: day 3, right: day 5).

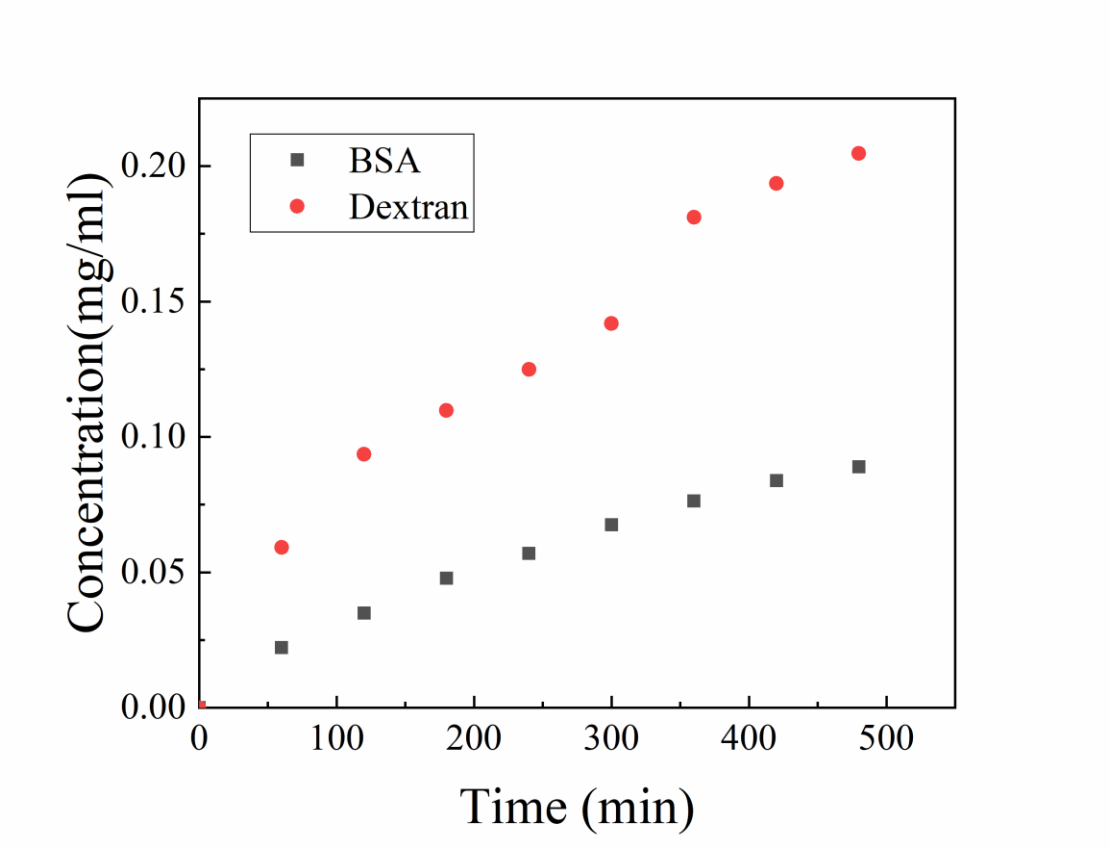

Figure S6. BSA and Dextran concentration change with time

Solute distribution in hydrogel

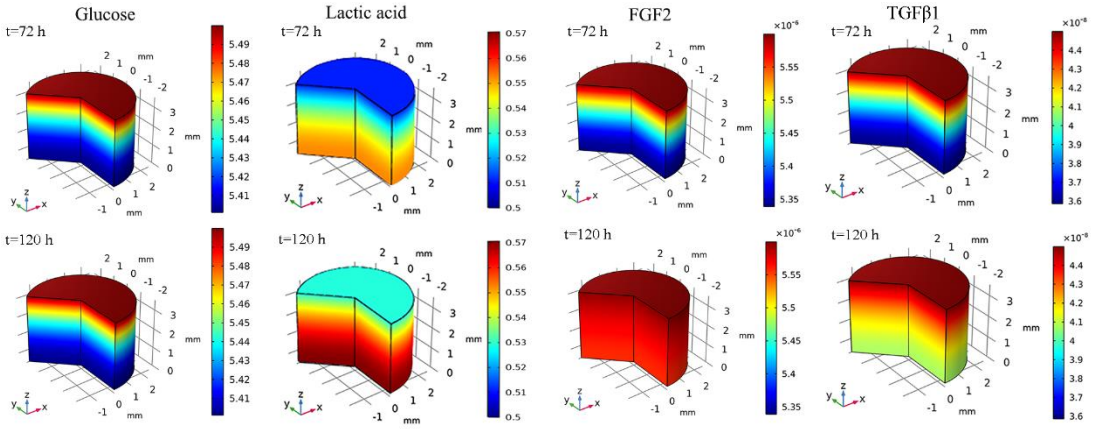

Figure S7. Solute distribution in hydrogel at 72 and 120 h

Table S1. Global parameters and variables for the COMSOL simulation.

Parameter	Value	Unit	Annotation
T	310	K	Temperature
$C_{g0,glucose}$	2.25	mol m^{-3}	Initial glucose conc. in gel
$C_{m0,glucose}$	5.5	mol m^{-3}	Initial glucose conc. in media
$C_{g,glucose}$	Variable	mol m^{-3}	Local glucose conc. in gel
$R_{glucose}$	1.108×10^{-5}	mol s^{-1} m^{-3}	Glucose uptake rate
$C_{g0,\ FGF2}$	2.8×10^{-6}	mol m^{-3}	Initial FGF2 conc. in gel
$C_{m0,\ FGF2}$	5.6×10^{-6}	mol m^{-3}	Initial FGF2 conc. in media
$C_{g,\ FGF2}$	Variable	mol m^{-3}	Real-time conc. of FGF2 in gel
$C_{g0,\ lacticacid}$	0	mol m^{-3}	Lactate conc. in gel
$C_{m0,\ lacticacid}$	0	mol m^{-3}	Lactate conc. in media
$C_{g,\ lacticacid}$	Variable	mol m^{-3}	local lactic acid conc. in gel
$C_{m,\ lacticacid}$	Variable	mol m^{-3}	local lactic acid conc. in media
$R_{lacticacid}$	1.108×10^{-5}	mol s^{-1} m^{-3}	Lactate production rate

Table S2. FTIR band assignment.

Wavenumber/cm^{-1}	Functional group assignment	Biomolecule
2970–2950	ν_{as} CH_3	Lipid
2935–2915	ν_{as} CH_2	Lipid
1742-1730	ν(C=O) carbonyl	Phospholipids
1674–1662	Amide I, turn&bands	Protein
1650–1648	Amide I, νC=O (70-85%) and νC-N (10-20%) α-helix	Protein
1641–1633	Amide I, νC=O (70-85%) and νC-N (10-20%) β-sheet	Protein
1570–1530	Amide II, δN-H (40-60%), νC-N (18-40%) and νC-C (10%)	Protein
1397	ν-COO-	Lipid
1379	δ_s CH_3	Lipid
1160	νC-O and δC-O-H	Carbohydrates
1099–1080	ν_s PO_2^-	DNA RNA phospholipids
1063	ν_s PO_2^-,νC-C,νC-N	B-DNA
996	RNA stretch and bend ring of uracil	RNA