

SUPPORTING INFORMATION

A Short Oxazolidine-2-one Containing Peptide Forms Supramolecular Hydrogels under Controlled Conditions

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Table of Contents

Table S1. Summary of the conditions tested for the critical gelation concentration (CGC) of gelator 1 after dissolution with water containing 1 eq. of NaOH	Page S3
Figure S1. Photographs of the trials for the measurement of the CGC of gelator 1 after dissolution in water containing 1 eq. of NaOH	Page S3
Figure S2. Zoom between 5 and 8.5 minutes of the HPLC chromatograms of the gels A-I after their formation.	Page S4
Figure S3. Photographs of the gels at a concentration of (a) 0.2 %, (b) 0.5 %, and (c) 1.0 % w/V obtained after dissolution with PB and addition of 1.2 eq. of GdL and comparison between the stiffness of the gels obtained with dissolution with NaOH and P	Page S5
Figure S4. Photographs of the gels at a concentration of (a) 0.2 %, (b) 0.5 %, and (c) 1.0 % w/V obtained after dissolution with PB and addition of 0.5 eq. of CaCl ₂ and comparison between the stiffness of the gels obtained with dissolution with NaOH and PB	Page S5
Table S2. Summary of the conditions tested for the critical gelation concentration (CGC) of gelator 1 after dissolution in phosphate buffer (PB) at pH 7.4	Page S6
Figure S5. Photographs of the trials for the measurement of the CGC of gelator 1 after dissolution in phosphate buffer (PB) at pH 7.4	Page S6
Figure S6. Single strain sweep experiments on the gels used for studying the CGC of 1 after dissolution with PB at pH 7.4 and addition of (a-c) GdL or (d) CaCl ₂ . The concentration of the gelator in each gel is reported above the corresponding graph	Page S7
Figure S7. Zoom between 5 and 8.5 minutes of the HPLC chromatograms of the gels J-O of 1 after their formation	Page S8

Figure S8. Strain sweep experiments ($\omega = 10 \text{ rad s}^{-1}$) on the gels A-I	Page S9
Figure S9. Absorption spectra of the gels A-I	Page S9
Figure S10. Strain sweep experiments ($\omega = 10 \text{ rad s}^{-1}$) on the gels J-O	Page S10
Figure S11. Absorption spectra of the gels J-O	Page S10
Figure S12. FT-IR spectra solution of 1 in 1.0 % concentration and of the corresponding gels C, I, L, O	Page S11
Figure S13. FT-IR spectra of solid 1 and of the xerogels C, I, L, O	Page S12
Table S3. Summary of the most representative peaks for the studied compounds	Page S13

Table S1. Summary of the conditions tested for the critical gelation concentration (CGC) of gelator **1** after dissolution with water containing 1 eq. of NaOH.

Gel	Conc (mM)	Conc (%)	pH ₀	Trigger (mM)	pH _f	Outcome
I	2.78	0.15	8.6	GdL (3.34)	3.6	Solution
II	2.78	0.15	8.4	CaCl ₂ (2.78)	4.7	Solution

pH₀ = starting pH (before trigger addition); pH_f = final pH

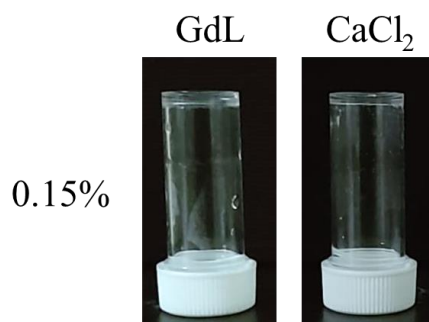


Figure S1. Photographs of the trials for the measurement of the CGC of gelator **1** after dissolution in water containing 1 eq. of NaOH, with the triggers.

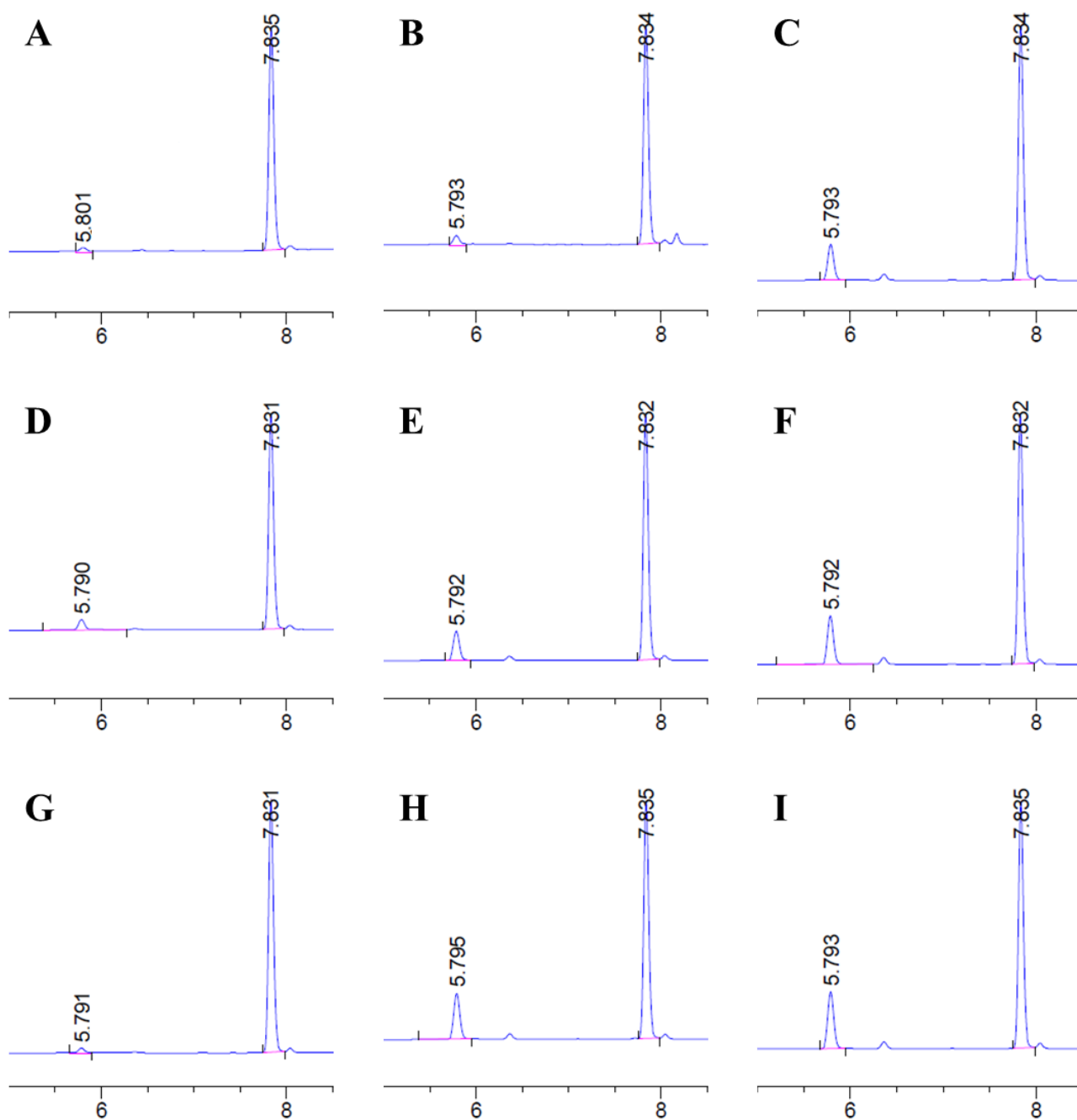


Figure S2. Zoom between 5 and 8.5 minutes of the HPLC chromatograms of the gels **A-I** after their formation. Boc-L-Phe-D-Oxd-L-Phe-OH elutes at 7.8 minutes, while Boc-L-Phe-OH elutes at 5.8 minutes. Products were detected with $\lambda = 210$ nm.

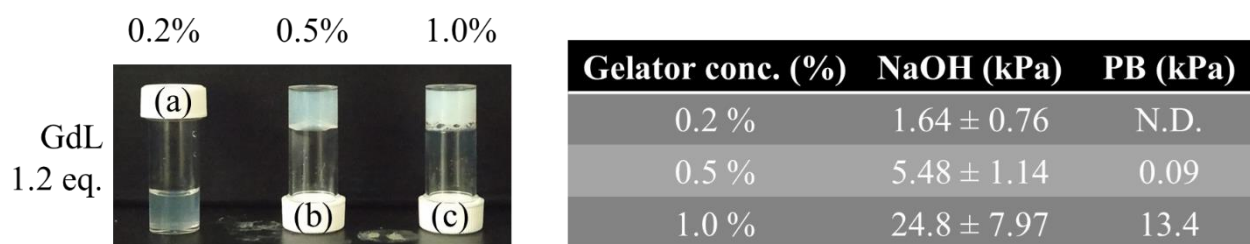


Figure S3. Left: photographs of the gels at a concentration of (a) 0.2 %, (b) 0.5 %, and (c) 1.0 % w/V obtained after dissolution with PB and addition of 1.2 eq. of GdL; right: comparison between the stiffness of the gels obtained with dissolution with NaOH and PB. Values of the stiffness with NaOH are done in triplicate and have standard deviation, while the ones with PB were done only once. N.D. = not determined.

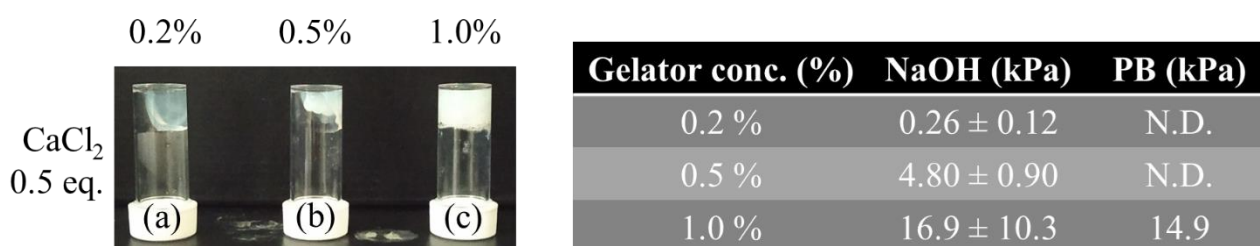


Figure S4. Left: photographs of the gels at a concentration of (a) 0.2 %, (b) 0.5 %, and (c) 1.0 % w/V obtained after dissolution with PB and addition of 0.5 eq. of CaCl₂; right: comparison between the stiffness of the gels obtained with dissolution with NaOH and PB. Values of the stiffness with NaOH are done in triplicate and have standard deviation, while the ones with PB were done only once. N.D. = not determined.

Table S2. Summary of the conditions tested for the critical gelation concentration (CGC) of gelator **1** after dissolution in phosphate buffer (PB) at pH 7.4.

Gel	Conc (mM)	Conc (%)	PB (mM)	pH ₀	Trigger (mM)	pH _f	Outcome	G' (Pa)	G'' (Pa)	LVER (%)	Crossover point (%)
III	2.78	0.15	7.2	6.9	GdL (5.56)	3.5	Gel	3221	380	1.5	N.D.
IV	1.86	0.10	4.8	7.0	GdL (3.72)	3.5	Gel	583	47.5	2.2	N.D.
V	0.93	0.05	2.4	7.0	GdL (1.86)	3.8	Gel	89.6	9.80	22	N.D.
V	0.93	0.03	1.4	7.0	GdL (1.86)	4.2	Solution	//	//	//	//
VI	2.78	0.15	7.2	6.9	CaCl ₂ (2.78)	5.2	Gel	507	69.6	1.5	N.D.
VII	1.86	0.10	4.8	6.9	CaCl ₂ (1.86)	5.0	Solution	//	//	//	//

pH₀ = starting pH (before trigger addition); pH_f = final pH; G' and G'' are taken at $\gamma = 0.046\%$ as at that strain none of the gel has inflections in the trend of their moduli; N.D. = not detected

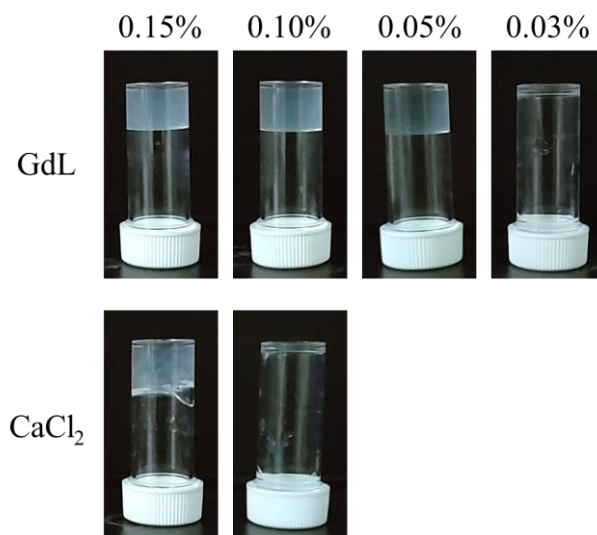


Figure S5. Photographs of the trials for the measurement of the CGC of gelator **1** after dissolution in phosphate buffer (PB) at pH 7.4.

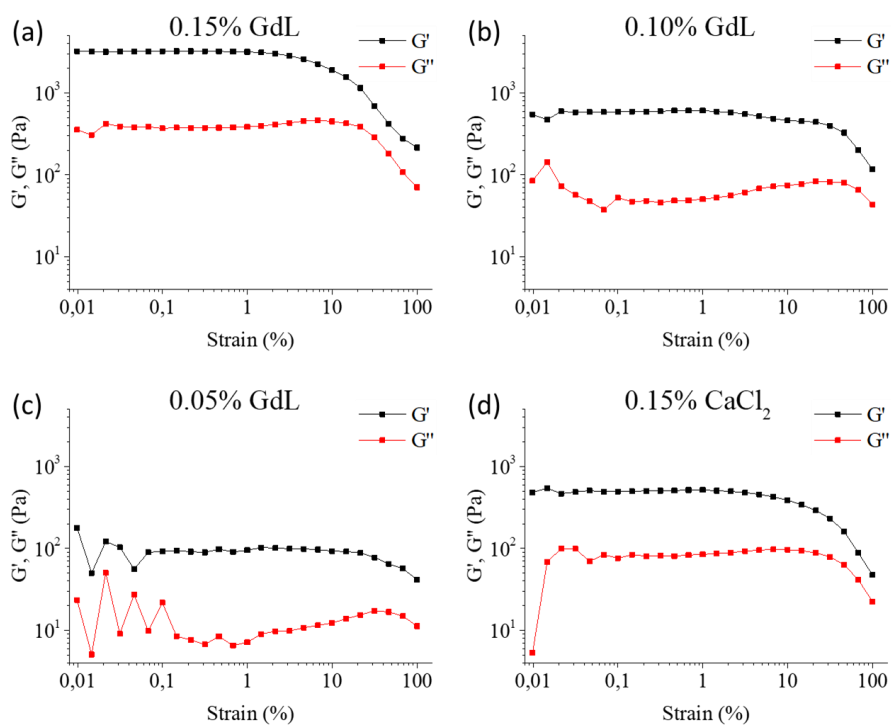


Figure S6. Single strain sweep experiments on the gels used for studying the CGC of **1** after dissolution with PB at pH 7.4 and addition of (a-c) GdL or (d) CaCl_2 . The concentration of the gelator in each gel is reported above the corresponding graph.

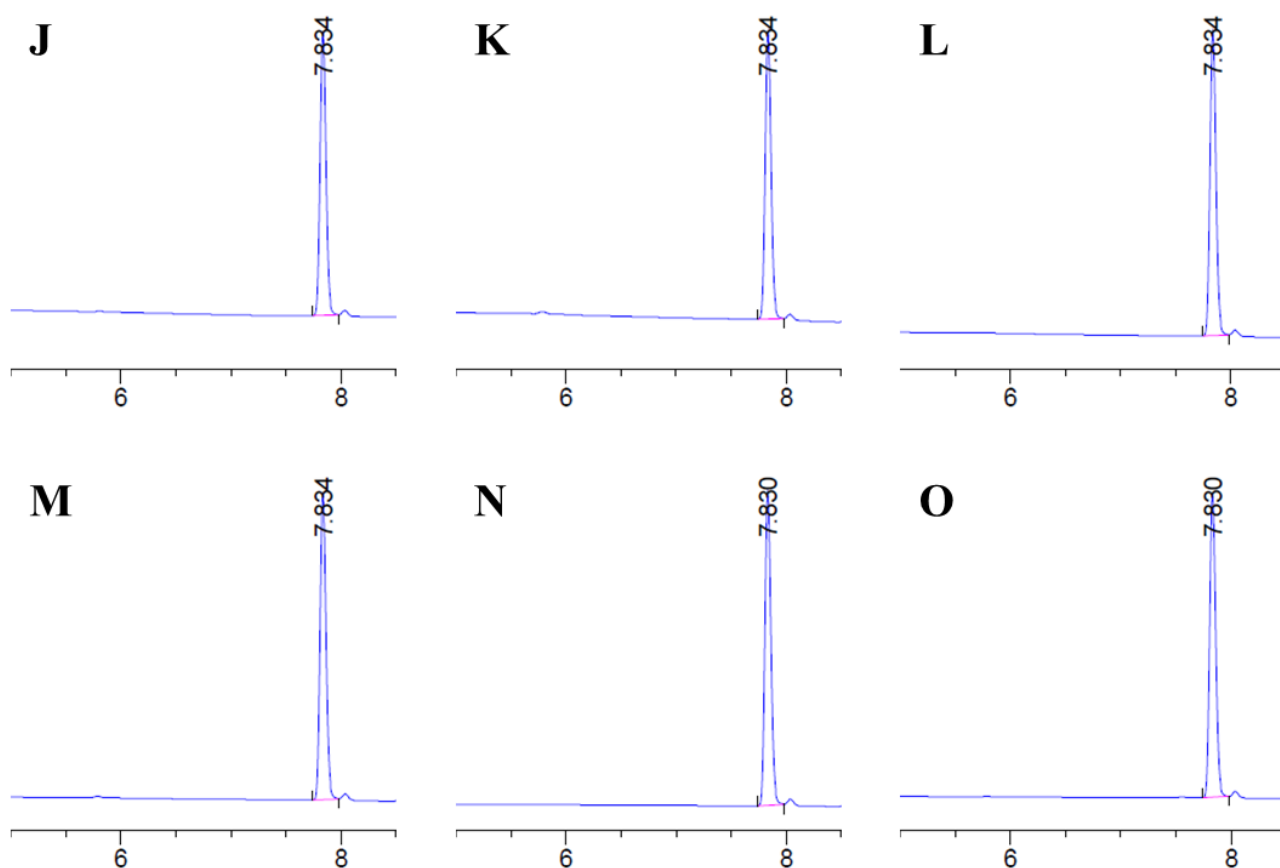


Figure S7. Zoom between 5 and 8.5 minutes of the HPLC chromatograms of the gels **J-O** after their formation. Boc-L-Phe-D-Oxd-L-Phe-OH elutes at 7.8 minutes, while Boc-L-Phe-OH elutes at 5.8 minutes. Products were detected with $\lambda = 210$ nm.

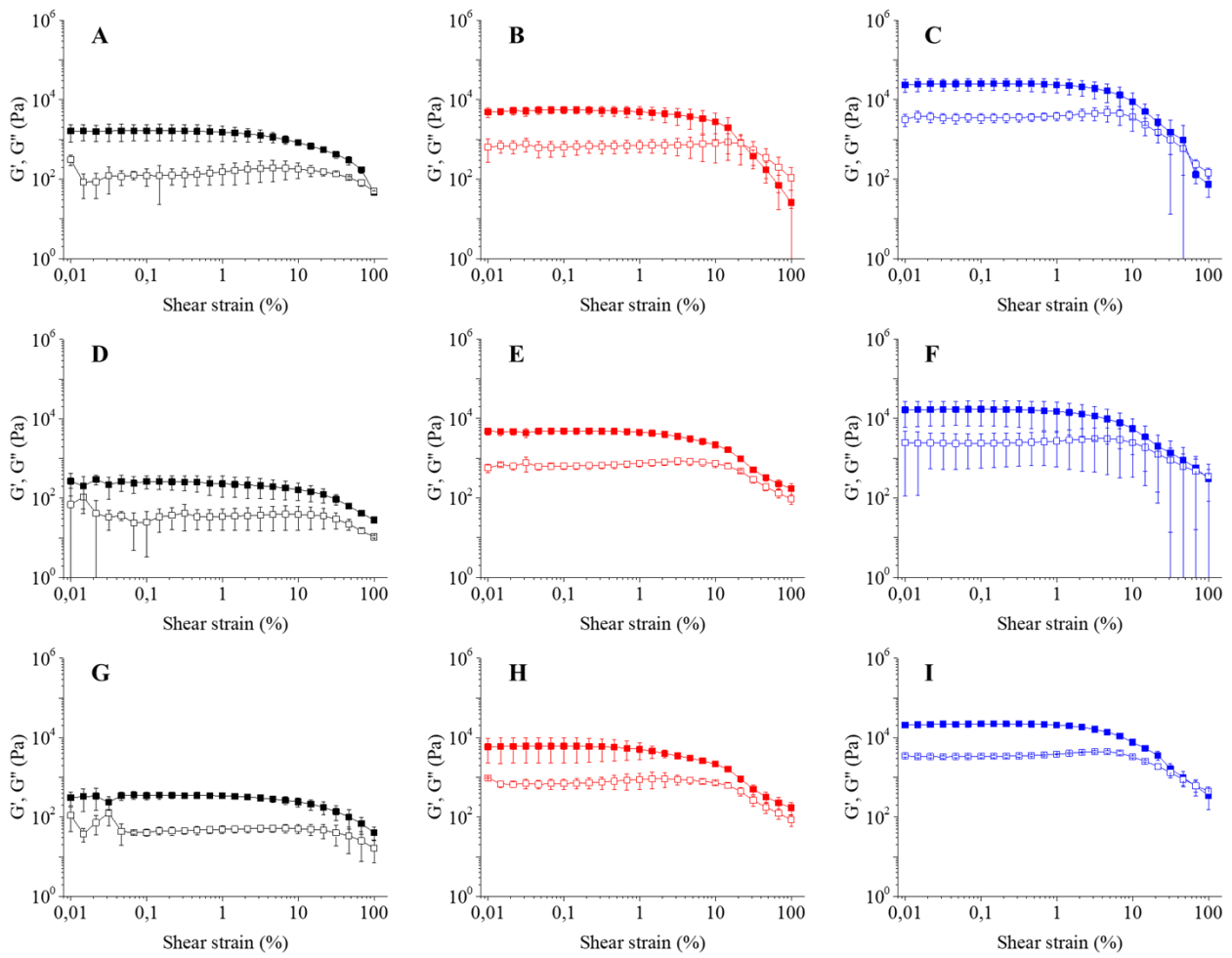


Figure S8. Strain sweep experiments ($\omega = 10 \text{ rad s}^{-1}$) on the gels **A-I**.

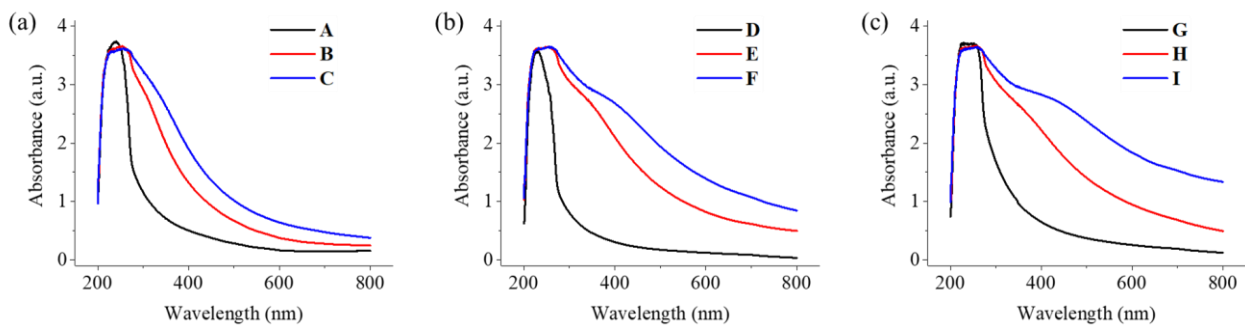


Figure S9. Absorption spectra of the gels (a) **A-C**, (b) **D-F**, and (c) **G-I**.

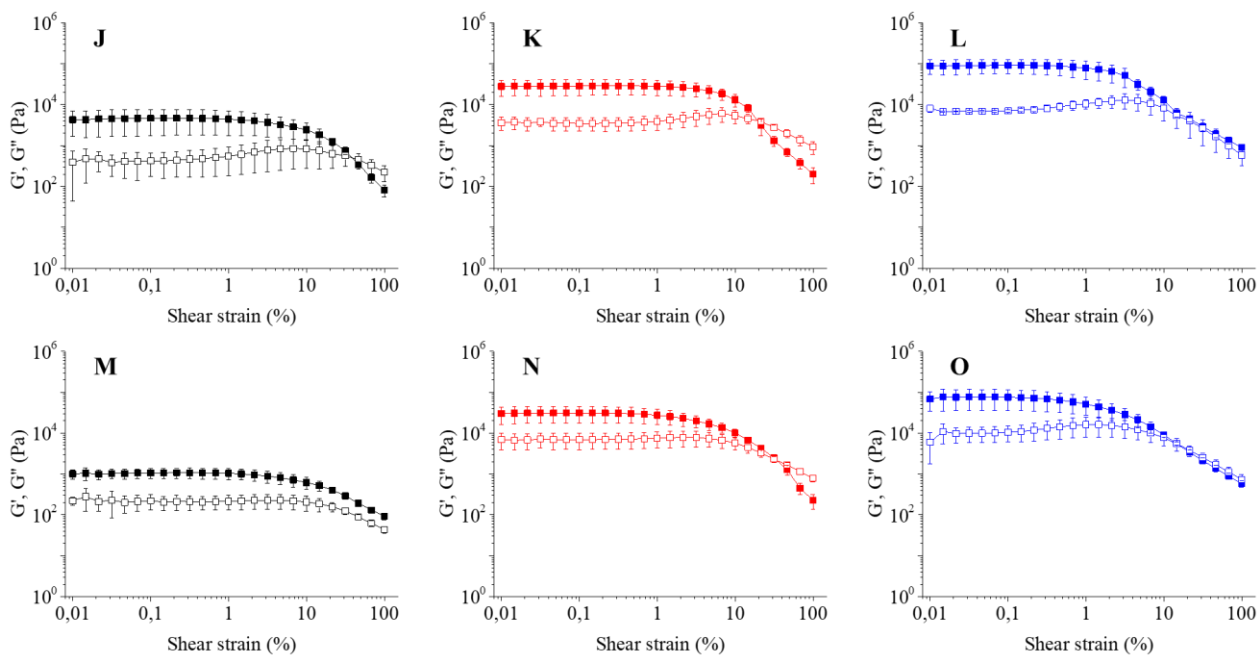


Figure S10. Strain sweep experiments ($\omega = 10 \text{ rad s}^{-1}$) on the gels **J-O**.

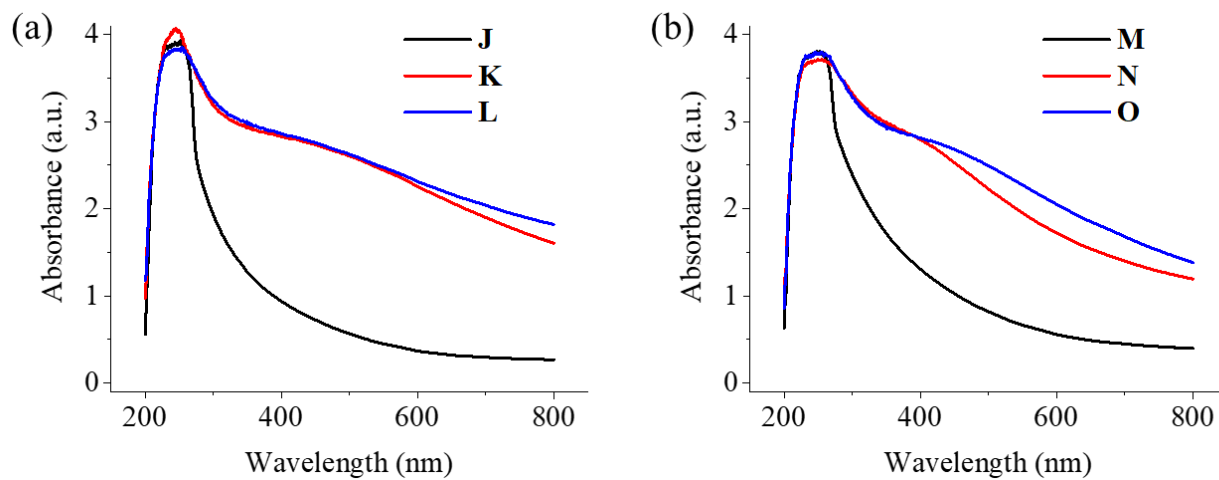


Figure S11. Absorption spectra of the gels (a) **J-L**, and (b) **M-O**.

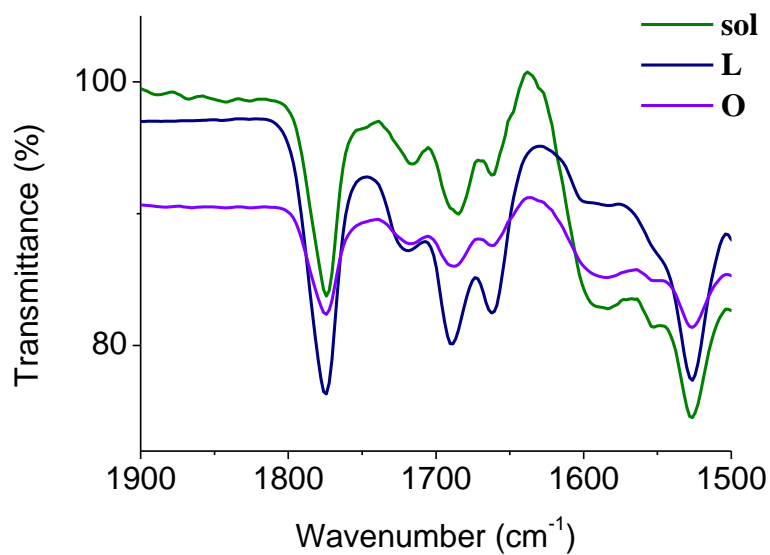
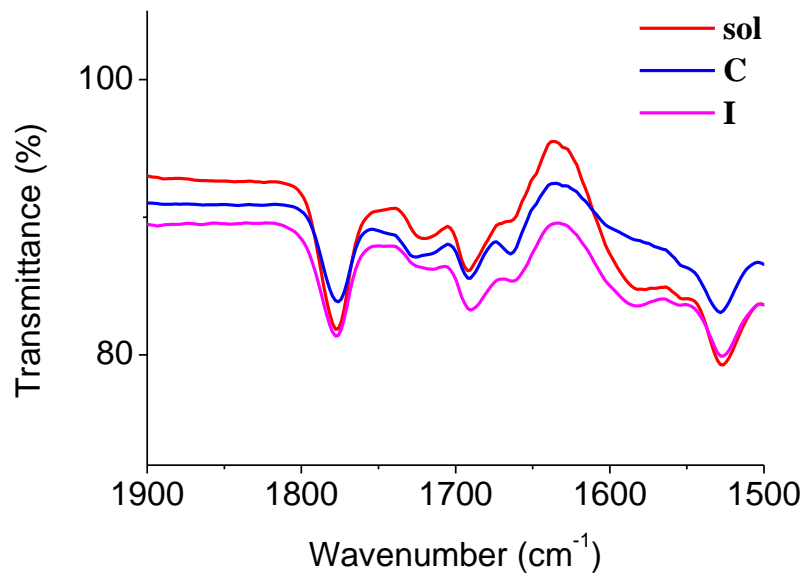


Figure S12. FT-IR spectra solution of **1** in 1.0 % concentration and of the corresponding gels **C**, **I**, **L**, **O**

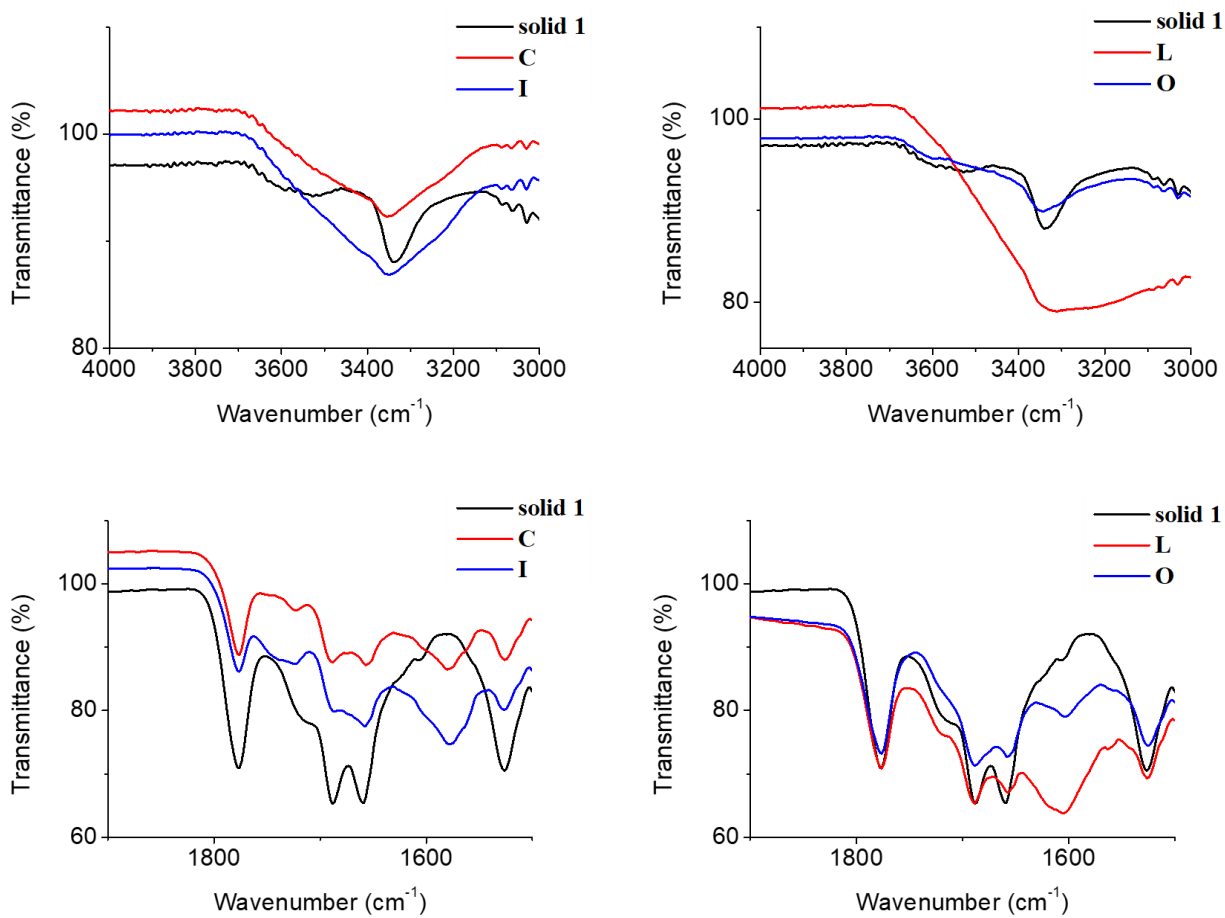


Figure S13. FT-IR spectra of solid **1** and of the xerogels **C**, **I**, **L**, **O**.

Table S3. Summary of the most representative peaks for the studied compounds.

General conditions	Product	Peaks of interest						
3 mM in CH ₂ Cl ₂	Boc-L-Phe-D-Oxd-L-Phe-OBn ^a	3432 3350	1788	1740	1700	1684		
1% in NaOH	1 solution in NaOH	-	1777	1721	1692	1664	1583	1527
	gel C	-	1776	1727	1690	1664	-	1528
	gel I	-	1778	1720	1689	1662	1586	1527
1% in PBS	1 solution in PBS	-	1774	1717	1684	1662	1592	1526
	gel L	-	1775	1721	1689	1661	1599	1526
	gel O	-	1773	1717	1687	1661	1589	1526
Solid	1	3340	1776	1714	1688	1659	-	1525
Xerogel NaOH	xerogel C	3348	1777	1723 w	1687	1654	1578	1526
	xerogel I	3351	1777	1724	1689	1657	1577	1526
Xerogel PBS	xerogel L	3322	1776	1719 w	1689	1657	1561 w	1526
	xerogel O	3344	1777	-	1688	1657	1603	1524
Sol. NaOD	sol-d	3403	1782	1719	1686	-	1596	-
	C-d	-	1778	1719	1685	-	1603	-
	O-D	-	1777	1721	1687	-	1584	-

^a L. Milli, N. Castellucci, C. Tomasini, *European J. Org. Chem.* **2014**, 2014, 5954–5961

w = weak peak