Electronic Supplementary Material (ESI) for Chemical Society Reviews.

Peptide Hydrogen-bonded Organic Frameworks

Thangavel Vijayakanth,*[a] Sneha Dasgupta,[b] Pragati Ganatra,[c] Sigal Rencus-Lazar,[a] Aamod V. Desai,[d] Shyamapada Nandi,[e] Rahul Jain,[b] Santu Bera,[f] Andy I. Nguyen,*[c] Ehud Gazit,*[a,g] Rajkumar Misra*[b]

[a.] Shmunis School of Biomedicine and Cancer Research, George S. Wise Faculty of Life Sciences, Tel Aviv University, Tel Aviv–6997801, Israel.
[b.] Department of Medicinal Chemistry, National Institute of Pharmaceutical Education and Research (NIPER), Mohali, S.A.S. Nagar (Mohali) 160062, India.
[c.] Department of Chemistry, University of Illinois Chicago, Chicago, Illinois 60607, United States.
[d.] School of Chemistry, University of St Andrews, North Haugh, St Andrews KY16 9ST, United Kingdom.
[e.] Chemistry Division, School of Advanced Sciences, Vellore Institute of Technology, 600127, Chennai, India.
[f.] Department of Chemistry, Ashoka University, Sonipat, Haryana 131029, India.
[g.] Sagol School of Neuroscience, Tel Aviv University, 6997801 Tel Aviv, Israel.
*Corresponding authors' email: vijayakantht@mail.tau.ac.il; andyn@uic.edu; ehudg@post.tau.ac.il; rkmisra@niper.ac.in

Table S1. Summary of properties and functionality in peptide-based hydrogen-bonded porous frameworks (P-HPFs)

P-HPFs name	No of hydrophobic residues	No of hydrophilic residues	Percentage of hydrophobic
VA	2	0	100
AV	2	0	100
AI	2	0	100
IA	2	0	10
VV	2	0	100
VI	2	0	100
IV	2	0	100
LS	1	1	50
FF	2	0	100
FG	2	0	100
FL	2	0	100
FW	2	0	100
LL	2	0	100
LF	2	0	100
IL	2	0	100
WG	2	0	100
Abu-Abu	2	0	100
Abu-Nva	2	0	100
Abu-Val	2	0	100
Abu-Leu	2	0	100
Abu-Ile	2	0	100
Nva-Abu	2	0	100

Nva-Nva	2	0	100
Nva-Val	2	0	100
Nva-Leu	2	0	100
Nva-Ile	2	0	100
HYF	2	0	100
DYF	2	1	75
YFD	2	1	75
F-^{D}Nva-F	3	0	100
SP1	8	1	88.89
SP2	4	0	100
SP3	14	13	51.85
SP4	12	14	46.15
SP5	14	12	53.85
SP6	13	13	50
SP7	11	15	42.31
SP8	10	6	62.5
F1	7	4	63.63
F2	5	5	50
F3	8	4	66.67
F4	15	0	100

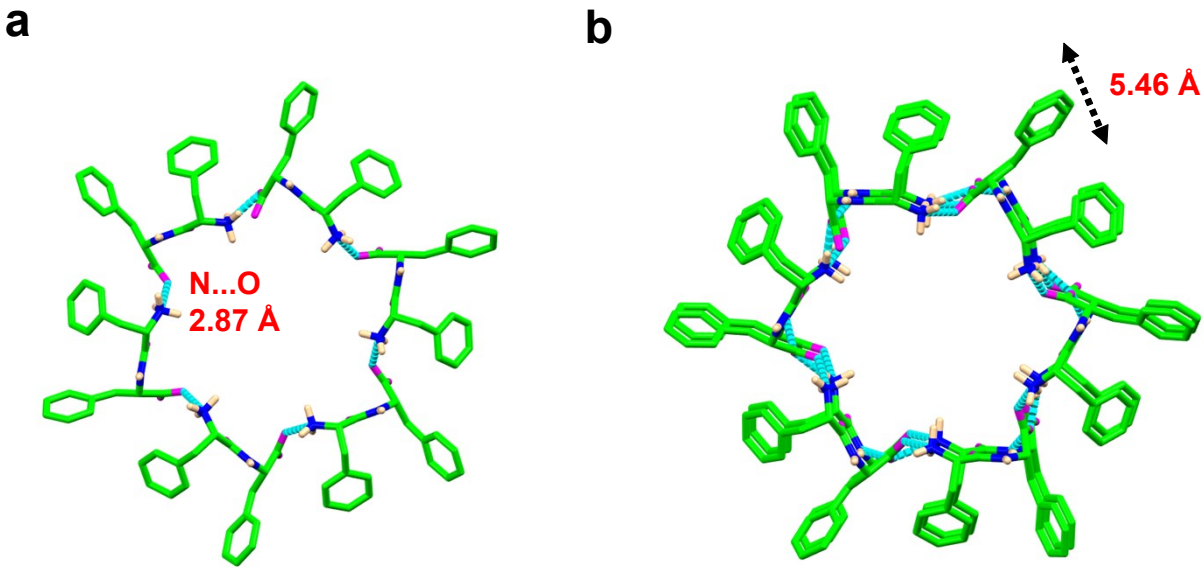

Figure S1. Unit-cell packing diagram of FF showing the formation of molecular rings by six FF molecules and its donor-acceptor interactions (a) and its pi-pi stacking modes (b). The hydrophilic channels formed by six FF molecules are shown and the solvent water molecules are removed for structural clarity.

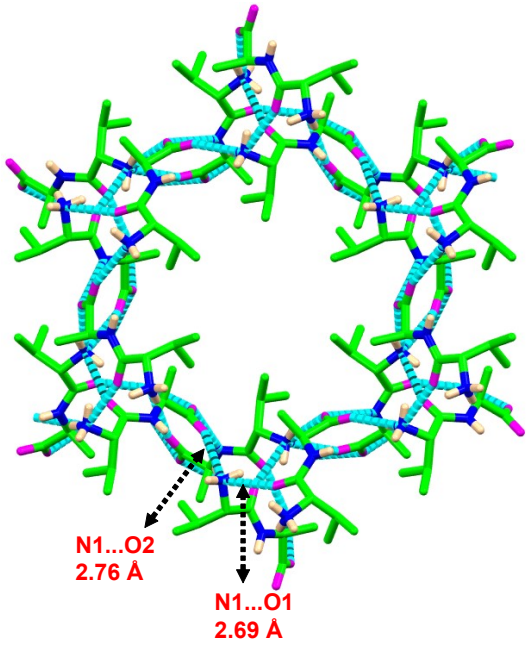

Figure S2. Unit-cell packing diagram of AV displaying a porous framework mediated via head-to-tail hydrogen-bonded interactions between ammonium (NH_3^+) and carboxylate (COO^-) residues.

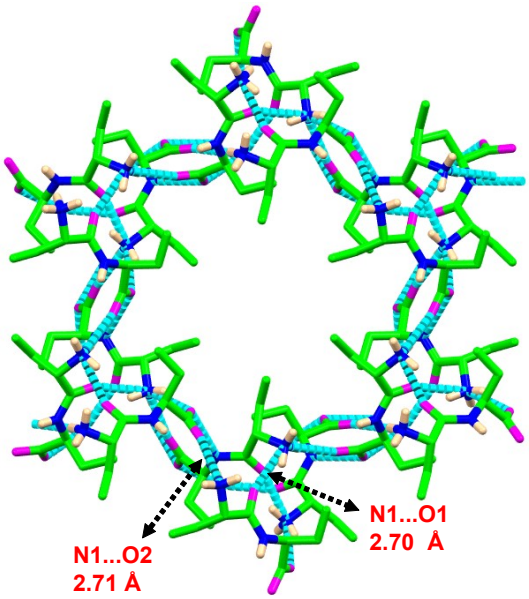

Figure S3. Unit-cell packing diagram of Abu-Abu displaying a porous framework mediated via head-to-tail hydrogen-bonded interactions between ammonium (NH_3^+) and carboxylate (COO^-) residues.

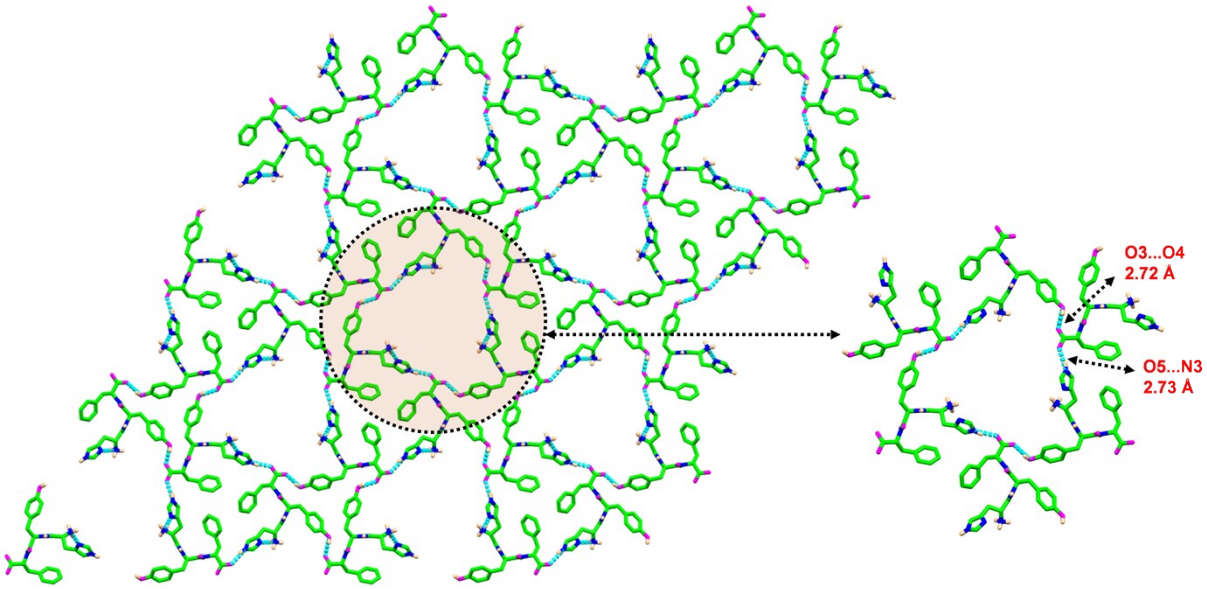

Figure S4. Higher-order crystal packing structure of HYF displaying hydrogen-bonded porous assemblies. The highlighted part shows the hydrogen-bonded porous framework channels formed by six HYF molecules and the solvent water molecules are removed for structural clarity.

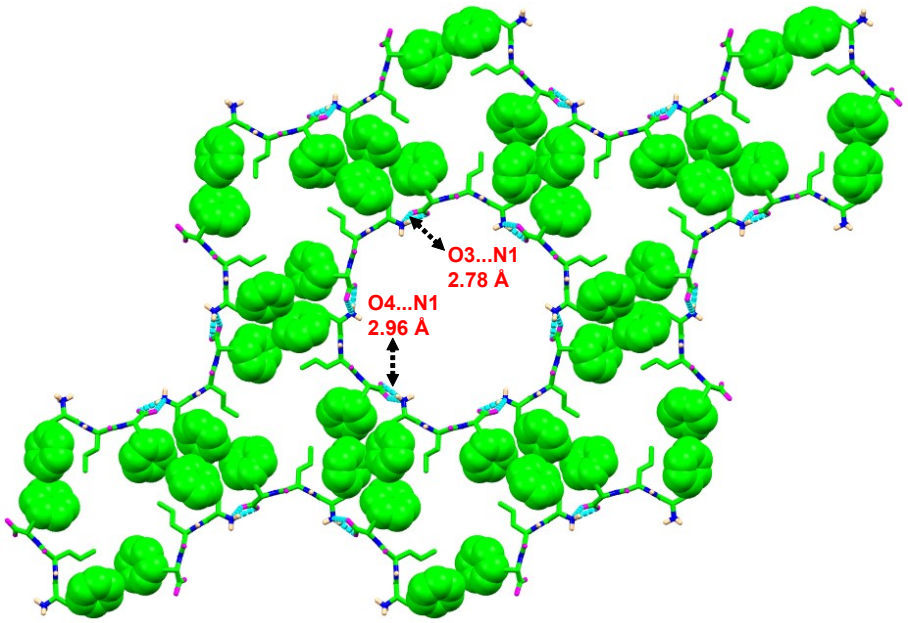

Figure S5. Higher-order crystal structure of F-^{D}Nva-F displaying a porous framework mediated via head-to-tail hydrogen-bonded interactions between ammonium (NH_3^+) and carboxylate (COO^-) residues. The aromatic phenyl rings are highlighted in the space-filling model.

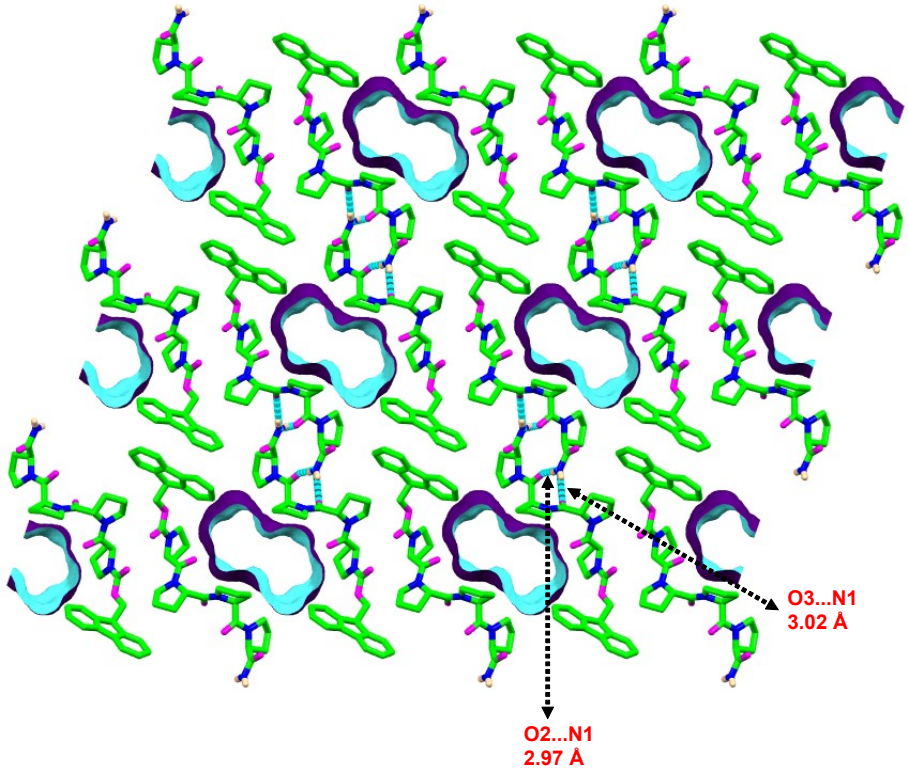

Figure S6. Higher-order crystal packing diagram of PP4 displaying hydrogen-bonded porous framework and the solvent-accessible channels (viewed along the b-axis). The solvent ethanol molecules are removed for structural clarity.

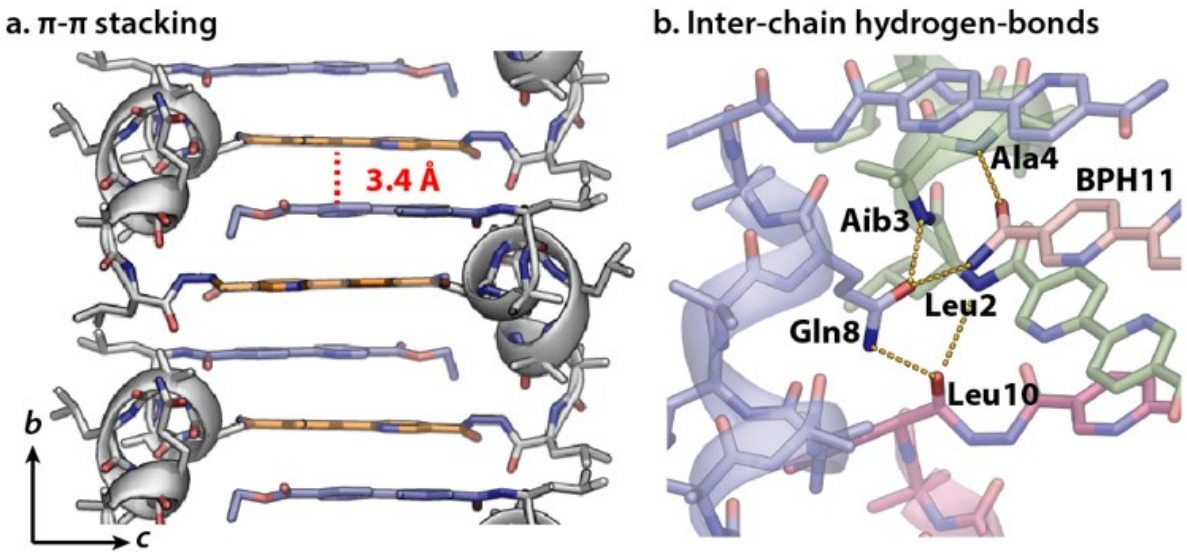

Figure S7. Views of the π-π stacking and inter-chain H-bonding contributing to the structure of **UIC-1** (**SP1**).