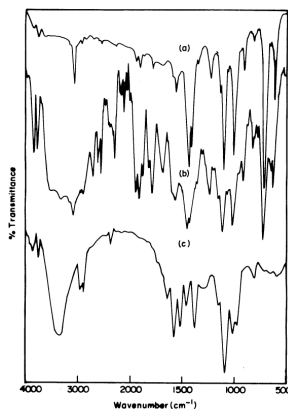# Novel Saccharide-Pyridine based gelators: selective gelation and diversity in superstructures

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Table S1: Chemical shifts (ppm) and coupling constants (Hz) of the anomeric proton (Ano-H) and N-glycosylamine proton (Gly-NH). * Ano-H peak overlapped with the saccharide-OH groups.

Compound no	δ. (Ano-H), $^3JH_1,H_2$	δ. (Gly-NH), $^3JH_1,H_2$	Yield(%)
7	5.09 (t), 9.3 Hz	6.46 (d), 7.8 Hz	69
8	5.04 (t), 8.7 Hz	7.03 (d), 9.3 Hz	65
9	6.52 (d), 9 Hz	6.4 (d), 9 Hz	48
10	6.41 (d), 8.7 Hz	7.28 (d), 9 Hz	61
11	5.01 (t), 8.7 Hz	6.49 (d), 8.7 Hz	69
12	6.96 (d), 6 Hz	5.25 (d), 6 Hz	23
13	4.71 (d),…*	5.86 (d), 6.6 Hz	71
14	4.64 (t), 7.5 Hz	5.86 (d), 7.2 Hz	64
15	6.96 (d), 6 Hz	6.82 (d), 6 Hz	60

Figure S2: FT-IR spectra of compound **11** (a), 1,2-dichlorobenzene; (b), gel phase (1,2-dichlorobenzene) and (c), solid phase.

Scheme S3: Different regions in the chosen molecules which have the tendency to interact with other molecules.
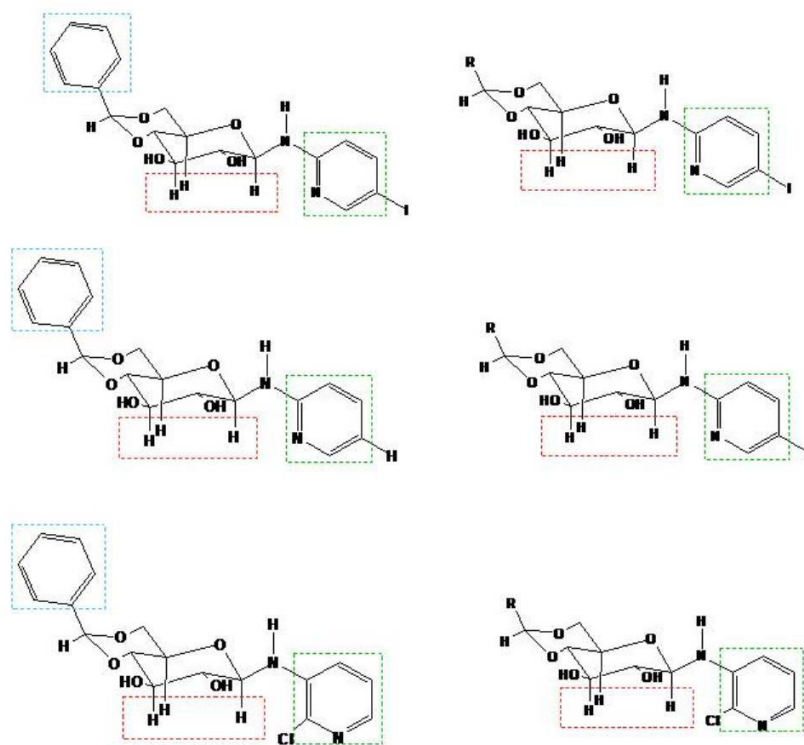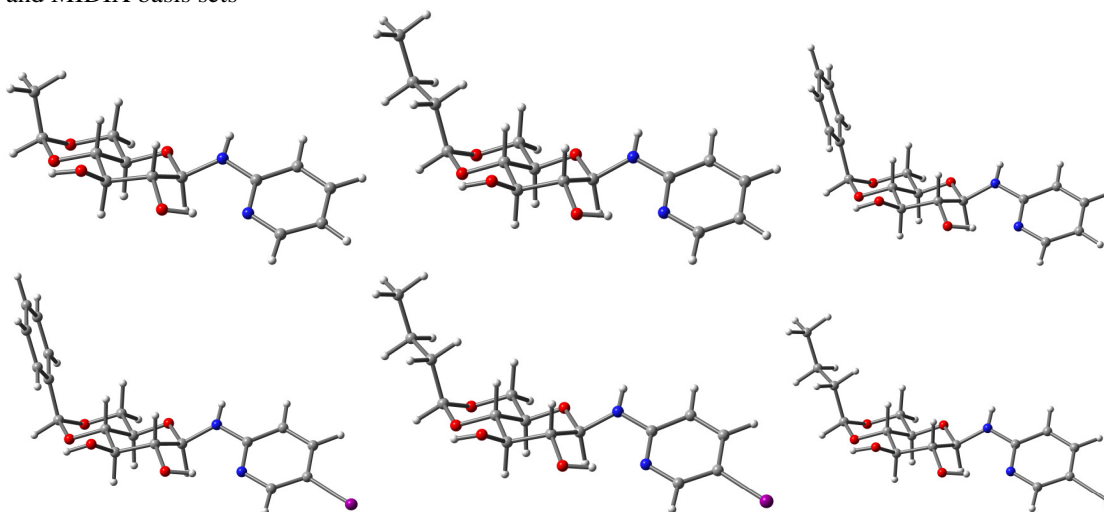

FIGURE S4: Optimized geometries of all the molecules obtained from B3LYP calculation using 6-31G* and MIDIX basis sets
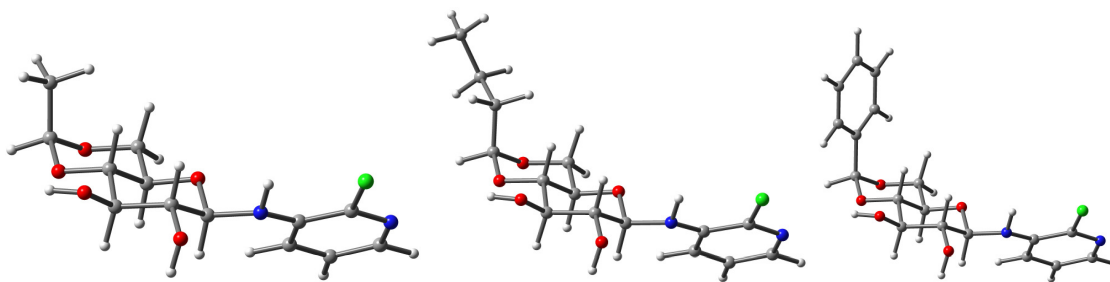
Table S5: Stabilization energy of various proposed interactions obtained from MP2 level of calculation using 6-31G* and MIDIX basis sets.

Species	Orientation	BSSE uncorrected SE (kcal/mol)	BSSE corrected SE (kcal/mol)
Py-NH$_2$-H	Parallel-displaced	6.7	2.1
Py-Cl-NH$_2$	Parallel-displaced	9.3	4.3
Py-NH$_2$-I	Parallel-displaced	12.8	7.2
Bz-Bz	Parallel	2.1	-0.1
Bz-Bz	Parallel-displaced	3.2	0.1
Sug-Py-NH$_2$-H	CH-π	7.6	2.2
Sug-Py-Cl-NH$_2$	CH-π	7.1	1.9
Sug-Py-NH$_2$-I	CH-π	8.3	3.1
Sug-Bz	CH-π	5.1	1.9

FIGURE S6: Molecular electrostatic potential maps of all the molecules obtained from B3LYP calculation using 6-31G* and MIDIX basis sets. The given electrostatic potential maps are ±0.04 au isosurface value.

7 8 9

10 11 12

13 14 15