Supporting information:

Directing spatial disposition of ferrocene around homoadenine tetrads

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Crystal structure refinement details for ferrocene conjugate 1: The compound **1** was crystallized by the slow evaporation of methanol and chloroform mixture. For the compound, X-ray data was collected on a Bruker SMART CCD4 X-ray diffraction instrument. The crystal was solved by direct methods and refined by using full-matrix least-squares on F^2 (SHELX97). The structure was expanded using Fourier techniques. All other non-hydrogen atoms were refined anisotropically. Hydrogen atoms are placed at geometrically idealized positions. The crystal data and structural refinement parameters for both the conjugates are given in **Table 1**. CCDC contains the supplementary crystallographic data for this paper with a deposition number of **CCDC 654334** for compound **1**. Copies of this information can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK. [Fax: +44-1223/336-033; E-mail: deposit@ccdc.cam.ac.uk].

Figures:

The Figure S1 shows the formation of adenine ribbon with the help of eight intermolecular hydrogen bonding which are further interconnected with CH…O interaction thus forming a two dimentional network of adenine ribbons.

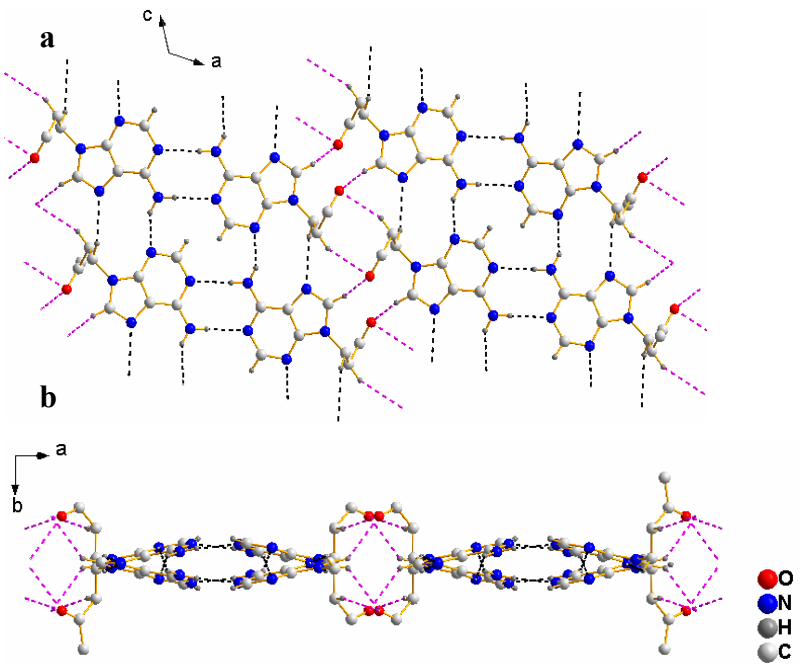

Figure S1: (a) Shows that the adenine ribbons are further connected to each other through CO…H hydrogen bonding forming a 2D network of adenine ribbons. (b) lateral view of the same structure (in all figures ferrocene moeity is omitted for clarity).

Figure S2 shows the different view of the crystal lattice which shows the spatial dispotition of ferrocene because of hydrogen bonding interactions and π–π stacking.

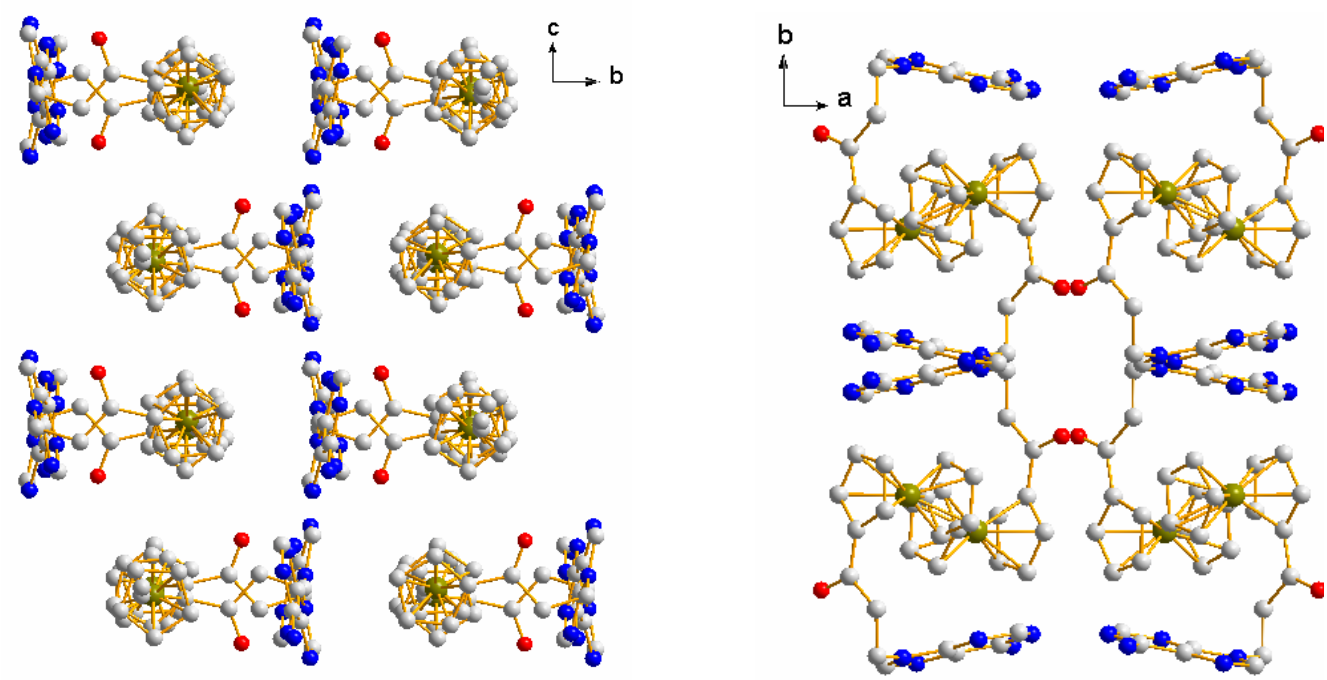

Figure S2: (a) view along a-axis, (b) view along c-axis.

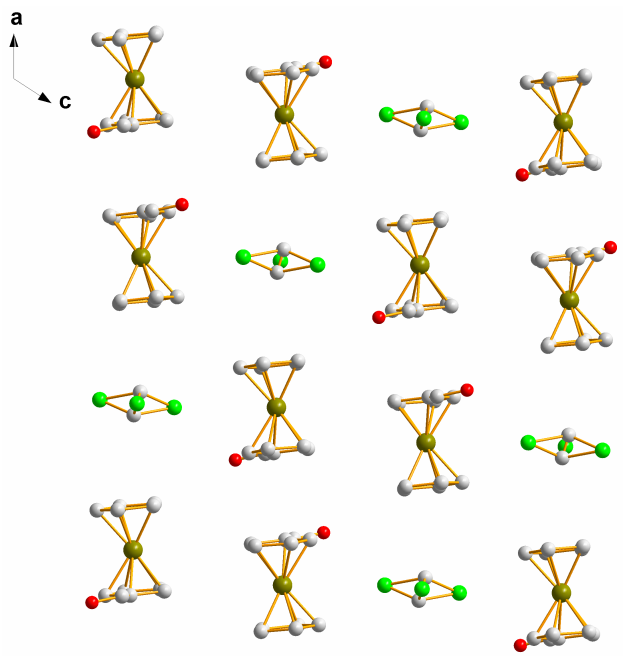

Figure S3: Linear arrangement of ferrocene units which are π stacked and also shows the entrapment of chloroform molecule in the crystal lattice (chloroform molecules are disordered).

Table S1: Crystal structural refinement parameters for 1.

Identification code	**1**
Empirical formula	C18.50 H17.50 Cl1.50 Fe N5 O
Formula weight	434.90
Temperature	100(2) K
Wavelength	0.71073 Å
Space group	C 2/c
a/Å	18.0660(17)
b/Å	18.2911(17)
c/Å	13.0640(13)
α(degree)	90.00
β(degree)	122.807(2)
γ(degree)	90.00
Volume ($Å^3$)	3628.41(56)
Z, Calculated density	8, 1.592 mg/m^3
Absorption coefficient	1.072 mm^{-1}
F(000)	1784
Crystal size	0.2 ×0.2 × 0.2 mm
Θ range	2.23 to 28.29 deg.
Limiting indices	-23 ≤h≤21, -18≤ k≤24, -17≤ l≤17
Reflections collected/unique	11919/4481 [R(int) = 0.0512]
Completeness to theta	= 28.29 99.5 %
Absorption correction	Psi-scan
Data/restraint /parameters	4481/ 0 / 248
Goodness-of-fit on F^2	1.323
Final R indices [I>2sigma(I)]	R1 = 0.0555, wR2 = 0.1168
R indices (all data)	R1 = 0.0827, wR2 = 0.1592
Largest diff. peak and hole	0.954 and -0.892 $e.Å^{-3}$

Table S2: Hydrogen bond distances and angles for compound 1.

No.	D-H...A	Symmetry of A	d_{D-H}	$d_{H...A}$	$d_{D...A}$	#D-H...A
(1)	N6-H6A...N1	2-x, y, 1.5-z	0.86	2.13	2.987(6)	175
(2)	N6-H6B...N3	x, -y,-0.5+z	0.86	2.22	2.977(5)	146
(3)	C8-H8...O1	1-x, -y, 1-z	0.93	2.58	3.341(5)	139
(4)	C10-H10A...N7	x, -y, 0.5+z	0.97	2.55	3.292(5)	133
(5)	C11-H11A…O1	1-x, y, 1.5-z	0.97	2.58	3.483(5)	154

Where D=donor, A=acceptor, d=distance between atoms (in Å) and #angles are in degree.