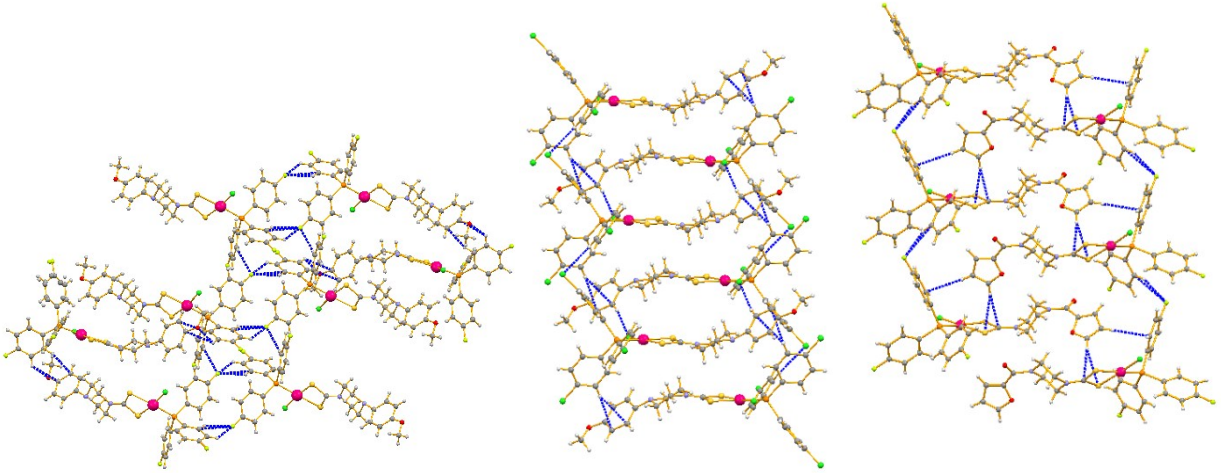
Supplementary Material

Crystal packing

These compounds provide an ideal platform to see the effect of various weak CH···X [X = O, F, Cl and π] non-covalent interactions on the solid state-self-assembly particularly in the absence of strong hydrogen bonds.[1-10] The crystal structure of compounds **1-3** revealed 3D-networks, composed of various 1D-supramolecular chains stabilized by variety of weak non-covalent interactions. The molecules are arranged in head to head fashion in 1D-chains of compound **1** stabilized by C-H···F [(C(18)-H(18)···F(2A) 2.529 Å, (C(17)-H(17)···F(2A) 2.648 Å, (C(30)-H(30)···F(2A) 2.622 Å], C-H···O [(C(15)-H(15)···O(1) 2.705 Å] and C-H···π [(C(15)-H(15)···C(9) 2.884 Å, (C(14)-H(14)···C(10) 2.825 Å] interactions (Fig. S1a, Table S1), antiparallel fashion in compound **2** stabilized by C-H···Cl [(C(18)-H(18)···Cl(4) 2.889 Å, (C(11)-H(11)···Cl(1) 2.768 Å] and C-H···π [(C(23)-H(23)···C(10) 2.882 Å, (C(23)-H(23)···C(11) 2.881 Å] interactions (Fig. S1b), and slightly displaced antiparallel fashion in compound **3** stabilized by C-H···F [(C(24)-H(24)···F(2) 2.434 Å], C-H···S [(C(9)-H(9)···S(1) 2.901 Å] and C-H···π [(C(9)-H(9)···C(1) 2.876 Å, (C(10)-H(10)···C(18) 2.846 Å] interactions (Fig. S1c). The 1D-supramolecular extend themselves in three dimensions by means of C-H···Cl [(C(5)-H(5B)···Cl(1) 3.017 Å], C-H···S [(C(4)-H(4B)···S(2) 3.068 Å], C-H···O [(C(2)-H(2B)···O(1) 2.814 Å] and C-H···π [(C(2)-H(2A)···C(9) 2.935 Å] interactions in compound **1** (Fig. S2a), by means of C-H···Cl [(C(29)-H(29)···Cl(2) 3.262 Å, (C(3)-H(3A)···Cl(1) 3.017 Å], halide···π [Cl(2)···C(29) 3.436 Å] and C-H···π [(C(15)-H(15)···C(21) 2.848 Å, (C(15)-H(15)···C(22) 2.963 Å] interactions in compound **2** (Fig. S2b), and by means of C-H···O [(C(19)-H(19)···O(1) 2.631 Å, (C(18)-H(18)···O(1) 2.708 Å, (C(13)-H(13)···O(1) 2.668 Å], C-H···S [(C(3)-H(3B)···S(2) 3.068 Å], C-H···π [(C(5)-H(5A)···C(8) 2.996 Å, (C(5)-H(5A)···C(10) 2.768 Å, (C(13)-H(13)···C(8) 2.911 Å] interactions in compound **3** (Fig. S2c, Table S1) to provide an overall 3D-network structures.



(a) (b) (c)

Figure S1: The 1D-supramolecular chains in 3D-crystal packing of compounds **1-3**.

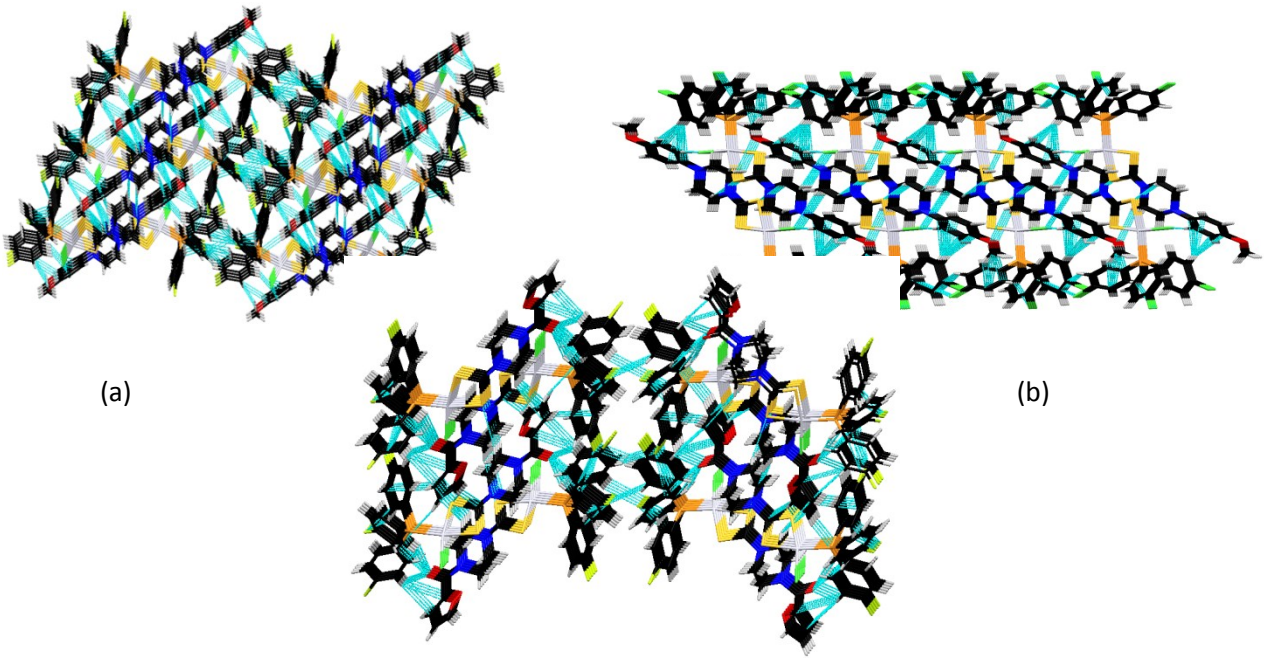


Figure S2: The 3D-crystal packing of **1** along *b*-axis (a), **2** along *b*-axis (b) and **3** along a-axis (c).

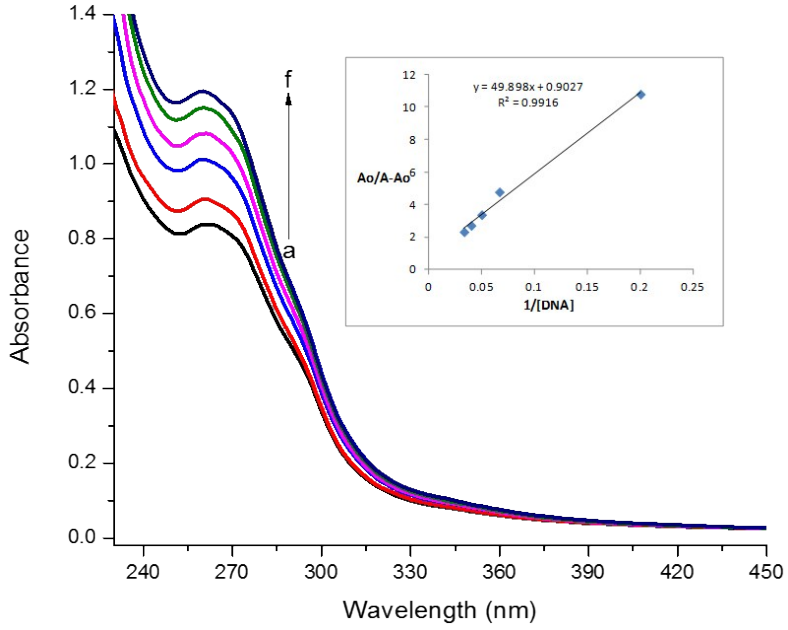


Figure S3: Absorbance of 35µM complex (**1**) in the absence (a) and presence of (b) 5µM, (c) 15µM, (d) 20µM, (e) 25µM and (f) 30 µM DNA. The inset graph represents the plot of A0/A-A0 vs. 1/[DNA] $(\mu M)^{-1}$ for calculation of binding constant (K) and Gibb's free energy (ΔG)

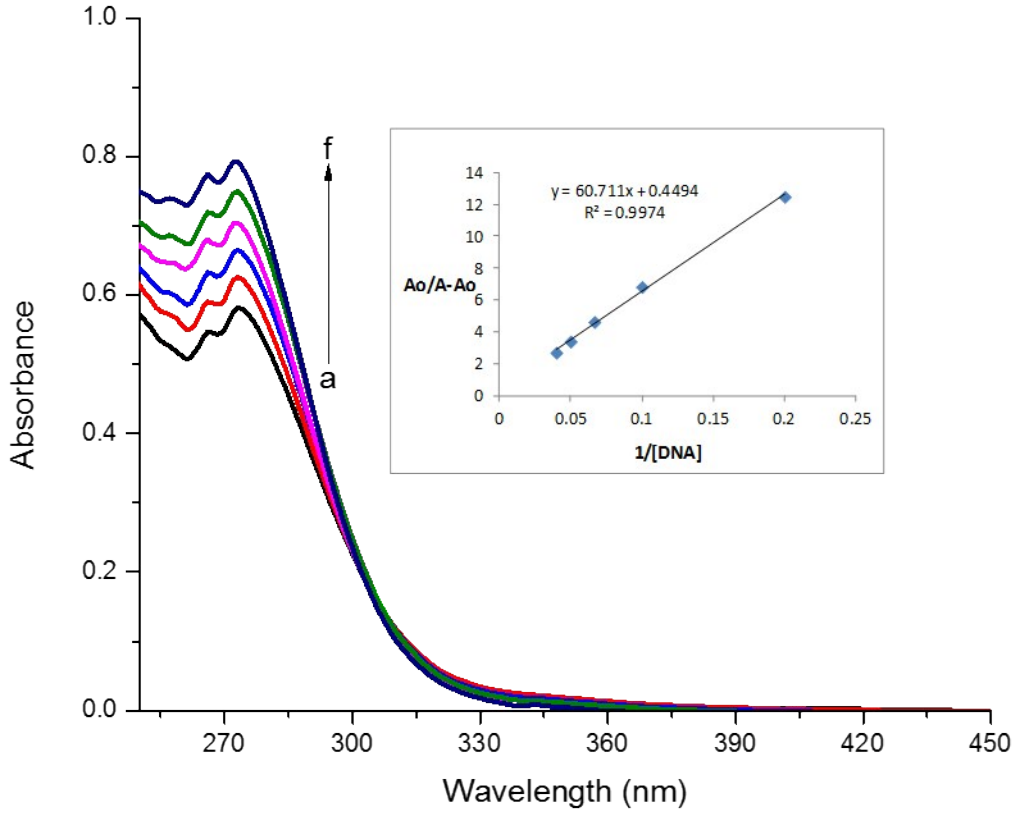


Figure S4: Absorbance of 25μM complex (**2**) in the absence (a) and presence of (b) 5μM, (c) 10μM, (d) 15μM, (e) 20μM and (f) 25μM DNA. The inset graph represents the plot of A0/A-A0 vs. 1/[DNA] $(\mu M)^{-1}$ for calculation of binding constant (K) and Gibb's free energy (ΔG)

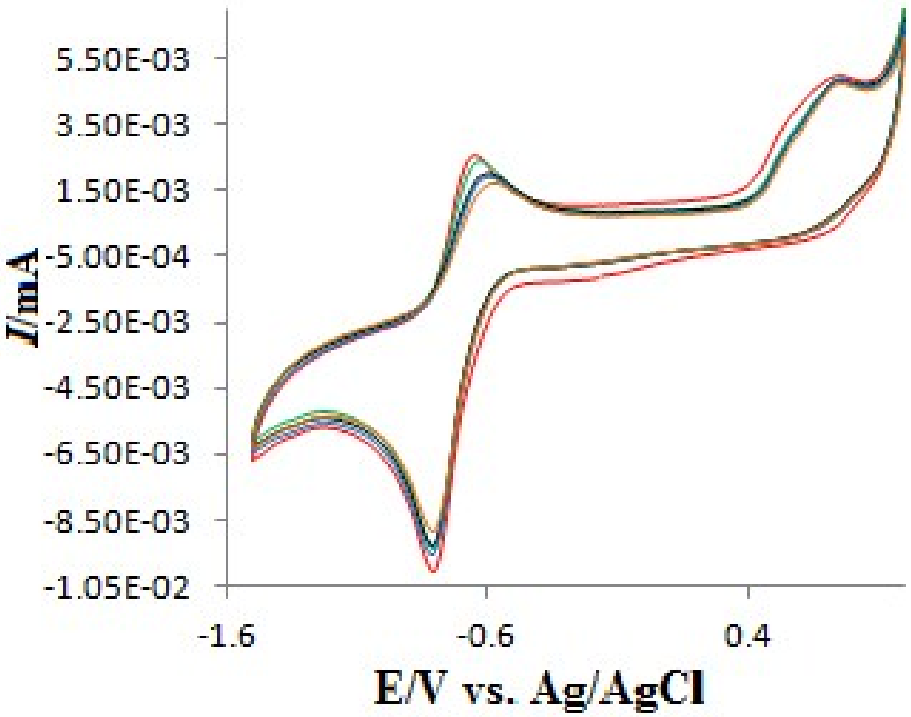


Figure S5: Cyclic voltamograms of 1 mM complex **2** with 0.5 M TBAP as supporting electrolyte in the absence (red) and presence of 20 μM DNA (green), 40 μM DNA (black), 60 μM DNA (blue) and 80 μM DNA (orange) showing a decrease in I from I^o

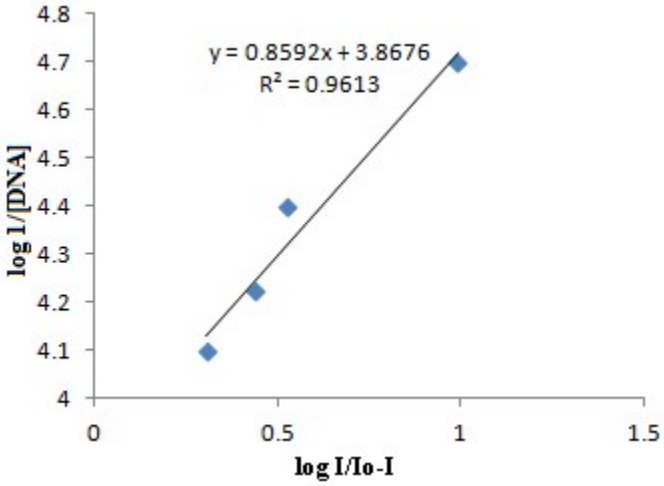


Figure S6: Representative plot of log (I/Io-I) versus log (1/[DNA]) for determination of binding constant of complex (**2**).

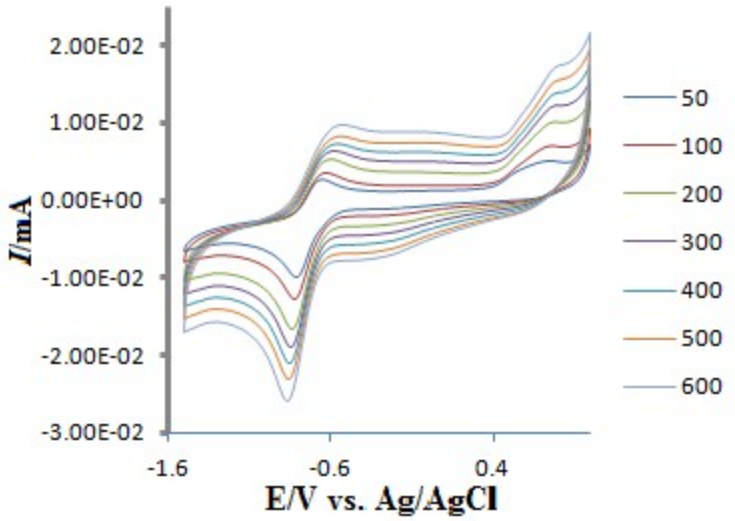


Figure S7: Representative cyclic voltammogram of 1mM complex **2** at different (50-600 mVs^{-1}) scan rates in DMSO with 0.5 M TBAP as supporting electrolyte.

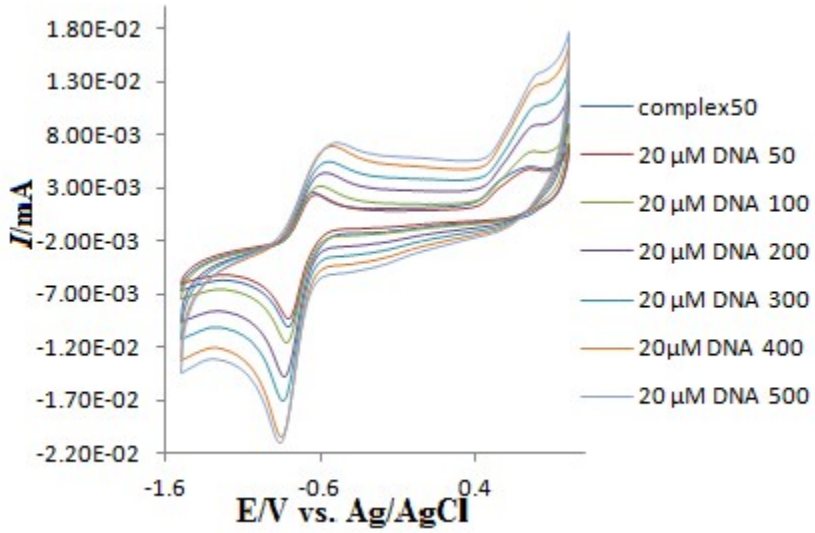


Figure S8: Representative cyclic voltammogram of 1mM complex **2** in the presence of 20 µM DNA at different (50-500 mVs^{-1}) scan rates in DMSO with 0.5 M TBAP as supporting electrolyte.

Table S1: Various weak non-covalent interactions forming 1D and 3D networks for crystal packing

Complex	C-H···X		C-H···O		C-H···π		C-H···S		C-H···Cl		X··· π	
	1D	3D	1D	3D	1D	3D	1D	3D	1D	3D	1D	3D
(**1**)	2.529 Å 2.648 Å 2.622 Å	-	2.705 Å	2.814 Å	2.884 Å 2.825 Å	2.935 Å	-	3.068 Å	-	3.017 Å	-	-
(**2**)	2.889 Å 2.768 Å	3.262Å	-	-	2.882 Å 2.881 Å	2.848 Å 2.963 Å	-	-	-	3.017 Å	-	3.436 Å
(**3**)	2.434 Å	-	-	2.631 Å 2.708 Å 2.668 Å	2.876 Å 2.846 Å	2.996 Å 2.768 Å 2.911 Å	2.901 Å	3.068 Å	-	-	-	-

X= F(**1, 3**), Cl (**2**)

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