Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

The interaction of the (7-chloroquinolin-4-yl)-(2,5-dimethoxyphenyl)-aminehydrochloridedihydrate with serum albumin proteins, inputs from spectroscopic, molecular docking and X-ray diffraction studies

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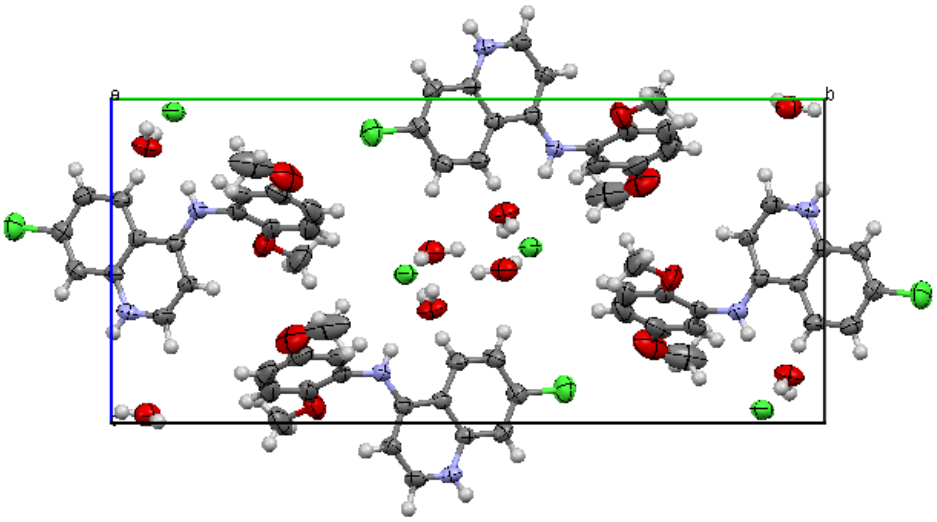

Figure S1: Unit Cell diagram of CQDPA along *a*-axis

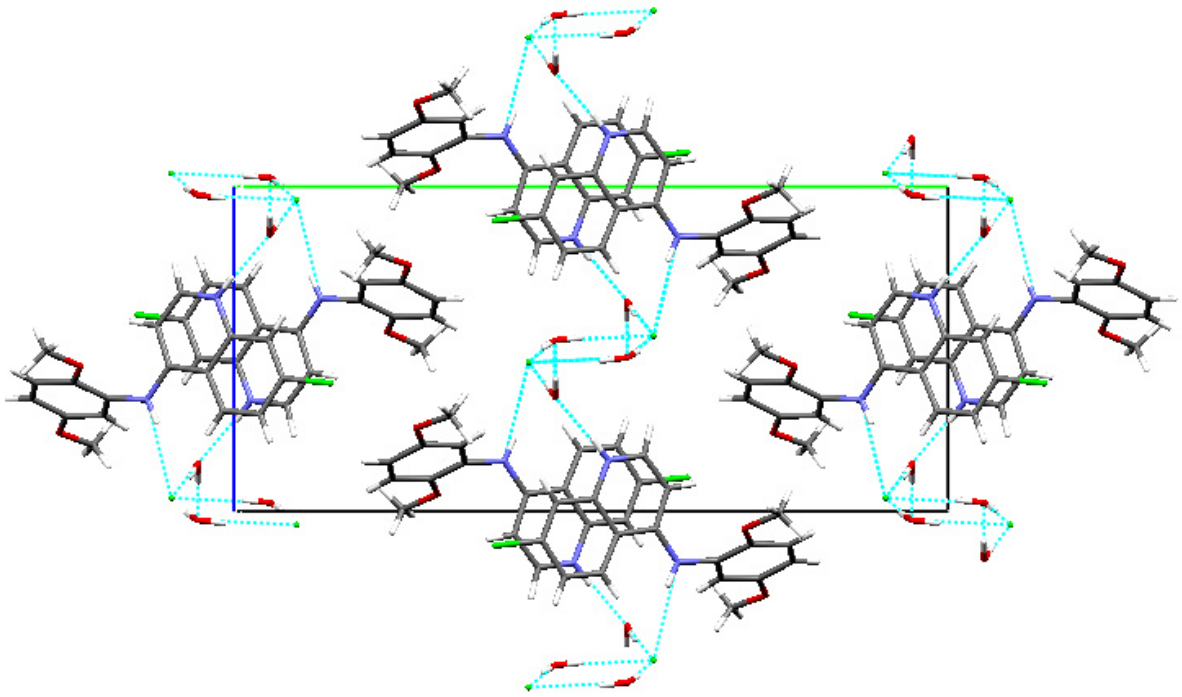

Figure S2: Packing diagram of CQDPA along *c*-axis showing hydrogen bonding.

Table S1: Hydrogen bond geometry (Å, °) for CQDPA

D-H…A	D-H(Å)	H…A(Å)	D-A(Å)	D-H…A(°)	Symmetry code
O4-H4A…Cl2	0.904	3.145	2.249	170.24(3.79)	x, y, z
N2-H2A…Cl2	0.793	3.270	2.496	165.45(3.57)	x, y, z
C1-H1…O3	1.013	3.360	2.453	148.58(2.95)	x, y, z
C4-H4…Cl2	0.906	3.596	2.715	164.40(2.49)	x, y, z
C11-H11…O4	0.897	3.510	2.642	163.09(2.68)	x, y, z
O3-H3B…Cl2	0.834	3.209	2.381	172.00(4.72)	-x+2,-y,-z+1
C7-H7…O4	0.914	3.407	2.722	132.46(2.47)	-x+2,-y,-z+1
N1-H1A…O4	0.854	2.754	1.905	172.75(3.44)	x,+y,+z-1
O3-H3A…O3	0.887	3.198	2.326	167.95(4.69)	x,+y,+z-1
O4-H4B…O3	0.891	2.767	1.876	177.58(5.13)	x+1,+y,+z+1

C5-H5…Cl2	0.924	3.786	2.871	170.89(3.25)	-x+2,-y,-z+2

Table 2: Bond angles [°] for CQDPA

C12-O1-C17	117.83 (0.55)	C15-O2-C16	118.11 (0.46)
H3A-O3-H3B	104.04 (4.71)	H4A-O4-H4B	110.32 (4.50)
C1-N1-C8	121.24 (0.31)	C1-N1-H1A	124.17 (2.32)
C8- N1- H1A	114.51 (2.48)	C3-N2-C10	125.46 (0.29)
C3- N2- H2A	119.07 (2.75)	C10-N2-H2A	115.41 (2.65)
N1- C1- C2	122.56 (0.34)	N1-C1-H1	114.70 (1.93)
C2-C1-H1	122.69 (2.14)	C1-C2-C3	120.14 (0.33)
C1-C2-H2	120.55 (1.69)	C3-C2-H2	119.23 (1.70)
N2-C3-C2	121.79 (0.31)	N2-C3-C9	120.38 (0.28)
C2-C3-C9	117.80 (0.29)	C5-C4-C9	121.89 (0.33)
C5-C4-H4	120.91 (1.81)	C9-C4-H4	117.18 (1.95)
C4-C5-C6	118.94 (0.34)	C4-C5-H5	118.53 (2.36)
C6-C5-H5	122.52 (2.50)	Cl1-C6-C5	118.47 (0.27)
Cl1-C6-C7	119.57 (0.27)	C5-C6-C7	121.96 (0.36)
C6-C7-C8	119.21 (0.32)	C6-C7-H7	121.55 (2.00)
C8-C7-H7	119.24 (1.84)	N1-C8-C7	119.61 (0.30)
N1-C8-C9	119.33 (0.29)	C7-C8-C9	121.06 (0.30)
C3-C9-C4	124.20 (0.29)	C3-C9-C8	118.91 (0.28)
C4-C9-C8	116.88 (0.29)	N2-C10-C11	118.81 (0.35)
N2-C10-C15	119.87 (0.29)	C11-C10-C15	121.24 (0.39)
C10-C11-C12	120.81 (0.44)	C10-C11-H11	121.02 (2.20)
C12-C11-H11	117.99 (2.03)	O1-C12-C11	125.33 (0.50)
O1-C12-C13	116.46 (0.53)	C11-C12-C13	118.22 (0.44)
C12-C13-C14	120.94 (0.59)	C12-C13-H13	113.91 (2.78)

C14-C13-H13	125.15 (2.95)	C13-C14-C15	121.56 (0.55)
C13-C14-H14	122.03 (2.53)	C15-C14-H14	116.38 (2.41)
C10-C15-C14	117.18 (0.33)	O2-C15-C10	116.33 (0.38)
O2-C16-H16A	107.56 (3.06)	O2-C15-C14	126.49 (0.43)
O2-C16-H16B	104.86 (3.64)	O2-C16-H16C	106.98 (4.09)
H16A-C16-H16B	104.15 (4.90)	H16A-C16-H16C	116.24 (5.04)
H16B-C16-H16C	116.24 (5.69)	O1-C17-H17A	108.84(3.05)
H17B-C17-H17C	112.24 (4.64)		

Table 3: Torsion angles [°] for CQDPA

C17 -O1-C12-C11	-8.99 (0.87)	C17-O1-C12-C13	170.95 (0.62)
C12-O1-C17-H17A	-57.61 (3.40)	C12-O1-C17-H17B	-174.50 (3.89)
C12-O1-C17-H17C	61.39 (3.00)	C16-O2-C15-C10	-176.34 (0.46)
C16-O2-C15-C14	3.53 (0.72)	C15-O2-C16-H16A	47.43 (3.31)
C15-O2-C16-H16B	-63.01 (3.95)	C15-O2-C16-H16C	172.98 (4.26)
C8-N1-C1-C2	-0.12 (0.56)	C8-N1-C1-H1	-177.58 (2.24)
H1A-N1-C1-C2	-176.68 (2.93)	H1A-N1-C1-H1	5.87 (3.70)
C1-N1-C8-C7	178.86 (0.34)	C1-N1-C8-C9	-0.68 (0.50)
H1A-N1-C8-C7	-4.27 (2.69)	H1A-N1-C8-C9	176.19 (2.66)
C10-N2-C3-C2	-6.32 (0.54)	C10-N2-C3-C9	175.41 (0.32)
H2A-N2-C3-C9	-7.30 (3.15)	H2A-N2-C3-C2	170.96 (3.13)
C3-N2-C10-C11	119.14 (0.42)	C3-N2-C10-C15	-64.08 (0.51)
H2A-N2-C10-C11	-58.23 (3.05)	H2A-N2-C10-C15	118.54 (3.03)
N1-C1-C2-H2	177.05 (1.99)	N1-C1-C2-C3	0.14 (0.58)
H1-C1-C2-C3	177.40 (2.41)	H1-C1-C2-H2	-5.69 (3.15)
C1-C2-C3-N2	-177.70 (0.34)	C1-C2-C3-C9	0.61 (0.51)

H2-C2-C3-C9	-176.34 (1.95)	H2-C2-C3-N2	5.35 (2.01)
N2-C3-C9-C4	-2.53 (0.50)	N2-C3-C9-C8	176.97 (0.31)
C2-C3-C9-C4	179.13 (0.33)	C2-C3-C9-C8	-1.37 (0.46)
C9-C4-C5-H5	-178.32 (2.77)	C9-C4-C5-C6	0.41 (0.56)
H4-C4-C5-C6	179.30 (2.21)	H4-C4-C5-H5	0.57 (3.56)
C5-C4-C9-C3	177.64 (0.34)	C5-C4-C9-C8	-1.87 (0.51)
H4-C4-C9-C8	179.20 (2.13)	H4-C4-C9-C3	-1.29 (2.18)
C4-C5-C6-Cl1	-178.84 (0.29)	C4-C5-C6-C7	1.64 (0.57)
H5-C5-C6-Cl1	-0.16 (2.91)	H5-C5-C6-C7	-179.68 (2.88)
Cl1-C6-C7-H7	-1.99 (2.30)	Cl1-C6-C7-C8	178.41 (0.27)
C5-C6-C7-C8	-2.08 (0.55)	C5-C6-C7-H7	177.52 (2.27)
C6-C7-C8-N1	-179.03 (0.33)	C6-C7-C8-C9	0.50 (0.52)
H7-C7-C8-C9	179.11 (2.21)	H7-C7-C8-N1	1.36 (2.25)
N1-C8-C9-C3	1.41 (0.46)	N1-C8-C9-C4	-179.05 (0.31)
C7-C8-C9-C3	-178.12 (0.31)	C7-C8-C9-C4	1.42 (0.48)
N2-C10-C11-H11	2.31 (2.52)	N2-C10-C11-C12	177.32 (0.40)
C15-C10-C11-C12	0.59 (0.65)	C15-C10-C11-H11	-174.42 (2.47)
C11-C10-C15-O2	178.90 (0.37)	C11-C10-C15-C14	-0.98 (0.64)
C10-C11-C12-O1	-178.87 (0.47)	C10-C11-C12-C13	1.20 (0.73)
H11-C11-C12-C13	176.35 (2.41)	H11-C11-C12-O1	-3.72 (2.49)
O1-C12-C13-C14	177.44 (0.56)	O1-C12-C13-H13	-2.84 (3.16)
C11-C12-C13-C14	-2.63 (0.87)	C11-C12-C13-H13	177.09 (3.10)
C12-C13-C14-C15	2.28 (0.95)	C12-C13-C14-H14	-179.68 (2.90)
H14-C14-C15-O2	1.55 (2.82)	H14-C14-C15-C10	-178.59 (2.73)

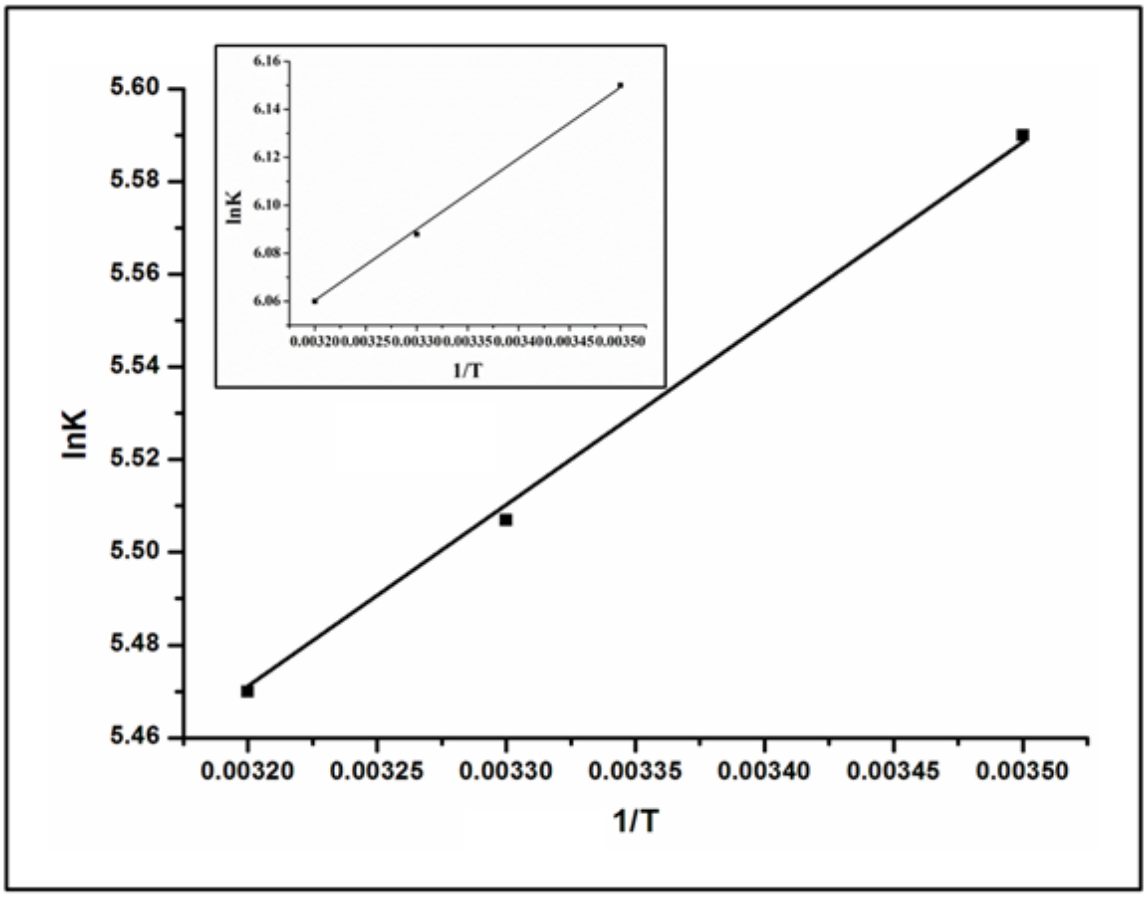

Figure S3: Van't Hoff plot for the interaction of BSA with (7-chloroquinolin-4-yl)-(2,5-dimethoxyphenyl)-amine at pH=7.40; **(inset):** Van't Hoff plot for the interaction of HSA with (7-chloroquinolin-4-yl)-(2,5-dimethoxyphenyl)-amine at pH= 7.40.