Table S1. [(TZD)(DCQ]-serotonin interactions results by DS.

Name	Distance	Category	Type
ASN343:HD21 - [(TZD)(DCQ]:O	2.88554	Hydrogen Bond	Conventional Hydrogen Bond
[(TZD)(DCQ]:C - ASP155:OD2	3.31333	Hydrogen Bond	Carbon Hydrogen Bond
[(TZD)(DCQ]:CL - SER159:O	3.69785	Hydrogen Bond	Carbon Hydrogen Bond
[(TZD)(DCQ]:CL - SER242:O	3.25597	Hydrogen Bond	Carbon Hydrogen Bond
[(TZD)(DCQ]:HN - TRP336	3.13951	Hydrogen Bond	Pi-Donor Hydrogen Bond
TRP336 - [(TZD)(DCQ]	4.87891	Hydrophobic	Pi-Pi T-shaped
PHE340 - [(TZD)(DCQ]	4.72846	Hydrophobic	Pi-Pi T-shaped Pi-
[(TZD)(DCQ] - PHE339	4.76266	Hydrophobic	Pi T-shaped
SER159:C,O;THR160:N - [(TZD)(DCQ]	5.28218	Hydrophobic	Amide-Pi Stacked
LEU229 - [(TZD)(DCQ]	5.08258	Hydrophobic	Alkyl
VAL235 - [(TZD)(DCQ]	4.95457	Hydrophobic	Alkyl
VAL366 - [(TZD)(DCQ]	5.15107	Hydrophobic	Alkyl
[(TZD)(DCQ]:CL - ILE135	4.65913	Hydrophobic	Alkyl
[(TZD)(DCQ]:CL - VAL156	3.80768	Hydrophobic	Alkyl
TYR139 - [(TZD)(DCQ]:CL	4.7308	Hydrophobic	Pi-Alkyl
TRP151 - [(TZD)(DCQ]	4.57405	Hydrophobic	Pi-Alkyl
TRP336 - [(TZD)(DCQ]:CL	3.79169	Hydrophobic	Pi-Alkyl
PHE339 - [(TZD)(DCQ]:CL	4.38122	Hydrophobic	Pi-Alkyl
PHE340 - [(TZD)(DCQ]	5.19771	Hydrophobic	Pi-Alkyl
[(TZD)(DCQ] - VAL156	5.49878	Hydrophobic	Pi-Alkyl
[(TZD)(DCQ] - LEU229	4.7862	Hydrophobic	Pi-Alkyl
[(TZD)(DCQ] - VAL366	4.23249	Hydrophobic	Pi-Alkyl

Table S2. TZD-serotonin interactions results by DS.

Name	Distance	Category	Type
TRP151:CH2 - [(TZD)(DCQ]	3.91922	Hydrophobic	Pi-Sigma
TRP151 - [(TZD)(DCQ]	5.26375	Hydrophobic	Pi-Pi T-shaped
[(TZD)(DCQ] - TRP336	4.8628	Hydrophobic	Pi-Pi T-shaped
[(TZD)(DCQ] - PHE340	4.6715	Hydrophobic	Pi-Pi T-shaped
VAL366 -[(TZD)(DCQ]	5.09644	Hydrophobic	Alkyl
[(TZD)(DCQ]:Cl - VAL366	4.04828	Hydrophobic	Alkyl
TRP151 - [(TZD)(DCQ]	5.26133	Hydrophobic	Pi-Alkyl
TRP336 - [(TZD)(DCQ]	4.77987	Hydrophobic	Pi-Alkyl
TRP336 - [(TZD)(DCQ]	4.78786	Hydrophobic	Pi-Alkyl
PHE340 - [(TZD)(DCQ]	4.80985	Hydrophobic	Pi-Alkyl
TRP367 - [(TZD)(DCQ]:Cl	4.70609	Hydrophobic	Pi-Alkyl
[(TZD)(DCQ] - VAL366	4.79115	Hydrophobic	Pi-Alkyl
[(TZD)(DCQ] - VAL156	5.41572	Hydrophobic	Pi-Alkyl

Table S3. The bond lengths of [(TZD)(DCQ)] obtained through DFT.

S. No.	[(TZD)(DCQ)] (RB3LYP/ 6-311G++)			
	Atom No.	Bond length (Å)	Atom No.	Bond length (Å)
1	R(1-20)	1.761	R(15-16)	1.353
2	R(2-18)	1.259	R(15-17)	1.54
3	R(3-8)	1.47	R(16-20)	1.537
4	R(3-9)	1.477	R(16-41)	1.071
5	R(3-12)	1.468	R(17-21)	1.357
6	R(4-10)	1.469	R(17-42)	1.071
7	R(4-11)	1.469	R(19-24)	1.524
8	R(4-15)	1.466	R(20-22)	1.354
9	R(5-7)	1.411	R(21-22)	1.542
10	R(5-14)	1.476	R(21-43)	1.069
11	R(5-18)	1.473	R(22-44)	1.071
12	R(6-18)	1.455	R(23-25)	1.374
13	R(6-19)	1.455	R(23-45)	1.07
14	R(6-23)	1.475	R(24-26)	1.352
15	R(7-19)	1.297	R(24-46)	1.07
16	R(8-10)	1.539	R(25-26)	1.554
17	R(8-27)	1.07	R(25-47)	1.068
18	R(8-28)	1.069	R(26-48)	1.073
19	R(9-11)	1.54	R(49-50)	1.543
20	R(9-29)	1.069	R(49-54)	1.537
21	R(9-30)	1.071	R(49-56)	1.256
22	R(10-31)	1.07	R(50-51)	1.355
23	R(10-32)	1.067	R(50-57)	1.759
24	R(11-33)	1.071	R(51-52)	1.539
25	R(11-34)	1.07	R(51-55)	1.071
26	R(12-13)	1.537	R(52-53)	1.542
27	R(12-35)	1.071	R(52-60)	1.292
28	R(12-36)	1.072	R(53-54)	1.354
29	R(13-14)	1.54	R(53-59)	1.071
30	R(13-37)	1.072	R(54-58)	1.762
31	R(13-38)	1.069	R(60-61)	1.69
32	R(14-39)	1.069	R(7-56)	2.038
33	R(14-40)	1.069		

Table S4. The bond angles of the [(TZD)(DCQ)] obtained through DFT.

S. No.	[(TZD)(DCQ)] (RB3LYP/ 6-311G++)			
	Atom No.	Bond Angle (Å)	Atom No.	Bond Angle (Å)
1	A(1-20-16)	119.8	A(13-12-35)	109.1
2	A(1-20-22)	120.3	A(13-12-36)	108.9
3	A(2-18-5)	125.4	A(12-13-14)	110.2
4	A(2-18-6)	125.8	A(12-13-37)	109.5

5	A(8-3-9)	110.2	A(12-13-38)	109
6	A(8-3-12)	108.6	A(35-12-36)	109.7
7	A(3-8-10)	109.8	A(14-13-37)	110.4
8	A(3-8-27)	109.5	A(14-13-38)	108.1
9	A(3-8-28)	109.4	A(13-14-39)	110.9
10	A(9-3-12)	108.4	A(13-14-40)	109.2
11	A(3-9-11)	110.2	A(37-13-38)	109.5
12	A(3-9-29)	109.5	A(39-14-40)	109.3
13	A(3-9-30)	109.1	A(16-15-17)	120
14	A(3-12-13)	110.7	A(15-16-20)	120.2
15	A(3-12-35)	108.4	A(15-16-41)	119.8
16	A(3-12-36)	110.1	A(15-17-21)	119.9
17	A(10-4-11)	108.9	A(15-17-42)	120.1
18	A(10-4-15)	109.7	A(20-16-41)	120
19	A(4-10-8)	109.1	A(16-20-22)	119.9
20	A(4-10-31)	109.6	A(21-17-42)	120
21	A(4-10-32)	109.4	A(17-21-22)	119.9
22	A(11-4-15)	110.3	A(17-21-43)	120.1
23	A(4-11-9)	109.1	A(19-24-26)	117.3
24	A(4-11-33)	109.7	A(19-24-46)	121.4
25	A(4-11-34)	109.5	A(20-22-21)	120.1
26	A(4-15-16)	118.9	A(20-22-44)	120
27	A(4-15-17)	121.1	A(22-21-43)	120
28	A(7-5-14)	113	A(21-22-44)	120
29	A(7-5-18)	102.4	A(25-23-45)	120.1
30	A(5-7-19)	111.7	A(23-25-26)	121
31	A(5-7-56)	123.9	A(23-25-47)	119.6
32	A(14-5-18)	105.6	A(26-24-46)	121.3
33	A(5-14-13)	106.9	A(24-26-25)	119
34	A(5-14-39)	110.6	A(24-26-48)	120.1
35	A(5-14-40)	109.9	A(26-25-47)	119.5
36	A(5-18-6)	108.8	A(25-26-48)	120.9
37	A(18-6-19)	99.4	A(50-49-54)	120.1
38	A(18-6-23)	116.7	A(50-49-56)	119.9
39	A(19-6-23)	112.7	A(49-50-51)	120.1
40	A(6-19-7)	111.8	A(49-50-57)	119.9
41	A(6-19-24)	121.7	A(54-49-56)	120
42	A(6-23-25)	120.2	A(49-54-53)	119.9
43	A(6-23-45)	119.8	A(49-54-58)	119.8
44	A(7-19-24)	126.5	A(49-56-7)	119.6
45	A(19-7-56)	124.4	A(51-50-57)	120
46	A(10-8-27)	109.1	A(50-51-52)	119.6
47	A(10-8-28)	109.5	A(50-51-55)	120.4
48	A(8-10-31)	110	A(52-51-55)	120
49	A(8-10-32)	109.3	A(51-52-53)	120.4
50	A(27-8-28)	109.5	A(51-52-60)	119.4

51	A(11-9-29)	109.5	A(53-52-60)	120.2
52	A(11-9-30)	108.9	A(52-53-54)	119.9
53	A(9-11-33)	109.2	A(52-53-59)	120.2
54	A(9-11-34)	109.9	A(52-60-61)	119.9
55	A(29-9-30)	109.5	A(54-53-59)	119.9
56	A(31-10-32)	109.5	A(53-54-58)	120.2
57	A(33-11-34)	109.4		

Table S5. Mulliken atomic charges of the [(TZD)(DCQ)] atoms.

S. No.	**Synthesized complex**			
	Mulliken atomic numbers	**Mulliken atomic charges**	**Mulliken atomic numbers**	**Mulliken atomic charges**
1	1Cl	-0.04942	32H	0.16865
2	2O	-0.54516	33H	0.17958
3	3N	-0.54281	34H	0.16717
4	4N	-0.66525	35H	0.13573
5	5N	-0.46077	36H	0.31159
6	6N	-0.6965	37H	0.17188
7	7N	-0.3286	38H	0.22389
8	8C	-0.13684	39H	0.22325
9	9C	-0.13969	40H	0.21835
10	10C	-0.20156	41H	0.19948
11	11C	-0.16839	42H	0.19277
12	12C	-0.13341	43H	0.17103
13	13C	-0.50297	44H	0.19276
14	14C	-0.09915	45H	0.2377
15	15C	0.25538	46H	0.21345
16	16C	-0.08244	47H	0.19118
17	17C	-0.13231	48H	0.1895
18	18C	0.78762	49C	0.59717
19	19C	0.40068	50C	-0.30143
20	20C	-0.26758	51C	-0.0586
21	21C	-0.1559	52C	0.2488
22	22C	-0.0655	53C	0.0574
23	23C	0.09151	54C	-0.35593
24	24C	-0.15677	55H	0.27504
25	25C	-0.21765	56O	-0.40821
26	26C	-0.11492	57Cl	0.1072
27	27H	0.1532	58Cl	0.04778
28	28H	0.19075	59H	0.24535
29	29H	0.17018	60N	-0.56297
30	30H	0.16677	61Cl	0.1523
31	31H	0.21561		

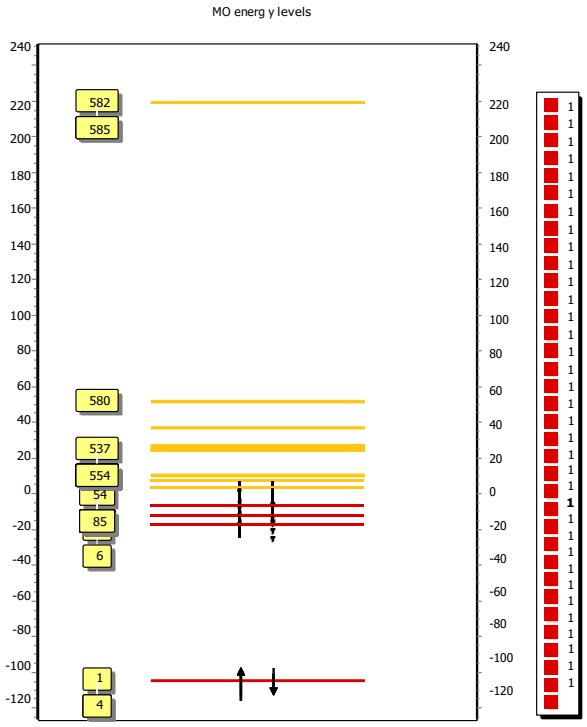

Figure S1. MO energy level diagram of the [(TZD)(DCQ)] complex.