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Supplementary Information

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Experimental, DFT, molecular docking and *in silico* ADMET studies of cadmium-benzenetricarboxylates

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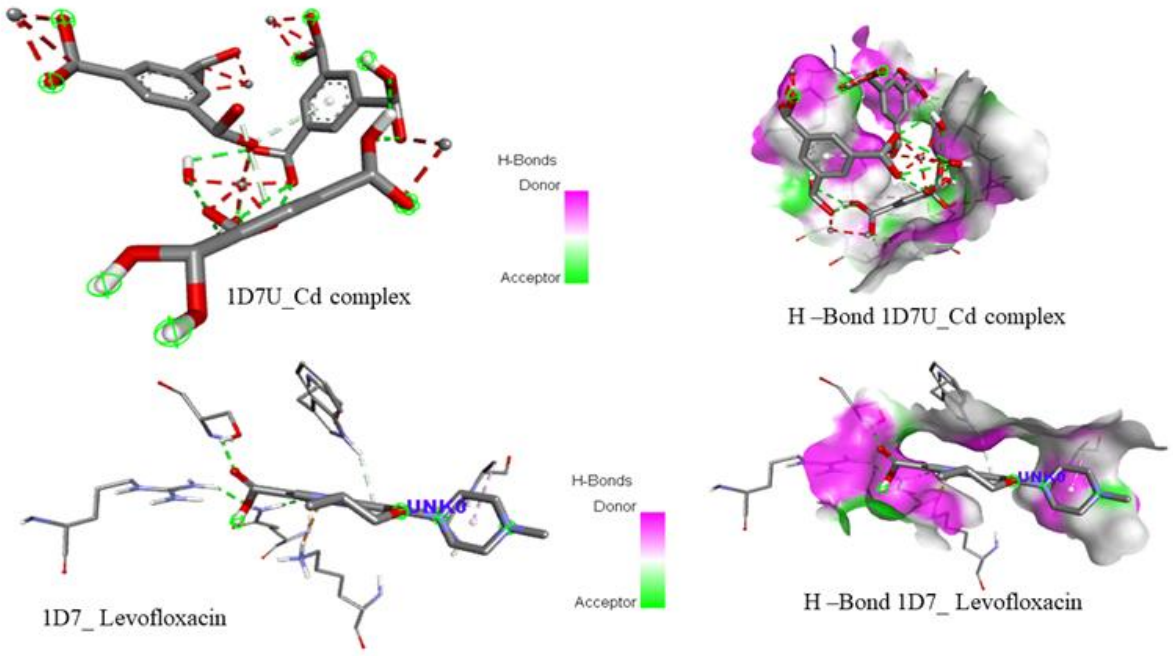

Figure S1. Interactions, H -Bond of the Cd complex and the standard drug with the receptor protein 2D7U.

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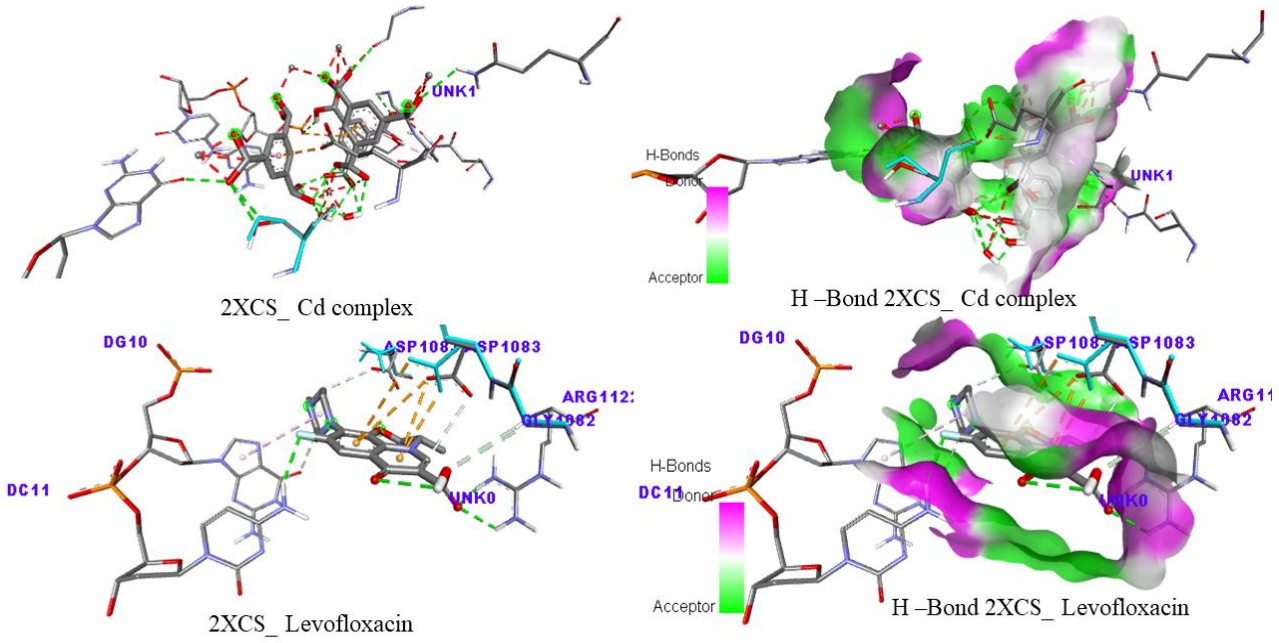

Figure S2. Interactions, H-bond of the Cd complex and the standard drug with the receptor protein 2XCS.

Table S1. Selected bond length (Å).

Atom	Atom	Length (Å)	Atom	Atom	Length (Å)
Cd1	$O7^2$	2.291(3)	C4	C5	1.392(5)
Cd1	C1	2.737(4)	C4	C8	1.494(4)
O3	C1	1.254(5)	C5	C6	1.383(5)
O4	C1	1.279(5)	C6	C7	1.392(5)
O5	C8	1.270(4)	C6	C9	1.481(5)
O6	C8	1.249(4)			

Table S2. Selected bond angle (°).

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O4	Cd1	$O5^1$	145.97(9)	C7	C2	C1	120.8(3)
O4	Cd1	$O6^1$	92.51(9)	C4	C3	C2	121.0(3)
O4	Cd1	$O7^2$	133.61(10)	C3	C4	C8	121.6(3)
O4	Cd1	C1	27.53(10)	C5	C4	C3	119.1(3)
$O5^1$	Cd1	O1	88.82(10)	C5	C4	C8	119.4(3)
$O5^1$	Cd1	O2	90.96(10)	C6	C5	C4	120.3(3)
$O5^1$	Cd1	O3	159.07(9)	C5	C6	C7	120.8(3)
$O5^1$	Cd1	$O6^1$	53.50(9)	C5	C6	C9	116.3(3)
$O5^1$	Cd1	$O7^2$	80.34(10)	C7	C6	C9	122.8(3)
$O5^1$	Cd1	C1	172.95(10)	C6	C7	C2	119.5(3)
$O6^1$	Cd1	C1	119.75(10)	O5	C8	C4	118.1(3)
$O7^2$	Cd1	O1	96.08(11)	O6	C8	O5	121.4(3)
$O7^2$	Cd1	O2	87.90(11)	O6	C8	C4	120.5(3)
$O7^2$	Cd1	O3	79.36(10)	O7	C9	O8	124.6(3)
$O7^2$	Cd1	$O6^1$	133.84(10)	O7	C9	C6	120.8(3)
$O7^2$	Cd1	C1	106.38(10)	O8	C9	C6	114.6(3)
C1	O3	Cd1	85.3(2)				

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Table S3. Atomic charges, Mulliken population analysis and natural population analysis.

Atoms	MPA	NPA
Cd	0.351858	0.19165
O	–0.160251	–0.15589
O	–0.197791	–0.21943
O	–0.129836	–0.11583
O	–0.169683	–0.16842
C	0.072627	0.15902
C	0.070250	0.15440
C	–0.001230	–0.00425
C	–0.067339	–0.03909
C	–0.068446	–0.04121
C	–0.006045	–0.02582
H	0.111999	0.07589
C	–0.005066	–0.02456
H	0.107752	0.07160
C	–0.064182	–0.03421
H	0.120903	0.08308
C	0.000951	0.00006
C	–0.069141	–0.04293
C	–0.070311	–0.04442
C	–0.004620	–0.02298
H	0.110747	0.07463
C	–0.005489	–0.02418
H	0.108542	0.07281
C	–0.064749	–0.03539
H	0.121100	0.08319
C	0.226919	0.30560
O	–0.122283	–0.13169
C	–0.011409	–0.03383
C	–0.065212	–0.03427
C	–0.062989	–0.03127
C	–0.005832	–0.02598
H	0.109237	0.07295
C	–0.004342	–0.02433
H	0.117572	0.07973
C	–0.060716	–0.02794
H	0.123710	0.08500
O	–0.109731	–0.09382
C	0.217715	0.28909
O	–0.185995	–0.20937
O	–0.242756	–0.26935
H	0.247392	0.25327
C	0.217902	0.28887
O	–0.183488	–0.20670
O	–0.242876	–0.26952
H	0.247830	0.25371
C	0.214235	0.28488
O	–0.193920	–0.21872
O	–0.246729	–0.27379
H	0.244788	0.25105
C	0.213358	0.28444
O	–0.196452	–0.22145
O	–0.246422	–0.27346
H	0.245099	0.25135
C	0.216048	0.28681
O	–0.187513	–0.21135

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O	–0.245395	–0.27236
H	0.246389	0.25250
C	0.217195	0.28877
O	–0.188226	–0.21202
O	–0.242992	–0.26973
H	0.246737	0.25266
H	0.091839	0.05796
H	0.113569	0.07441
O	–0.329324	–0.37112
H	0.258796	0.28798
O	–0.324794	–0.36555
H	0.249810	0.28012
H	0.272082	0.30149
H	0.268622	0.29725

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