

Electronic Supporting Information

Controlled Drug Delivery of Antileishmanial Chalcones from Layer-by-Layer (LbL) Self Assembled PSS/PDADMAC Thin Films

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Calibration curves of chalcones

The calibration curves were obtained from UV-Visible spectrophotometry for the quantitative analysis of drug released in the medium. For the experiment, we have prepared ten different concentrations of respective drugs with a concentration value ranging from 1 ppm to 10 ppm by dissolving the required amount of the drug into 50% aqueous ethanol. The absorbance was then recorded at their respective analytical wavelength (λ_{max}). For the drug 3-*m*B-4'-HC the λ_{max} was 323 nm while for the other i.e., 3-DC-4'-HC it was 325 nm. The calibration curves were shown in the Fig. S1.

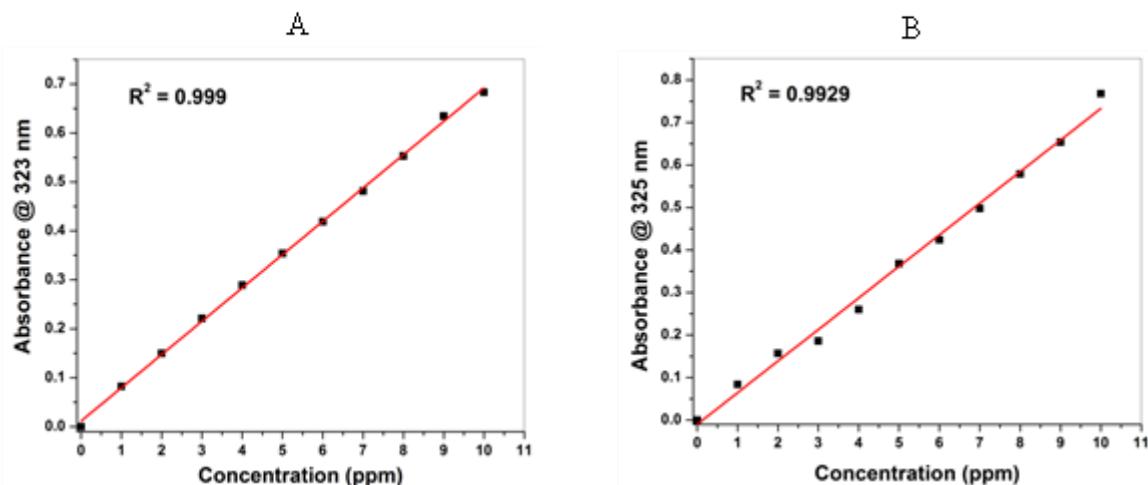


Fig. S1 Calibration curve of (A) 3-*m*B-4'-HC and (B) 3-DC-4'-HC.

Spectral data of chalcones

The synthesized chalcones were fully characterized by different spectroscopic methods including $^1\text{H-NMR}$, $^{13}\text{C-NMR}$, Fourier transformed infrared spectroscopy (FT-IR) and Mass spectrometer analysis. The spectroscopic data for chalcone 3-*m*B-4'-HC and 3-DC-4'-HC is given below.

3-*m*B-4'-HC i.e. 3-(3-Bromo-phenyl)-1-(4-hydroxy-phenyl)-propenone

¹H NMR: (400 MHz, DMSO- d6) δ/ppm 6.90 (2H, d, J=8 Hz, Ph- ring B), 7.4 (1H, t, J=8, 7.6 Hz Ph-ring A), 7.62 (2H, m, Ph- ring A & =C-H adjacent to C=O), 7.82 (1H, d, J=7.6 Hz, Ph- ring A), 7.98 (1H, d, J=15.6 Hz =C-H adjacent to ring A), 8.09 (2H, d, J=7.2 Hz, Ph- ring B), 8.18 (1H, s, Ph- ring A), 10.43 (1H, s, -OH Str.); ¹³C NMR (100 MHz, DMSO- d6) δ/ppm 115.35, 122.33, 123.65, 128.04, 128.92, 130.59, 130.85, 131.29, 132.68, 137.40, 140.88, 162.30, 186.93; FT-IR (cm⁻¹); 3260, 1651, 1598, 1564, 1342, 1226; ESI-MS (M, M+2): C₁₅H₁₁BrO₂, calcd.: 303, 305, found: 303.3882, 305.3832.

3-DC-4'-HC i.e. 3-(2,4-Dichloro-phenyl)-1-(4-hydroxy-phenyl)-propenone

¹H NMR: (400 MHz, DMSO- d6) δ/ppm 6.90 (2H, d, J=8.8 Hz, Ph- ring B), 7.54 (1H, dd, J=6.4, 2 Hz, Ph- ring A), 7.74 (1H, d, J=2 Hz, Ph- ring A), 7.90 (1H, d, J=15.6 Hz, =C-H adjacent to ring A), 8.00 (1H, d, J=15.6 Hz, =C-H adjacent to C=O), 8.08 (2H, d, J=8.8 Hz, Ph- ring B), 8.23 (1H, d, J=8.4 Hz, Ph- ring A), 10.49 (1H, s, -OH); ¹³C NMR (100 MHz, DMSO- d6) δ/ppm 115.42, 125.48, 127.85, 128.71, 129.39, 129.69, 131.35, 131.57, 136.03, 162.47, 186.69; FT-IR (cm⁻¹); 3131, 1602, 1553, 1226; ESI-MS (M+1): C₁₅H₁₀Cl₂O₂, calcd.: 293, found: 293.2704.

Complete *in-vitro* controlled release data

The *in-vitro* controlled release study of antileishmanial chalcones was performed by using UV-Visible spectrophotometer in phosphate buffer saline at pH 7.4. The details of the experiment were given in the manuscript under the Experimental section. All the measurements were performed thrice to minimize the error. The average values were used for plotting the release profiles of the drugs and the error was calculated as standard deviation. The complete data is given for both the drugs separately in Table-1 and Table-2 as shown below.

Table S1 Release data for 3-*m*B-4'-HC

S. No.	Time (min.)	Time interval (min.)	Absorbance at 323 nm			% Release (Eq. 5)			Average % Release
			Plate-1	Plate-2	Plate-3	Plate-1	Plate-2	Plate-3	
1.	0	0	0.1465	0.137	0.1786	0	0	0	0
2.	2	2	0.107	0.1206	0.166	26.96	11.97	7.05	15.3266
3.	5	3	0.0906	0.0986	0.1306	38.15	28.02	26.87	31.0133
4.	8	3	0.0743	0.0776	0.1136	49.28	43.35	36.39	43.0066
5.	11	3	0.0606	0.064	0.100	58.63	53.28	44.00	51.97
6.	14	3	0.053	0.057	0.0706	63.82	58.39	60.47	60.8933
7.	19	5	0.0456	0.0476	0.0603	68.87	65.25	66.23	66.7833
8.	24	5	0.042	0.0403	0.0536	71.33	70.80	69.98	70.7033
9.	29	5	0.038	0.0346	0.048	74.06	74.74	73.12	73.9733
10.	34	5	0.0356	0.026	0.0316	75.70	81.02	82.30	79.6733
11.	44	10	0.0316	0.026	0.0246	78.43	81.02	86.22	81.89
12.	59	15	0.0293	0.023	0.0213	80.00	83.21	88.07	83.76
13.	74	15	0.030	0.0193	0.0183	79.52	85.91	89.75	85.06
14.	104	30	0.0263	0.0156	0.0163	82.04	88.61	90.87	87.1733
15.	164	60	0.0273	0.014	0.012	81.36	89.78	93.28	88.14
16.	224	60	0.0243	0.0113	0.011	83.41	91.75	93.84	89.6666
17.	284	60	0.025	0.0113	0.0133	82.93	91.75	92.55	89.0766
18.	344	60	0.026	0.0123	0.0106	82.25	91.02	94.06	89.11
19.	584	240	0.0243	0.0096	0.0103	83.41	92.99	94.23	90.21

Table S2 Release data for 3-DC-4'-HC

S. No.	Time (min.)	Time interval (min.)	Absorbance at 325 nm			% Release (Eq. 5)			Average % Release
			Plate-1	Plate-2	Plate-3	Plate-1	Plate-2	Plate-3	
1.	0	0	0.167	0.203	0.171	0	0	0	0
2.	2	2	0.146	0.182	0.155	12.57	10.34	9.35	10.7533
3.	5	3	0.123	0.159	0.127	26.34	21.67	25.73	24.58
4.	8	3	0.107	0.146	0.116	35.92	28.07	32.16	32.05
5.	11	3	0.097	0.131	0.104	41.91	35.46	39.18	38.85
6.	14	3	0.087	0.115	0.095	47.90	43.34	44.44	45.2266
7.	19	5	0.077	0.102	0.086	53.89	49.75	49.70	51.1133
8.	24	5	0.069	0.097	0.079	58.68	52.21	53.80	54.8966
9.	29	5	0.063	0.094	0.074	62.27	53.69	56.72	57.56
10.	34	5	0.058	0.082	0.070	65.26	59.60	59.06	61.3066
11.	44	10	0.052	0.078	0.066	68.86	61.57	61.40	63.9433
12.	59	15	0.049	0.066	0.061	70.65	67.48	64.32	67.4833
13.	74	15	0.041	0.061	0.054	75.44	69.95	68.42	71.27
14.	104	30	0.040	0.055	0.049	76.04	72.90	71.34	73.4266
15.	164	60	0.035	0.049	0.041	79.04	75.86	76.02	76.9733
16.	224	60	0.040	0.044	0.040	76.04	78.32	76.60	76.9866
17.	284	60	0.027	0.040	0.040	83.83	80.29	76.60	80.24
18.	344	60	0.026	0.034	0.029	84.43	83.25	83.04	83.5733
19.	464	120	0.024	0.029	0.018	85.63	85.71	89.47	86.9366
20.	584	120	0.016	0.028	0.017	90.41	86.20	90.05	88.8866
21.	704	120	0.018	0.024	0.012	89.22	88.17	92.98	90.1233
22.	824	120	0.019	0.023	0.011	88.62	88.66	93.56	90.28
23.	944	120	0.019	0.022	0.012	88.62	89.16	92.98	90.2533