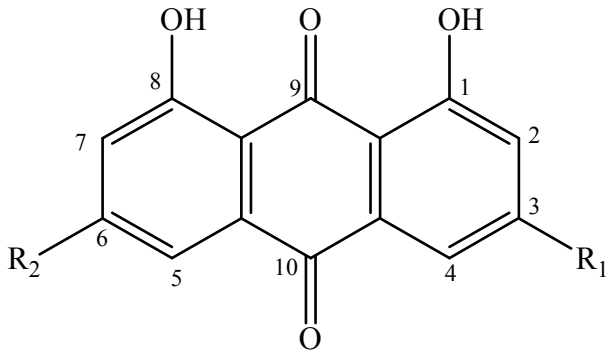
SUPPLEMENTARY DATA

1. Spectroscopic data of isolated compounds:



Compound	R_1	R_2
Rhein	COOH	H
Aloe emodin	CH_2OH	H
Emodin	OH	CH_3
Chrysophanol	CH_3	H
Physcion	OCH_3	CH_3

Rhein: mp 352-354°C (from MeOH). IR ($CHCl_3$): 3422, 3206, 1691, 1629cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$, Me_4Si) δ: 12.00 (1H, s, C_1–OH), 11.98 (1H, s, C_8–OH), 11.01(1H, broad, –COOH), 8.4 (1H, s, C_2–H),7.93 (1H, s, C_4–H), 7.81(1H, d, J = 7.5 Hz, C_7–H), 7.80 (1H, m, C_6–H), 7.38 (1H, d, J = 8.2 Hz, C_5–H),). ESI-MS ($M+1^+$): 285.00.

Aloe emodin: mp 222–224°C (from MeOH). IR ($CHCl_3$): 3600-3000 (broad), 1651, 1633cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$, Me_4Si) δ: 11.94 (1H, s, C_1–OH), 11.92 (1H, s, C_8–OH), 7.94 (1H, d, J = 6.8 Hz, C_5–H), 7.71 (1H, s, C_4–H), 7.38 (1H, m, C_6–H), 7.32 (1H, d, J = 8.4 Hz, C_7–H), 7.28 (1H, s, C_2–H), 5.58 (1H, s, –CH_2–OH), 4.62 (2H, s, –CH_2–). ESI-MS ($M+1^+$): 271.01.

Emodin: mp 252-254°C (from MeOH). IR ($CHCl_3$): 3389, 1676, 1610cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$, Me_4Si) δ: 12.27 (1H, s, C_3–OH), 12.11 (1H, s, C_1–OH), 12.01 (1H, s, C_8–OH), 7.70 (1H, s, C_5–H), 7.26 (1H, d, J = 2.1 Hz, C_4–H), 7.08 (1H, s, C_7–H), 6.67 (1H, d, J = 2.1 Hz, C_2–H), 2.35 (3H, s, CH_3); ESI-MS ($M+1^+$): 271.30.

Chrysophanol: mp 194-196°C (from MeOH). IR ($CHCl_3$): 3420, 1676, 1626cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$, Me_4Si) δ: 12.13 (1H, s, C_1–OH), 12.02 (1H, s, C_8–OH), 7.84 (1H, d, J = 7.1 Hz, C_5–H), 7.68 (1H, m, C_6–H), 7.67 (1H, s, C_4–H), 7.28 (1H, d, J = 8.2 Hz, C_7–H), 7.11(1H, s, C_2–H), 2.47 (3H, s, –CH_3). ESI-MS ($M+1^+$): 255.24.

Physcion: mp 207-209°C (from MeOH). IR ($CHCl_3$): 3423, 1609 (broad), 1364cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$, Me_4Si) δ: 12.11 (1H, s, C_1–OH), 12.00 (1H, s, C_8–OH), 7.64 (1H, s, C_5–H), 7.38 (1H, d, J = 2.1 Hz, C_4–H), 7.09 (1H, s, C_7–H), 6.70 (1H, d, J = 2.1 Hz, C_2–H), 3.93 (3H, s, –OCH_3), 2.46 (3H, s, –CH_3). ESI-MS ($M+1^+$): 285.26.

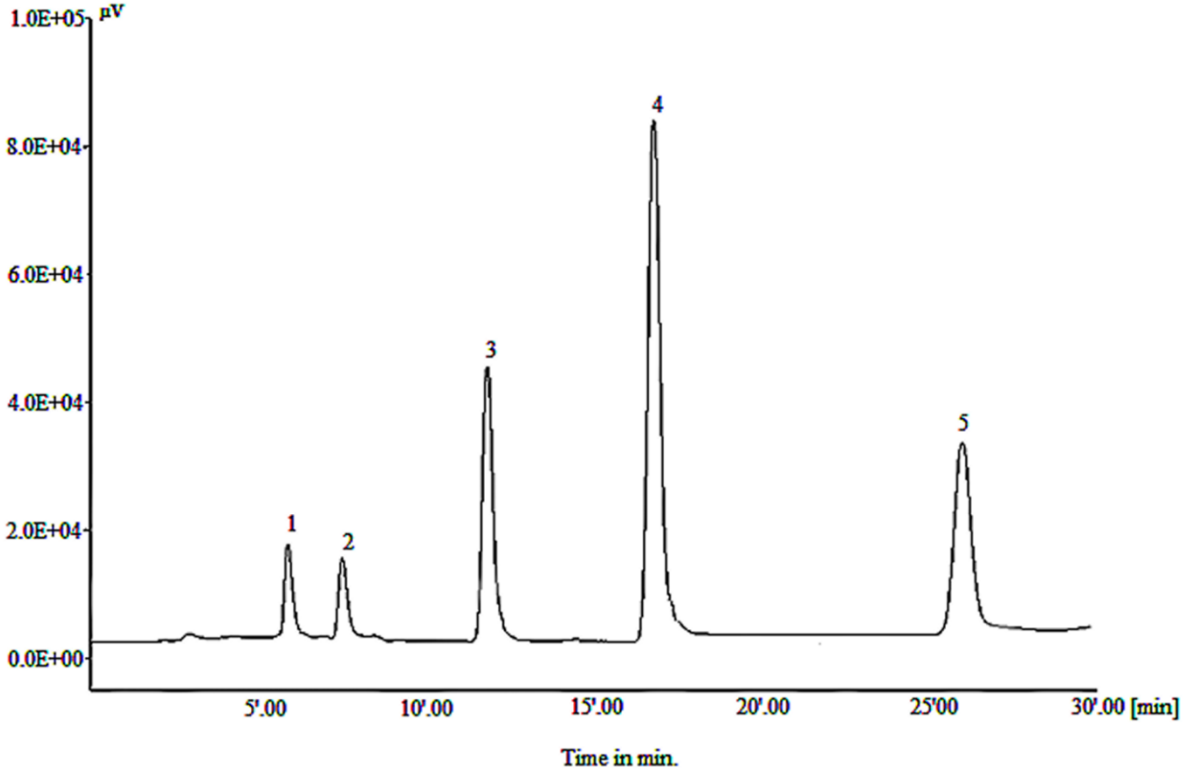


Fig.1: HPLC chromatogram of isolated 1,8-dihydroxyquinones: (1) aloe emodin – 5.8 min; (2) rhein – 7.4 min; (3) emodin – 11.9 min; (4) chrysophanol – 16.9 min; (5) physcion – 25.7 min. HPLC demonstrated a %purity > 98%.

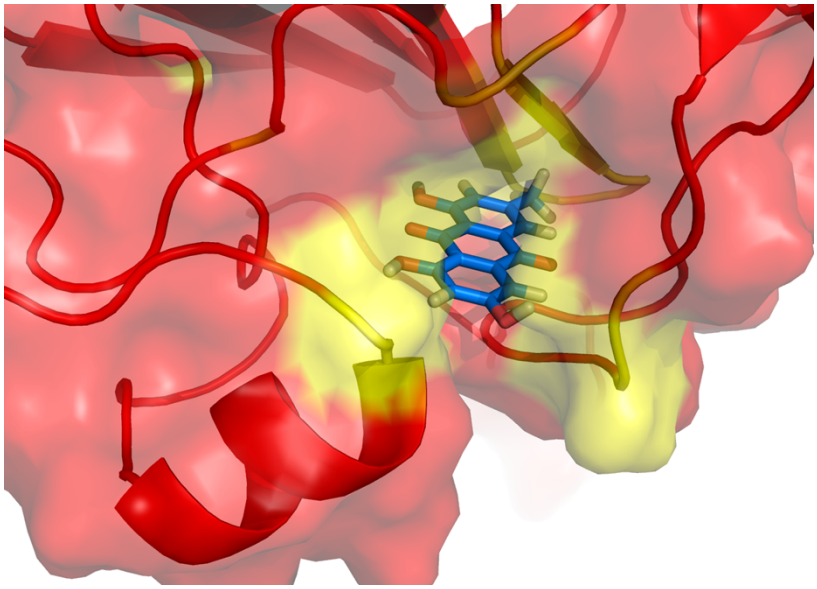


Fig.2: Surface representation of 'Quinone binding site' with favoured pose of most active emodin, interacting residue surface has been coloured in yellow for locating site. (Figure prepared using PyMol [http://www.pymol.org]).