

Elucidating the binding interaction of andrographolide with plasma proteins: biophysical and computational approach

Daniel Pushparaju Yeggoni[†], Christian Kuehne[‡], Aparna Rachamalla[¶], Rajagopal Subramanyam^{†*}

[†]Department of Plant Sciences, School of Life Sciences, University of Hyderabad, Hyderabad 500046, India

[‡]Institute of Laboratory Medicine, Clinical Chemistry and Pathobiochemistry, Charité-Universitätsmedizin Berlin, CVK, Augustenburger Platz 1, 13353, Berlin, Germany.

[¶]National Institute of Animal Biotechnology, Axis Clinicals Building, Miyapur, Hyderabad, 500049, India

*Corresponding author

RajagopalSubramanyam

Department of Plant Sciences

School of Life Sciences

University of Hyderabad 500 046 India

Tel: +91-40-23134572

Fax: +91-40-23010120

Email: srgsl@uohyd.ernet.in

Fig.SI 1.

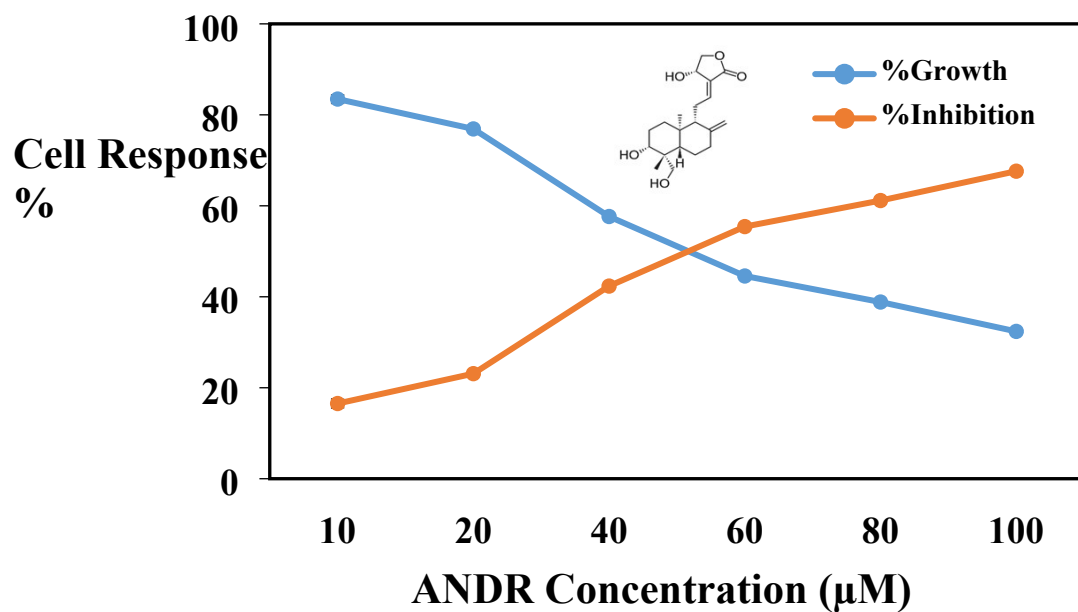


Fig.SI 1. Cell response of ANDR. ANDR showing anti-cancer properties (A) against breast cancer cells (MCF-7) in a dose dependent manner. Cell growth was measured by the MTT assay and the IC_{50} values were calculated accordingly.

Fig.SI 2.

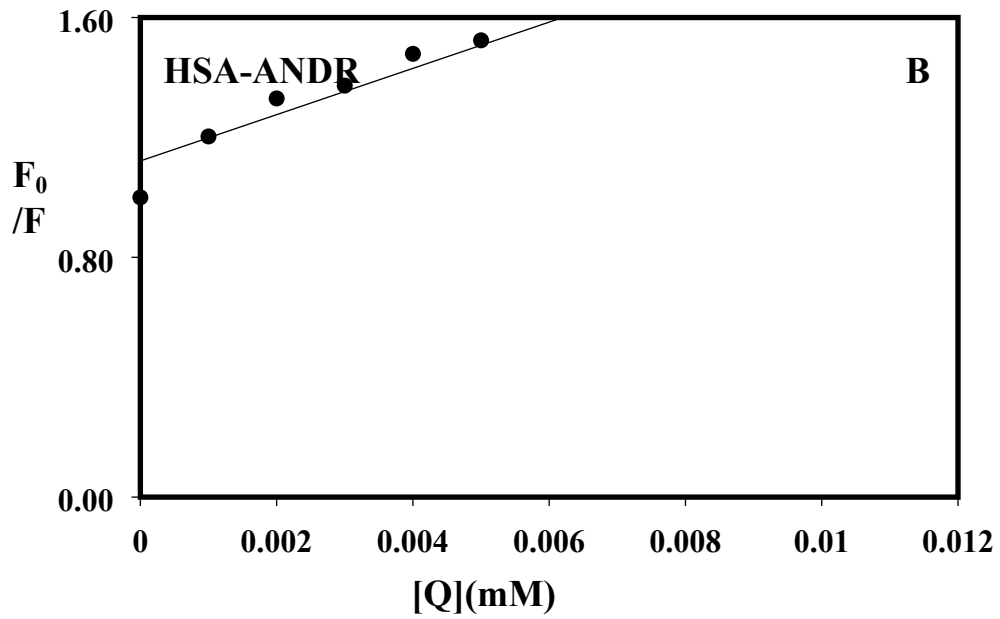


Fig.SI 2. Stern-Volmer plots of HSA-ANDR complexes showing fluorescence quenching constant (K_q). Here the plot is showing F_0/F against $[Q]$ for ANDR.

Fig.SI 3.

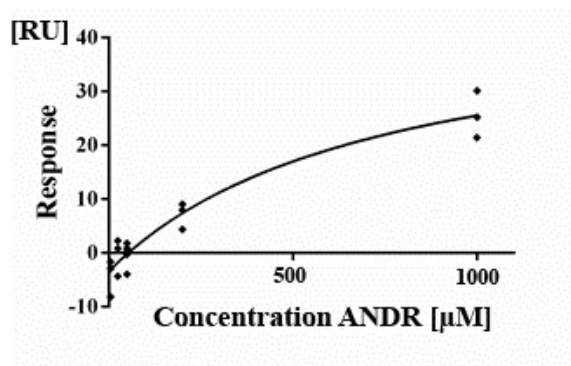
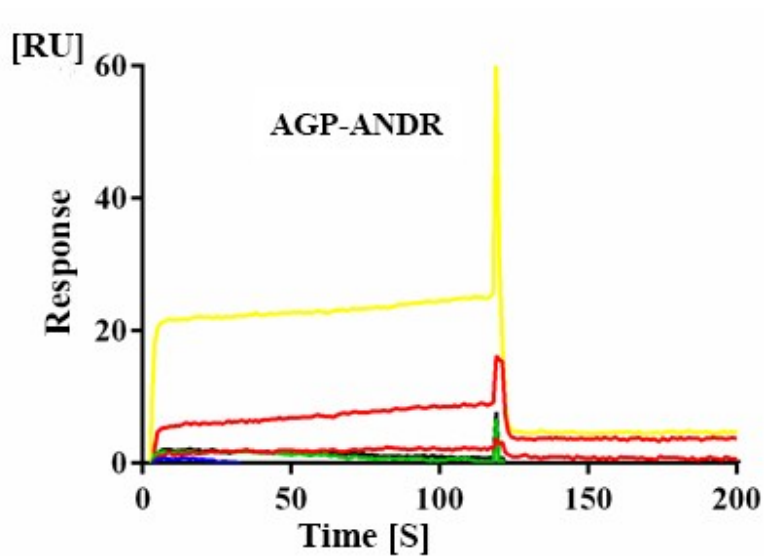


Fig.SI 3. Sensorgrams of ANDR binding to AGP immobilized on a CM 5 sensor chip (top) and respective R_{eq} values fitted to the steady state isotherm binding model (bottom). Increasing concentrations of the analyte are

denoted by different colors: 5 μM (blue), 25 μM (black), 50 μM (green),
200 μM (red) and 1000 μM (yellow) for ANDR-AGP.