Fig. S4 A: results of the first *in vitro* binding assay.
(First experimental verification)

I. *In vitro* binding assay of DHT and testosterone

![Chemical structure of DHT and testosterone](image1)

- (A) chemical structure of dihydrotestosterone (DHT) and testosterone.
- (B) result of *in vitro* assay.

II. *In vitro* binding assay of flutamide

![Chemical structure of flutamide](image2)

- (A) chemical structure of flutamide.
- (B) result of *in vitro* assay.

III. *In vitro* binding assay of bicalutamide

![Chemical structure of bicalutamide](image3)

- (A) chemical structure of bicalutamide.
- (B) result of *in vitro* assay.
IV. *In vitro* binding assay of nilutamide

(A) chemical structure of nilutamide. (B) Result of *in vitro* assay.

V. *In vitro* binding assay of spironolactone

(A) chemical structure of spironolactone. (B) Result of *in vitro* assay.

VI. *In vitro* binding assay of vitamin D3

(A) chemical structure of vitamin D3. (B) Result of *in vitro* assay.
VII. *In vitro* binding assay of ZINC 03849821

![Chemical structure of ZINC 03849821](image1)

**A** chemical structure of ZINC 03849821. **B** result of *in vitro* assay.

VIII. *In vitro* binding assay of ZINC 04369595

![Chemical structure of ZINC 04369595](image2)

**A** chemical structure of ZINC 04369595. **B** result of *in vitro* assay.

IX. *In vitro* binding assay of fluanisone

![Chemical structure of fluanisone](image3)

**A** chemical structure of fluanisone. **B** result of *in vitro* assay.
X. *In vitro* binding assay of ZINC 04026296

(A) chemical structure of ZINC 04026296. (B) result of *in vitro* assay.

XI. *In vitro* binding assay of 3-epiuzarigenin

(A) chemical structure of 3-epiuzarigenin. (B) result of *in vitro* assay.

XII. *In vitro* binding assay of MDPI 1011

(A) chemical structure of MDPI 1011. (B) result of *in vitro* assay.
XIII. In vitro binding assay of NSC 6129

(A) chemical structure of NSC 6129. (B) result of in vitro assay.

XIV. In vitro binding assay of MDPI 944

(A) chemical structure of MDPI 944. (B) result of in vitro assay.

XV. In vitro binding assay of P712100

(A) chemical structure of P712100. (B) result of in vitro assay.
XVI. *In vitro* binding assay of methandriol

(A) Chemical structure of methandriol. (B) Result of *in vitro* assay.

XVII. *In vitro* binding assay of cortexolone

(A) Chemical structure of cortexolone. (B) Result of *in vitro* assay.
(Second experimental verification)

XVIII. 

\textit{In vitro} binding assay of DSHS00507SC

\begin{figure}
\centering
\includegraphics[width=0.8\textwidth]{DSHS00507SC}
\caption{DSHS00507SC}
\end{figure}

\text{IC}_{50} \quad 22 \, \mu\text{M}

XIX. 

\textit{In vitro} binding assay of 4J-584S

\begin{figure}
\centering
\includegraphics[width=0.8\textwidth]{4J-584S}
\caption{4J-584S}
\end{figure}

\text{IC}_{50} \quad 22 \, \mu\text{M}

XX. 

\textit{In vitro} binding assay of T5853872

\begin{figure}
\centering
\includegraphics[width=0.8\textwidth]{T5853872}
\caption{T5853872}
\end{figure}

\text{IC}_{50} \quad 80 \, \mu\text{M}
XXI. *In vitro* binding assay of BAS01279920

![Graph showing in vitro binding assay for BAS01279920](image)

IC<sub>50</sub> > 200μM

XXII. *In vitro* binding assay of AN-652/43163258

![Graph showing in vitro binding assay for AN-652/43163258](image)

IC<sub>50</sub> > 200μM

Fig. S4 I-XXII: result of *in vitro* binding assay for each compound.