

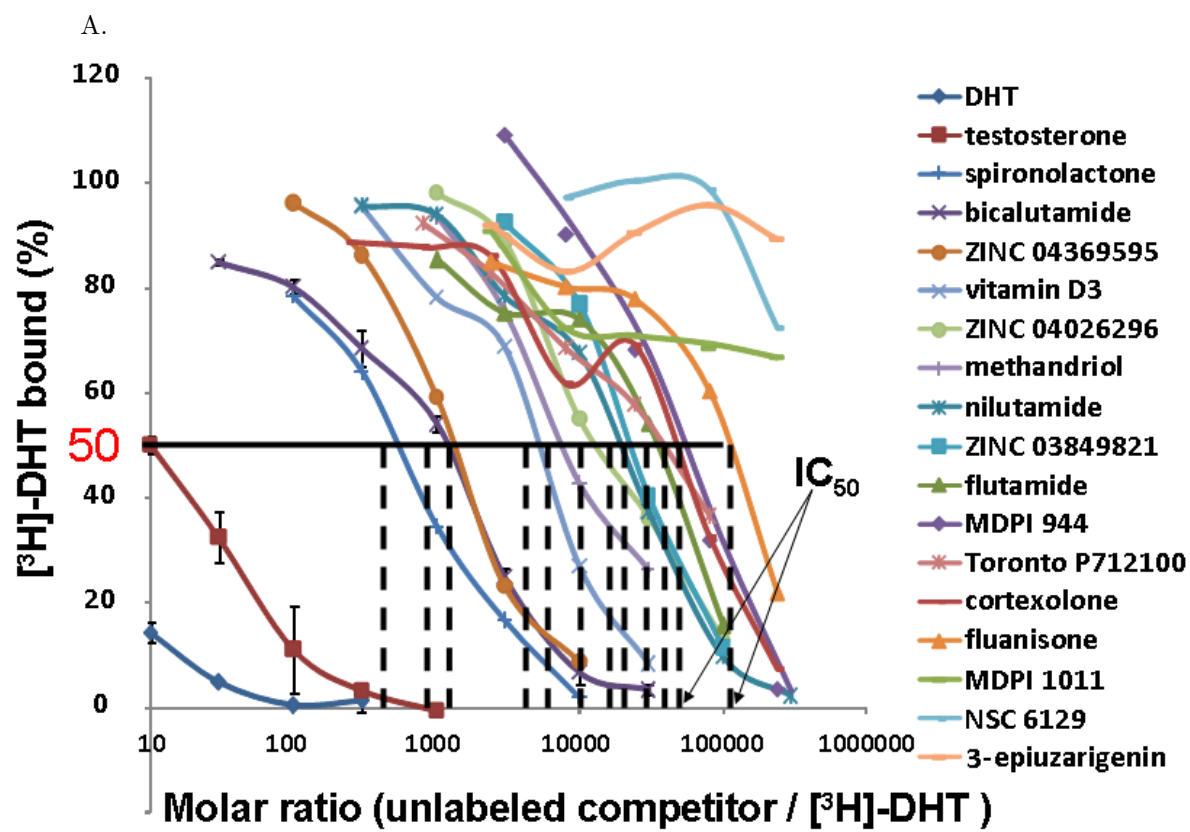
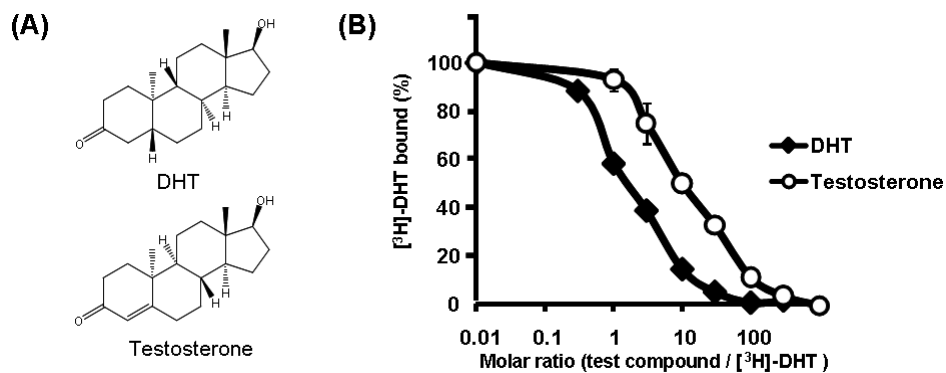
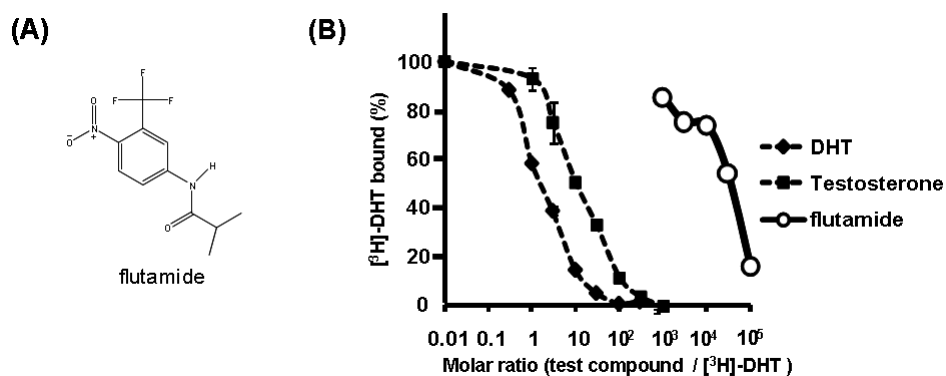


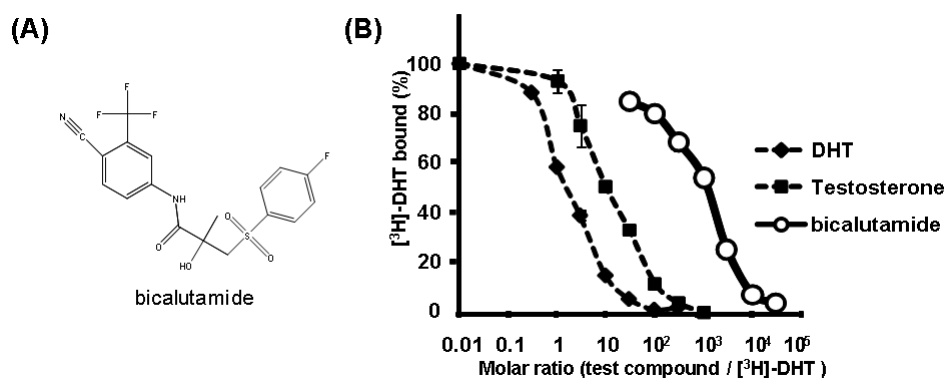
Fig. S4 A: results of the first *in vitro* binding assay.

(First experimental verification)I. *In vitro* binding assay of DHT and testosterone

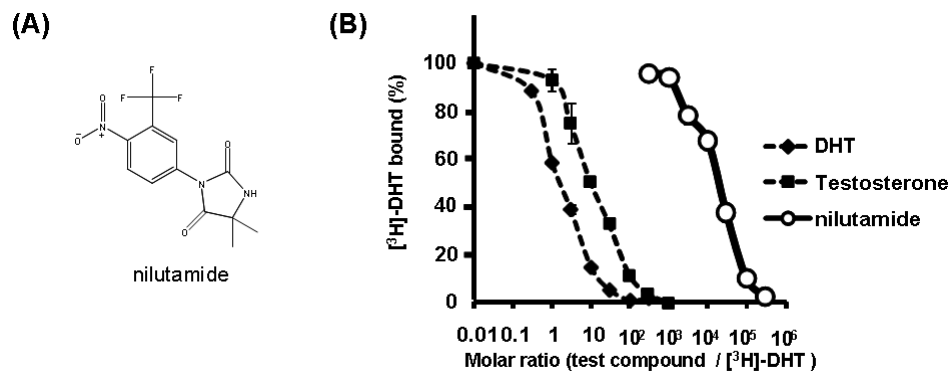
(A) chemical structure of dihydrotestosterone (DHT) and testosterone. (B) result of *in vitro* assay.

II. *In vitro* binding assay of flutamide

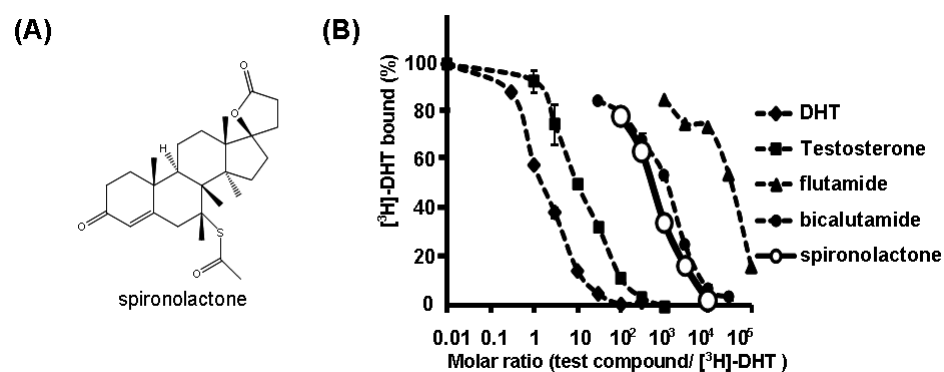
(A) chemical structure of flutamide. (B) result of *in vitro* assay.

III. *In vitro* binding assay of bicalutamide

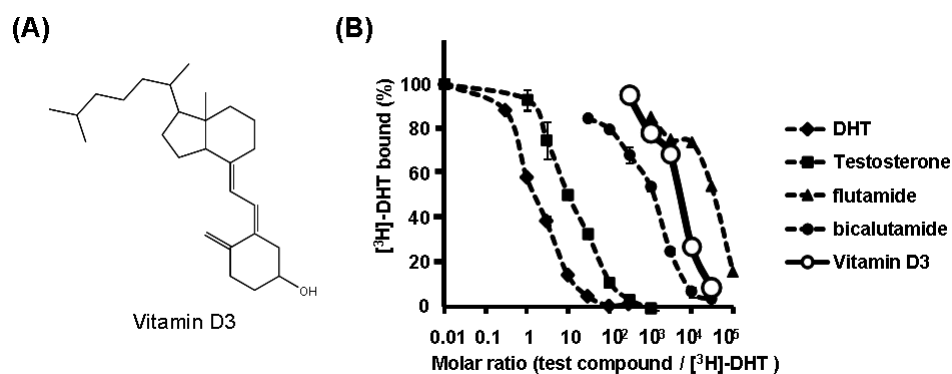
(A) chemical structure of bicalutamide. (B) result of *in vitro* assay.

IV. *In vitro* binding assay of nilutamide

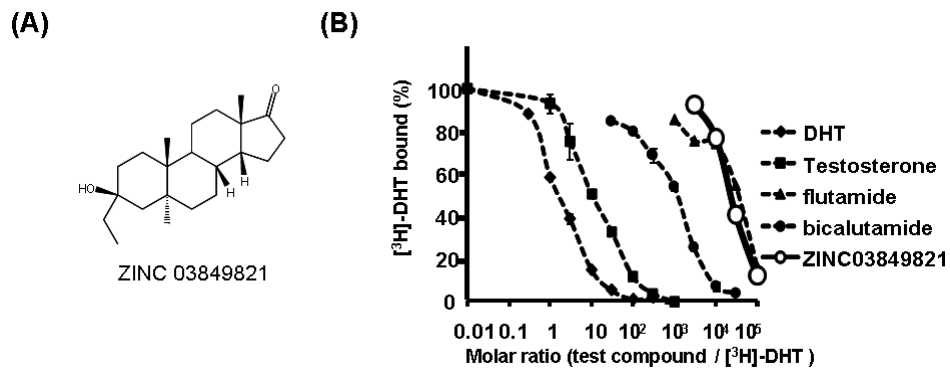
(A) chemical structure of nilutamide. (B) result of *in vitro* assay.

V. *In vitro* binding assay of spironolactone

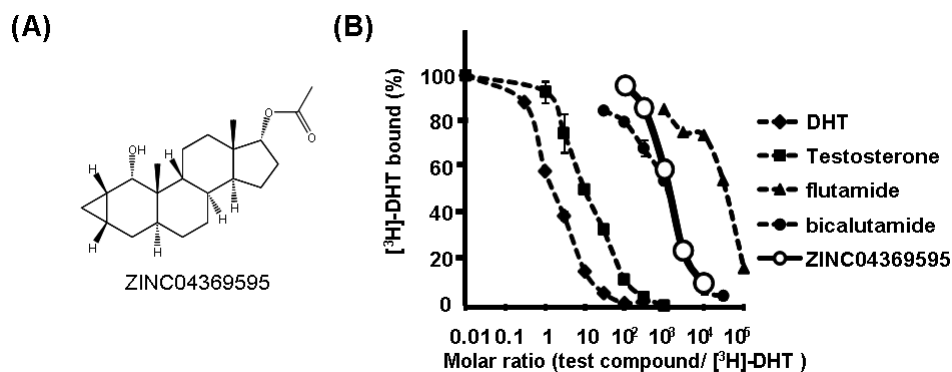
(A) chemical structure of spironolactone. (B) result of *in vitro* assay.

VI. *In vitro* binding assay of vitamin D3

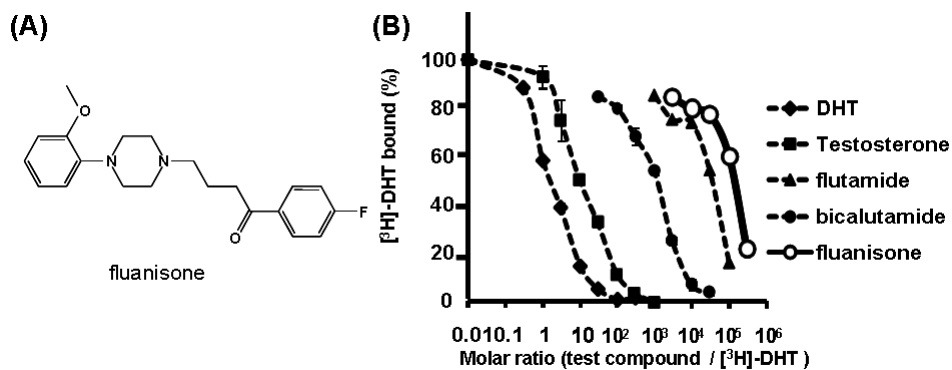
(A) chemical structure of vitamin D3. (B) result of *in vitro* assay.

VII. *In vitro* binding assay of ZINC 03849821

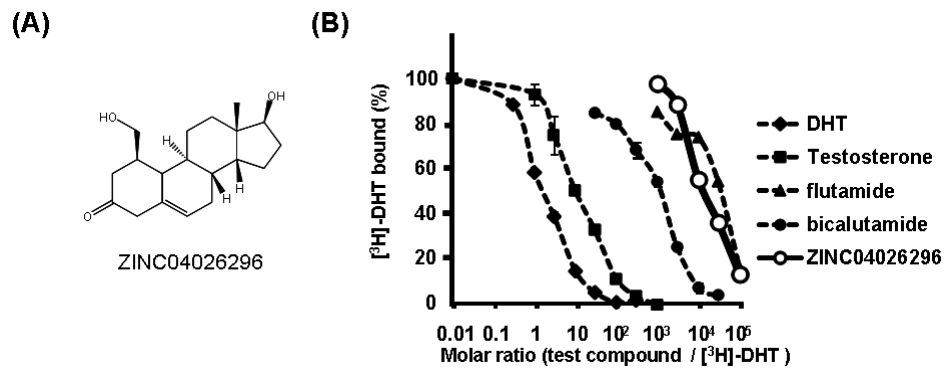
(A) chemical structure of ZINC 03849821. (B) result of *in vitro* assay.

VIII. *In vitro* binding assay of ZINC 04369595

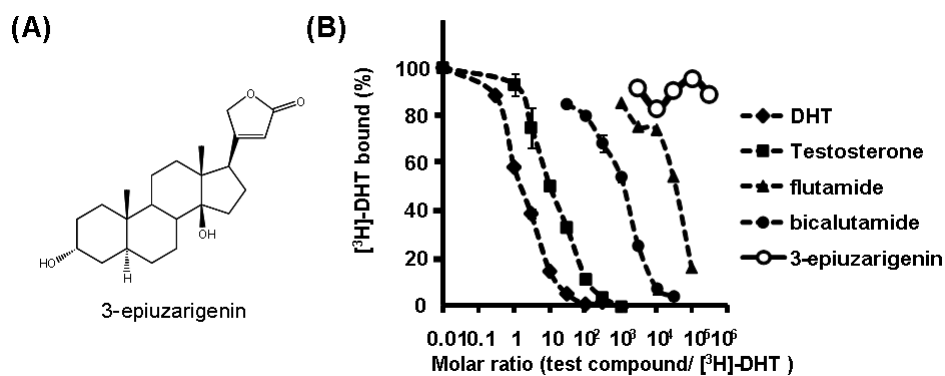
(A) chemical structure of ZINC 04369595. (B) result of *in vitro* assay.

IX. *In vitro* binding assay of fluanisone

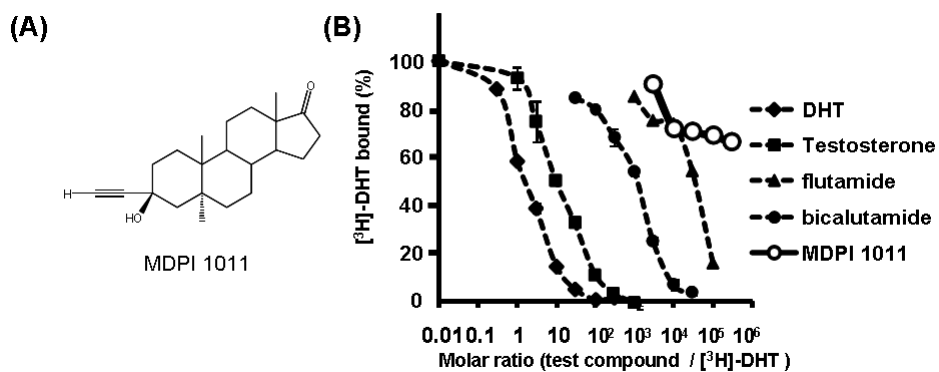
(A) chemical structure of fluanisone. (B) result of *in vitro* assay.

X. *In vitro* binding assay of ZINC 04026296

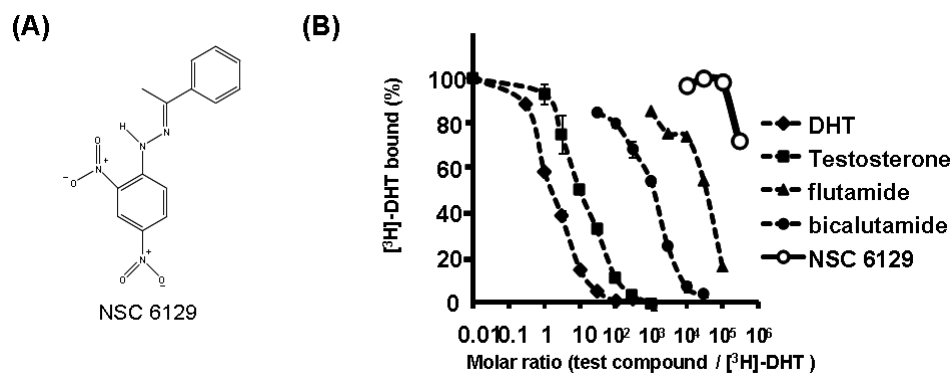
(A) chemical structure of ZINC 04026296. (B) result of *in vitro* assay.

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

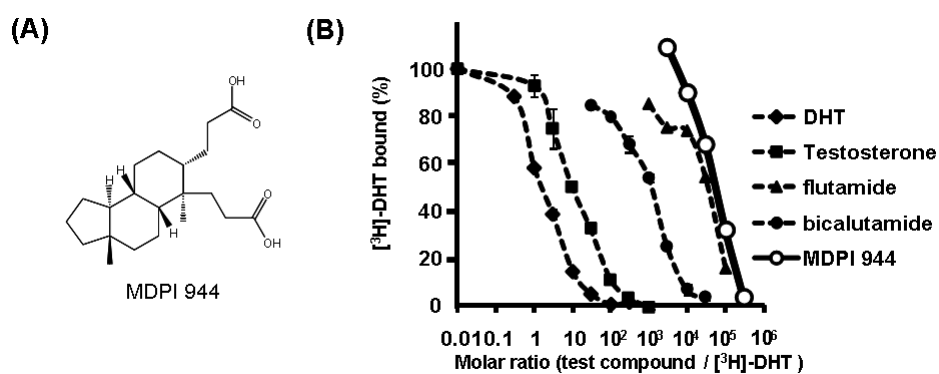
(A) chemical structure of 3-epiuzarigenin. (B) result of *in vitro* assay.

XII. *In vitro* binding assay of MDPI 1011

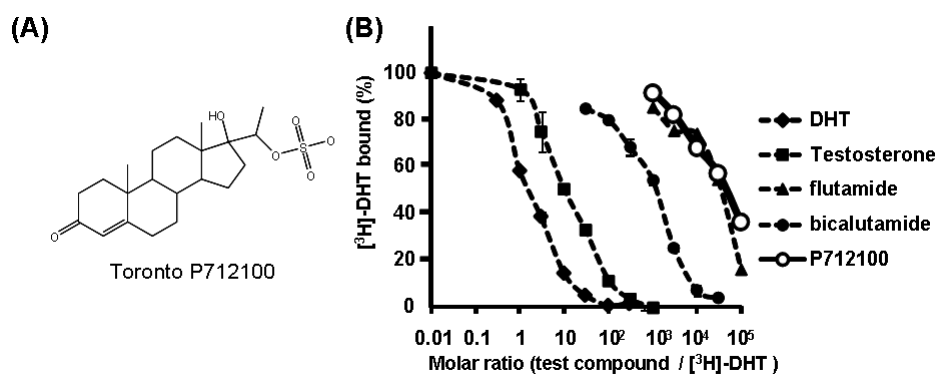
(A) chemical structure of MDPI 1011. (B) result of *in vitro* assay.

XIII. *In vitro* binding assay of NSC 6129

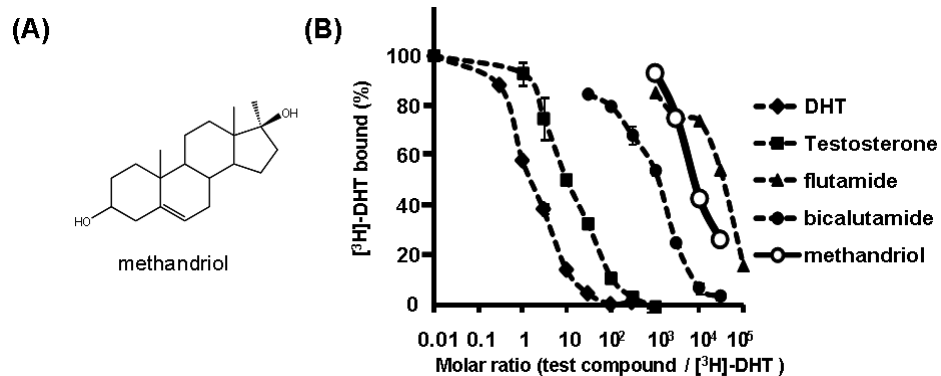
(A) chemical structure of NSC 6129. (B) result of *in vitro* assay.

XIV. *In vitro* binding assay of MDPI 944

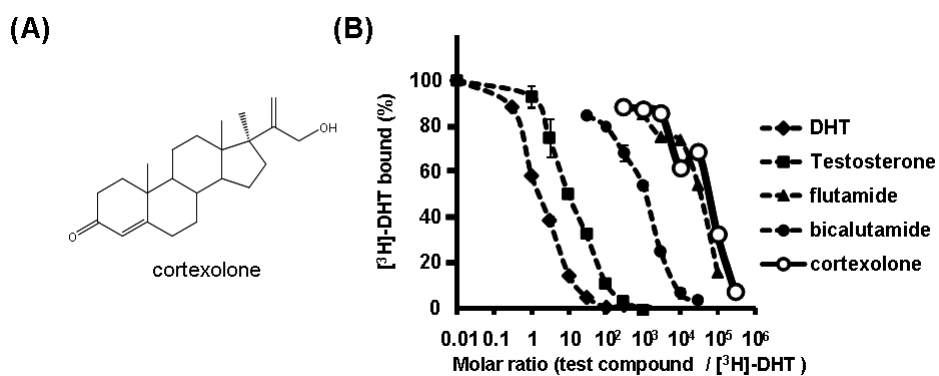
(A) chemical structure of MDPI 944. (B) result of *in vitro* assay.

XV. *In vitro* binding assay of P712100

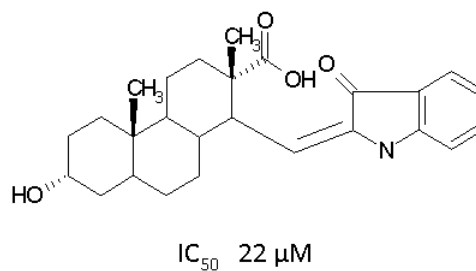
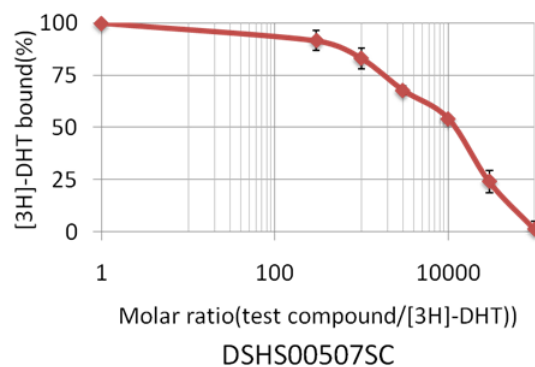
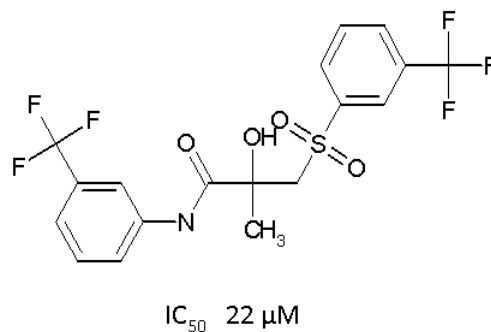
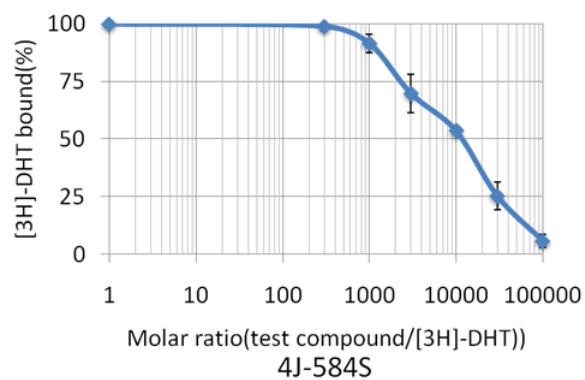
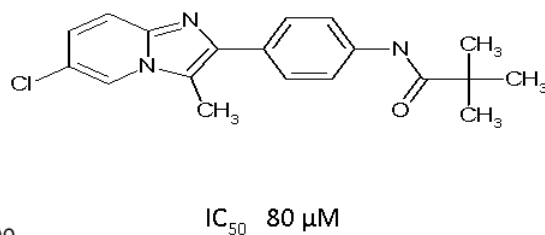
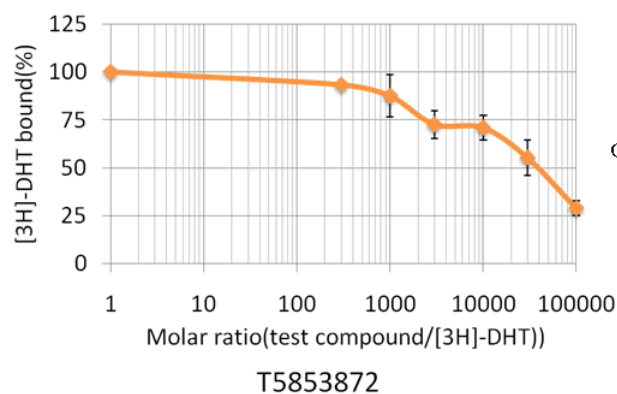
(A) chemical structure of P712100. (B) result of *in vitro* assay.

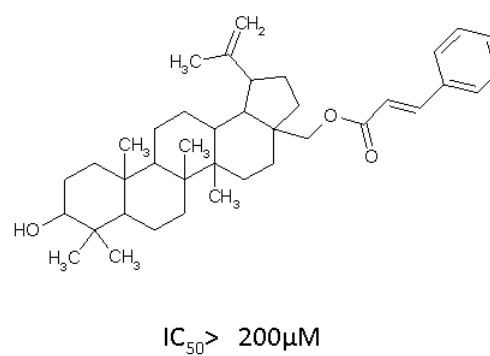
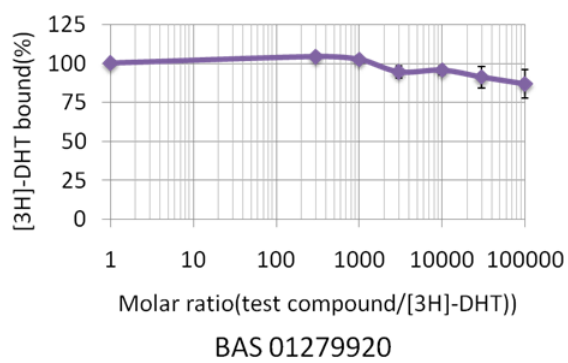
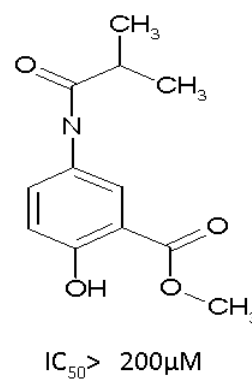
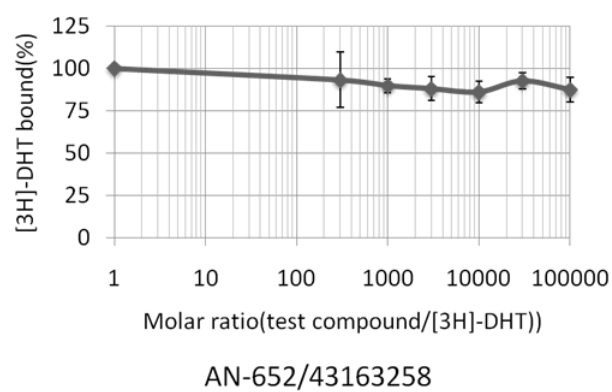
XVI. *In vitro* binding assay of methandriol

(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. *In vitro* binding assay of DSHS00507SCXIX. *In vitro* binding assay of 4J-584SXX. *In vitro* binding assay of T5853872

XXI. *In vitro* binding assay of BAS01279920XXII. *In vitro* binding assay of AN-652/43163258Fig. S4 I-XXII: result of *in vitro* binding assay for each compound.