Supporting Information

Antibody-Capped Mesoporous Nanoscopic Materials: Design of a Probe for the Selective Chromo-Fluorogenic Detection of Finasteride

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Chemical structures of steroids tested during selective studies.

Chemical structures of finasteride, dutasteride, finasteride metabolite, metenolone, oxandrolone, 16-β-hydroxystanozolol, 1-testosterone, androstanolone, testosterone and testosterone glucuronide are showed in Figure SI-1.
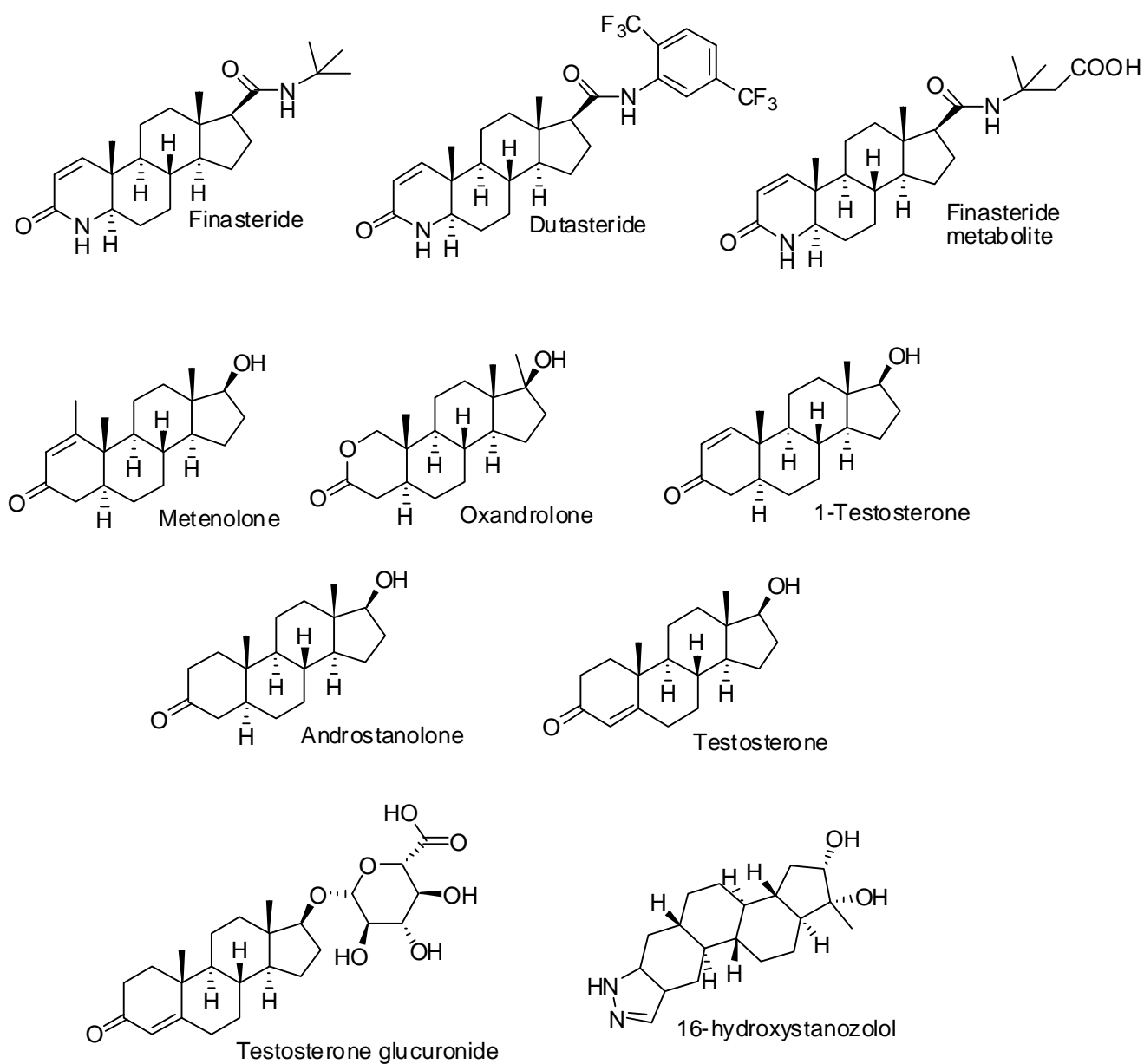

Figure SI-1. Chemical structures of substances tested during studies of selectivity.

Calculation of the average distance between immunoglobulin molecules.

With the aim of estimate the content of the antibody in the solid **S1-AB**, concentrations of IgG immunoglobulin (the most abundant type of antibody in plasma) were measured in serum I and in the aqueous solutions after the capping process via monitorization of the absorbance at 280 nm. Bearing in mind a typical MW for immunoglobulin of 150000 Da and the corresponding extinction molar coefficient of immunoglobulin, a content of 5.3 mg of IgG / mL of serum I was found. Taking into account the absorbance measurements, we can estimate than ca. 87% of the antibodies were incorporated in **S1-AB** when a dilution of sera of 1.25/100 was used. With this data, and knowing the concentration of IgG in serum I, it can be estimated that **S1-AB** material contains 1.16×10^{17} immunoglobulin molecules/g of solid using the following equation:

$$\frac{5.3 \text{ g IgG}}{1 \text{ L serum}} \cdot \frac{1.25 \text{ L serum}}{100 \text{ L solution}} \cdot \frac{0.5 \text{ L solution}}{1 \text{ g solid}} \cdot \frac{1 \text{ mol IgG}}{150000 \text{ g IgG}} \cdot \frac{6.022 \times 10^{23} \text{ molecules IgG}}{1 \text{ mol IgG}} \cdot \frac{87 \text{ molecules IgG retained}}{100 \text{ molecules IgG}} = \frac{1.16 \times 10^{17} \text{ molecules IgG retained}}{1 \text{ g solid}}$$

Additionally, and considering the typical external surface of an MCM-41 support (ca. 35 - 100 nm), an average distance between two immunoglobulin molecules of ca. 17 – 29 nm is calculated applying the following equation:

$$\frac{1}{\sqrt{\dfrac{1.16 \times 10^{17} \text{ molecules IgG retained}}{1 \text{ g solid}} \cdot \dfrac{1 \text{ g solid}}{(35-50) \times 10^{10} \text{ nm}^2}}} = \frac{17-29 \text{ nm}}{1 \text{ molecule IgG}}$$