

Human Metabolism of The Anabolic Steroid Methasterone: Detection and Kinetic Excretion of New Phase I Urinary Metabolites and Investigation of Phase II Metabolism by GC-MS and UPLC-MS/MS

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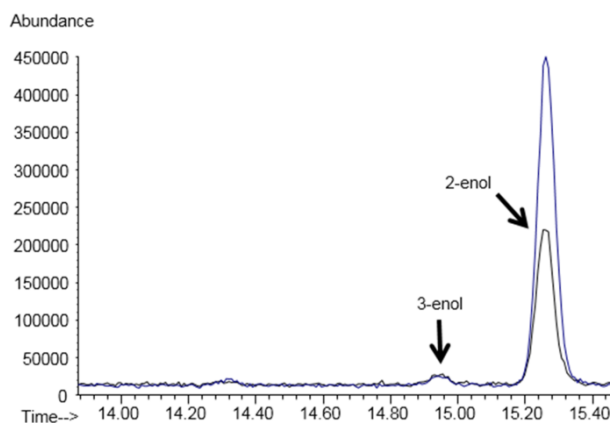


Figure S1. Overlay of total ion chromatograms obtained from the “nutritional supplement” capsule before (black) and after (blue) the addition of methasterone standards. The peaks of the 2-enol-TMS and 3-enol-TMS derivatives are shown.

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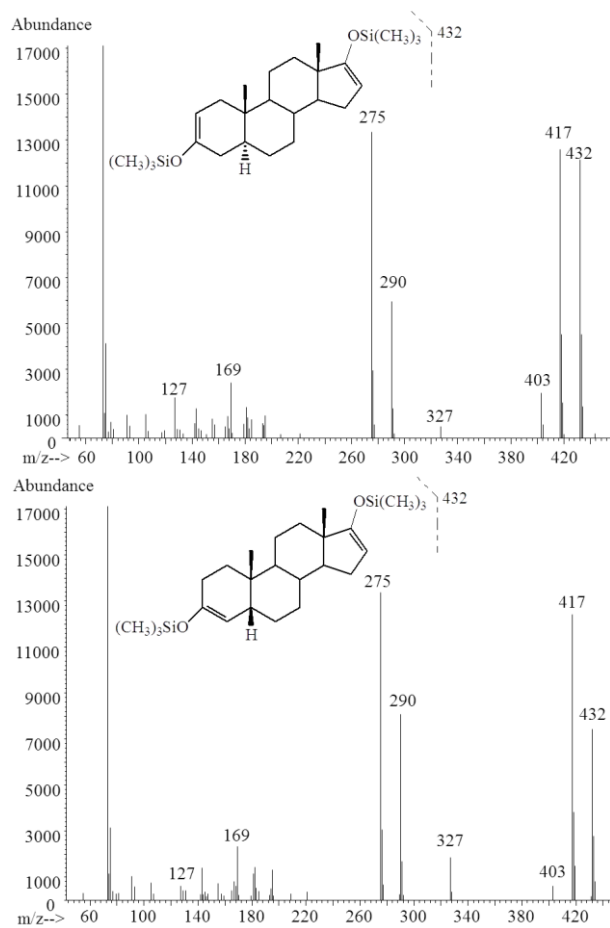


Figure S2. Mass spectra of 5 α -androstadiene 2-enol-TMS derivative (left) and 5 β -androstadiene 3-enol-TMS derivative (right).

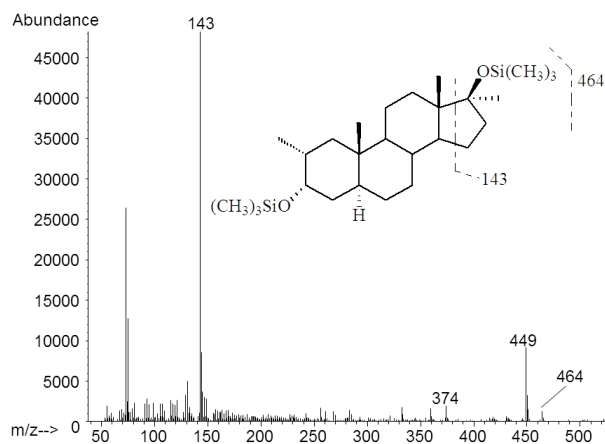


Figure S3. Postadministration urine mass spectrum at 13.3 min (where the M2 TMS derivative eluted) and its proposed fragmentation pathways.

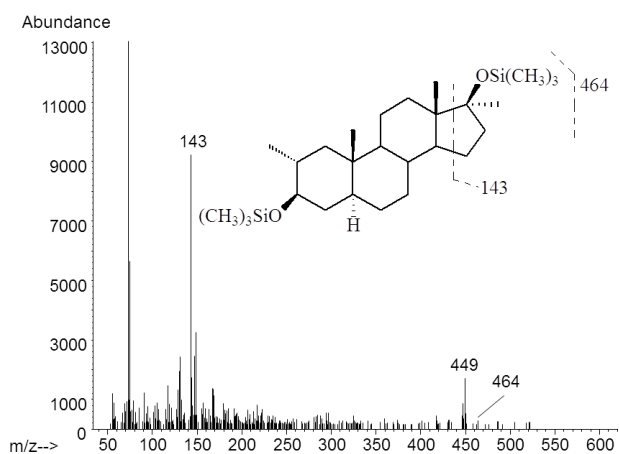


Figure S4. Postadministration urine mass spectrum at 13.8 min (where the M3 TMS derivative eluted) and its proposed fragmentation pathways.

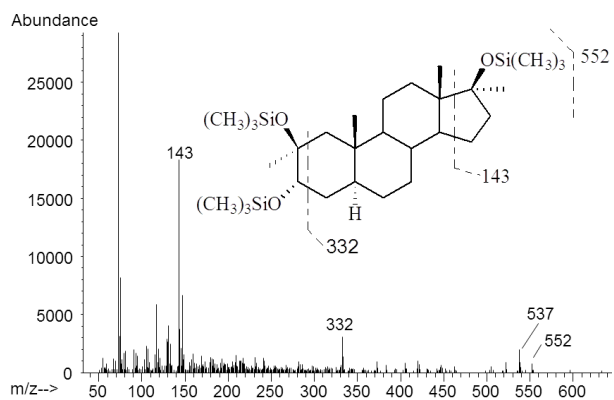


Figure S5. Postadministration urine mass spectrum at 17.2 min (where the M4 TMS derivative eluted) and its proposed fragmentation pathways.

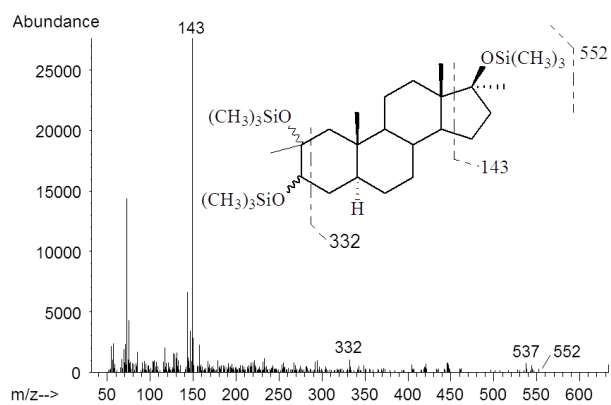


Figure S6. Postadministration urine mass spectrum at 16.8 min (where the M5 TMS derivative eluted) and its proposed fragmentation pathways.

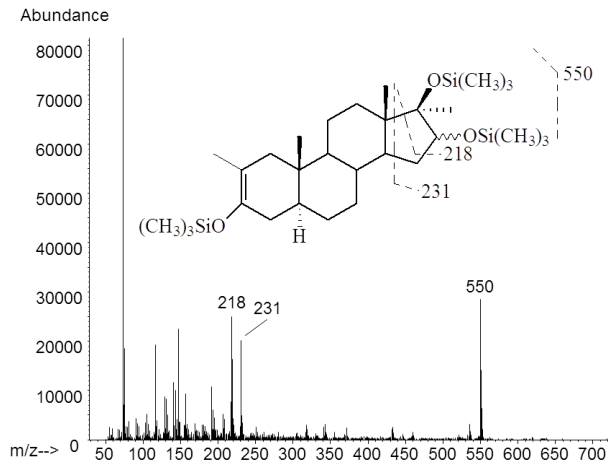


Figure S7. Postadministration urine mass spectrum at 19.0 min (where the M6 TMS derivative eluted) and its proposed fragmentation pathways.

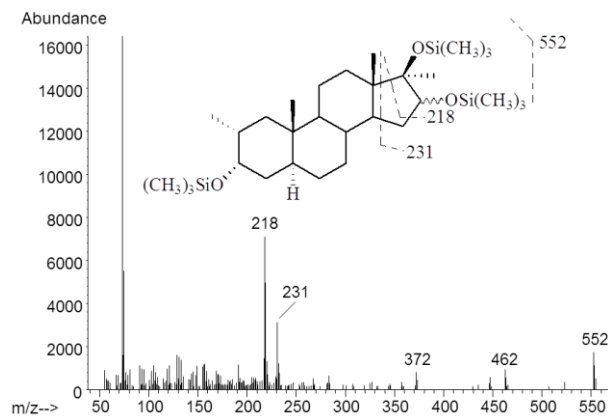


Figure S8. Postadministration urine mass spectrum at 18.1 min (where the M7 TMS derivative eluted) and its proposed fragmentation pathways.

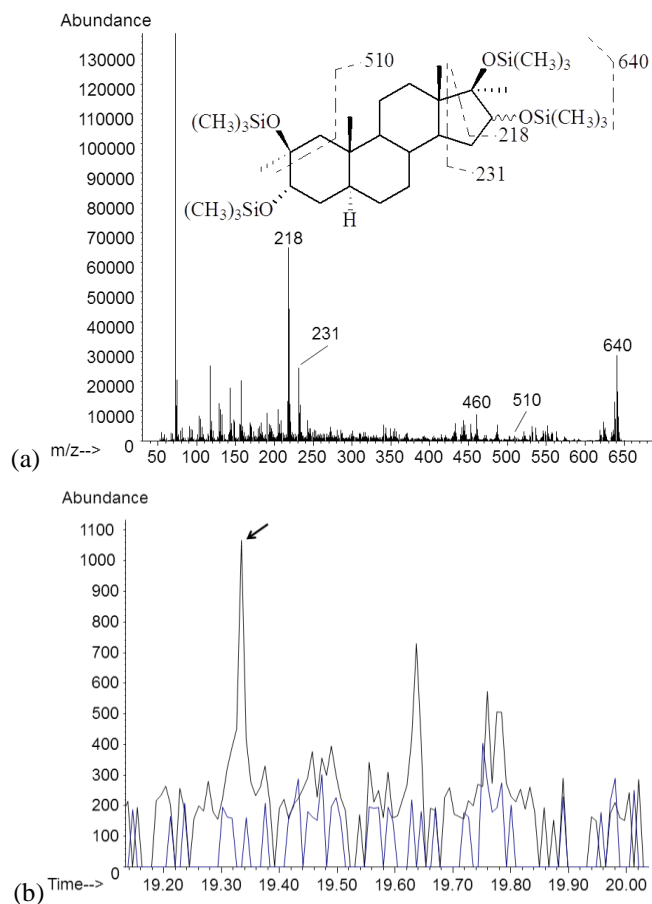


Figure S9. (a) Postadministration urine mass spectrum at 19.3 min (where the M8 TMS derivative eluted) and its proposed fragmentation pathways; (b) overlay of extracted ion chromatograms (m/z 510) obtained from postadministration urine sample (black) and blank urine (blue). The peak related to M8 is indicated by the arrow.

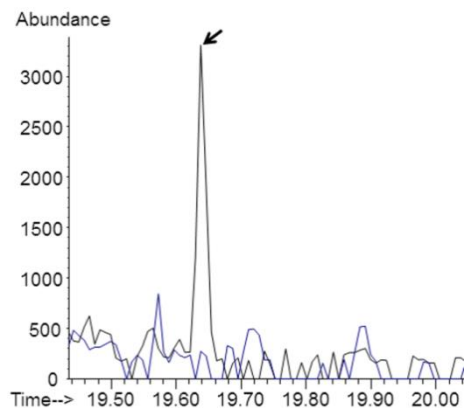


Figure S10. Overlay of extracted ion chromatograms (m/z 508) obtained from postadministration urine sample (black) and blank urine (blue). The peak related to M9 is indicated by the arrow.

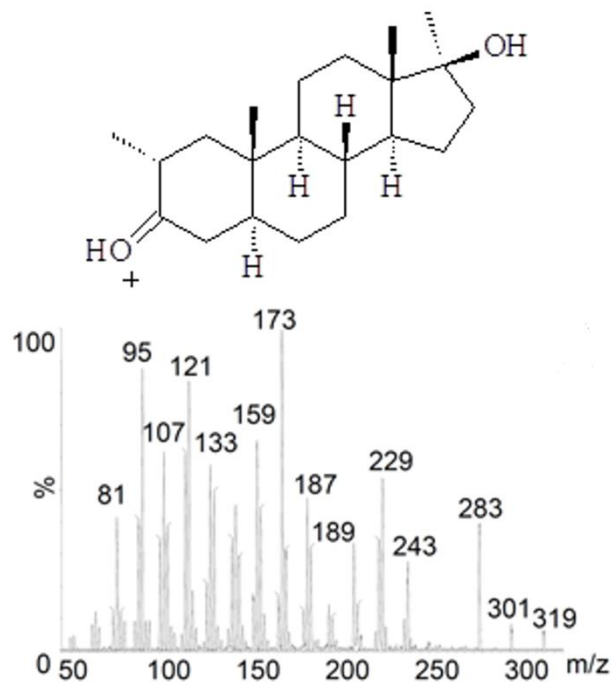


Figure S11. Product ion mass spectrum of m/z 319 at 9.9 min, where the pseudo-molecular ion $[M + H]^+$ of methasterone eluted. Its proposed chemical structure is shown.

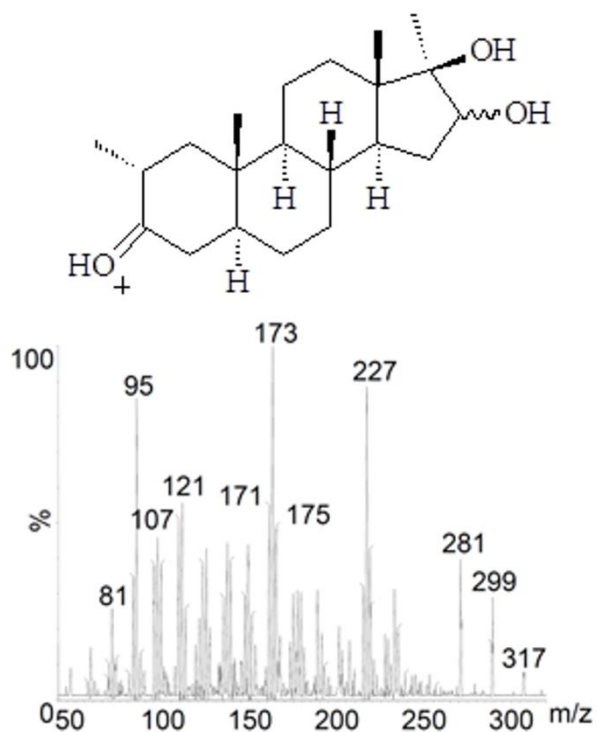


Figure S12. Product ion mass spectrum of m/z 335 at 8.0 min, where the pseudo-molecular ion $[M + H]^+$ of metabolite M6 eluted. Its proposed chemical structure is shown.