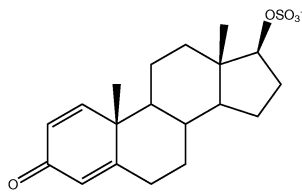
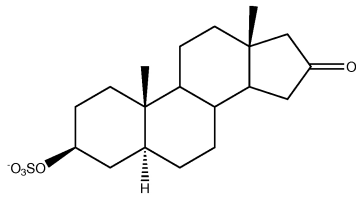


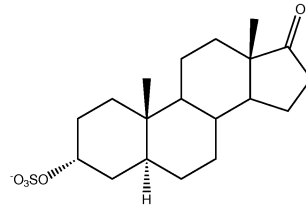
Fig. S1: Sulfates and glucuronidates in urine extracts and their enzymatic digestion. (A) Precursor ion scan for m/z 97, showing the presence of multiple sulfate precursors in the mock-treated sample. Inset, precursor scan of sample digested with sulfatase. (B) Precursor scan for m/z 97 in mock-treated sample and (inset) glucuronidase-treated sample. (C) Neutral loss scan of 176 (glucuronic acid) indicates the presence of multiple glucuronic acid conjugates. Inset, neutral loss scan after sulfatase digestion, demonstrating that sulfatase also contains glucuronidase activity. (D) Neutral loss 176 scan of mock-treated sample and (inset) glucuronidase-treated sample. (B) and (D) demonstrate that glucuronidase depletes the glucuronic acid conjugates but preserves the sulfated compounds. The samples used for precursor-ion and neutral-loss scans were from ODS-urine extracts dissolved in methanol at a concentration of $20\times$ relative to urine.



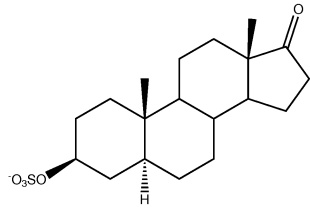
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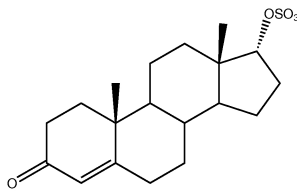
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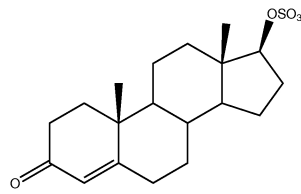
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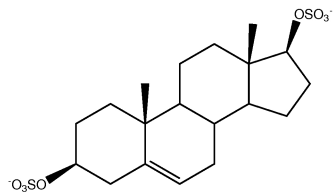
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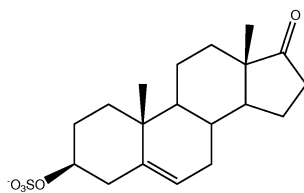
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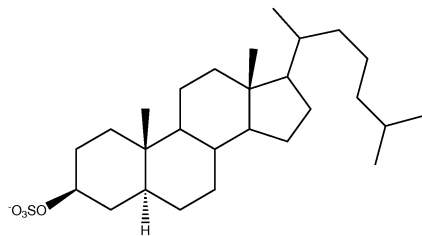
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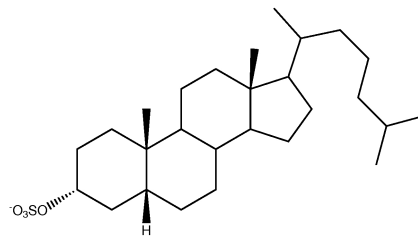
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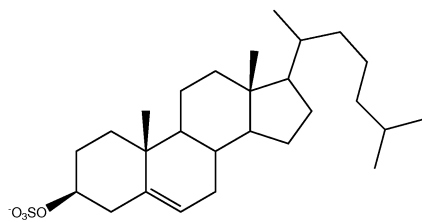
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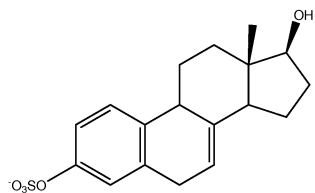
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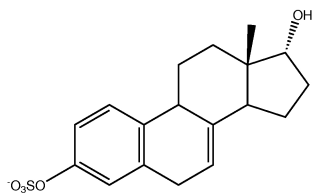
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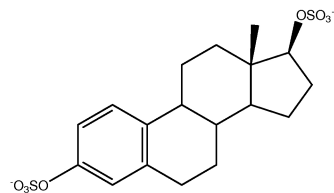
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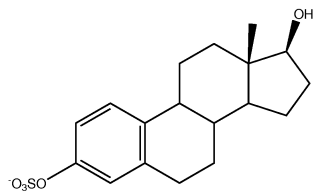
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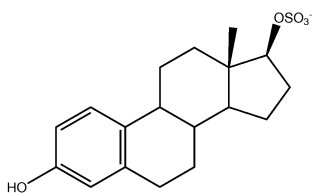
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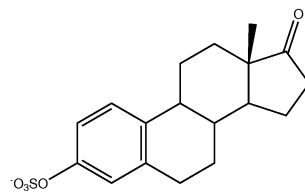
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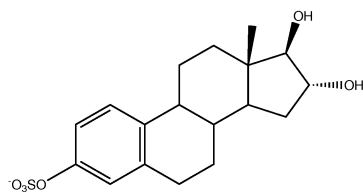
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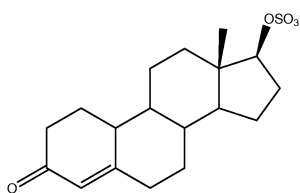
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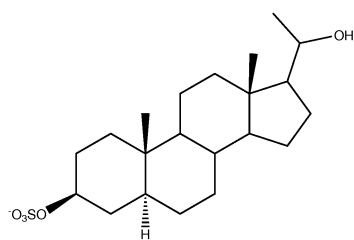
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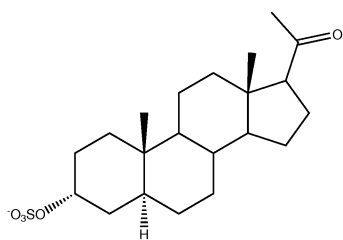
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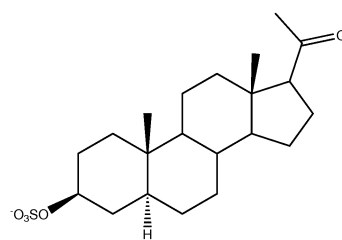
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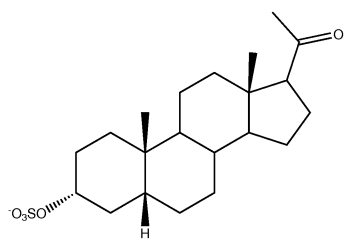
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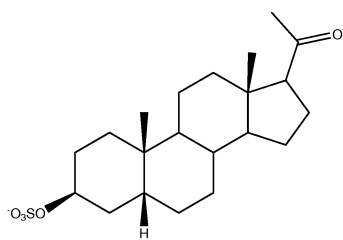
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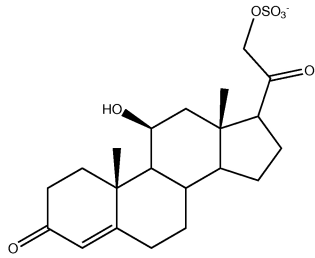
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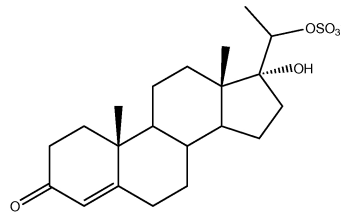
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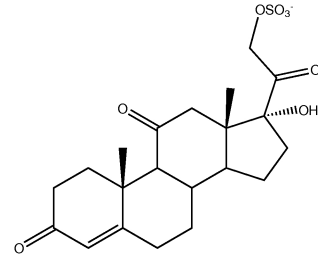
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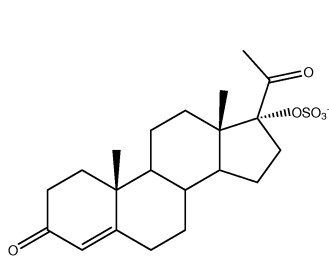
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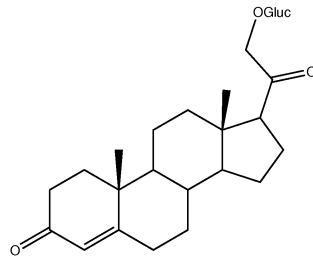
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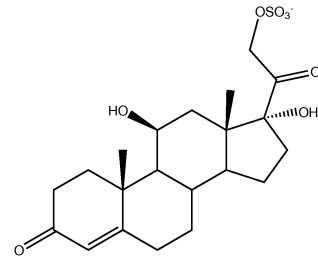
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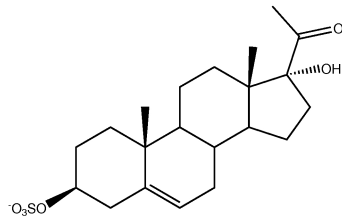
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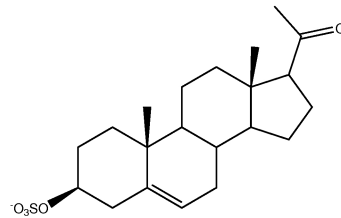
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Q3910



Q4765



Q5545

A0225 1, 4-ANDROSTADIEN-17 β -OL-3-ONE SULPHATE

A2398 5 α -ANDROSTAN-3 β -OL-16-ONE SULPHATE

A2460 5 α -ANDROSTAN-3 α -OL-17-ONE SULPHATE

A2534 5 α -ANDROSTAN-3 β -OL-17-ONE SULPHATE

A6940 4-ANDROSTEN-17 α -OL-3-ONE SULPHATE

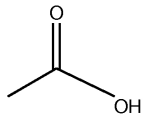
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A7864 5-ANDROSTEN-3 β , 17 β -DIOL DISULPHATE

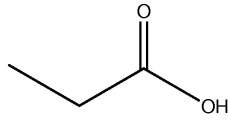
A8530 5-ANDROSTEN-3 β -OL-17-ONE SULPHATE

C4385 5 α -CHOLESTAN-3 β -OL SULPHATE

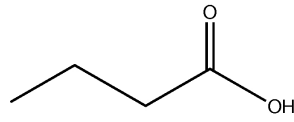
C5075 5 β -CHOLESTAN-3 α -OL SULPHATE
C6905 5-CHOLESTEN-3 β -OL SULPHATE
E0588 1, 3, 5(10), 7-ESTRATETRAEN-3, 17 β -DIOL 3-SULPHATE
E0893 1, 3, 5(10)-ESTRATRIEN-3, 17 α -DIOL 3-SULPHATE
E1050 1, 3, 5(10)-ESTRATRIEN-3, 17 β -DIOL DISULPHATE
E1100 1, 3, 5(10)-ESTRATRIEN-3, 17 β -DIOL 3-SULPHATE
E1103 1, 3, 5(10)-ESTRATRIEN-3, 17 β -DIOL 17-SULPHATE
E2335 1, 3, 5(10)-ESTRATRIEN-3-OL-17-ONE SULPHATE
E2732 1, 3, 5(10)-ESTRATRIEN-3, 16 α , 17 β -TRIOL 3-SULPHATE
E4105 4-ESTREN-17 β -OL-3-ONE SULPHATE
P2135 5 α -PREGNAN-3 β , 20 β -DIOL-3-SULPHATE
P3817 5 α -PREGNAN-3 α -OL-20-ONE SULPHATE
P3865 5 α -PREGNAN-3 β -OL-20-ONE SULPHATE
P8168 5 β -PREGNAN-3 α -OL-20-ONE SULPHATE
P8200 5 β -PREGNAN-3 β -OL-20-ONE SULPHATE
Q1570 4-PREGNEN-11 β , 21-DIOL-3, 20-DIONE 21-SULPHATE
Q1890 4-PREGNEN-17, 20 β -DIOL-3-ONE SULPHATE
Q2525 4-PREGNEN-17, 21-DIOL-3, 11, 20-TRIONE 21-SULPHATE
Q3383 4-PREGNEN-17-OL-3, 20-DIONE SULPHATE
Q3470 4-PREGNEN-21-OL-3, 20-DIONE GLUCOSIDURONATE
Q3910 4-PREGNEN-11 β , 17, 21-TRIOL-3, 20-DIONE 21-SULPHATE
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Q5545 5-PREGNEN-3 β -OL-20-ONE SULPHATE



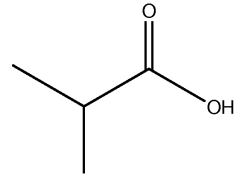
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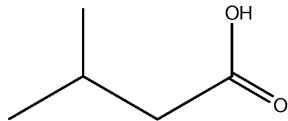
Propionic acid



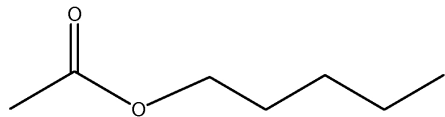
Butyric acid



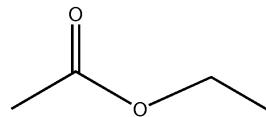
Isobutyric acid



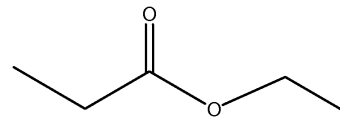
Isovaleric acid



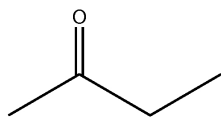
Pentyl acetate



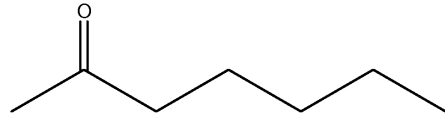
Ethyl acetate



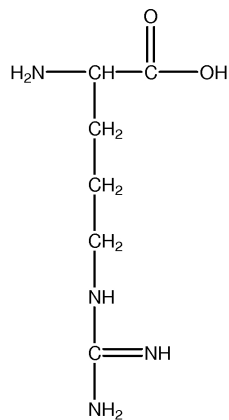
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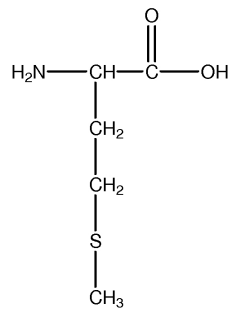
Butanone



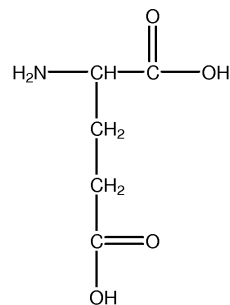
2-heptanone



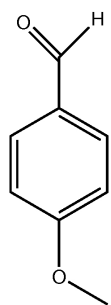
Arginine



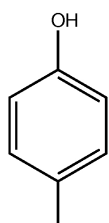
Methionine



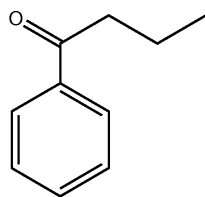
Glutamic acid



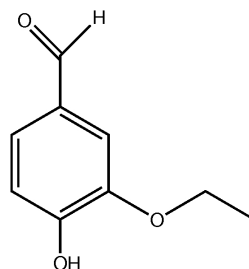
Aubepine



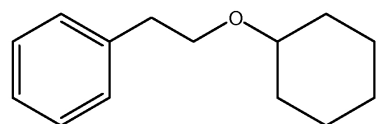
p-cresol



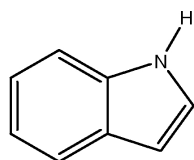
Butyrophenone



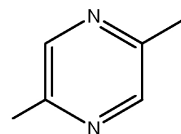
Ethyl vanilline



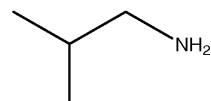
Phenafleur



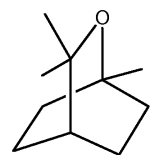
Indole



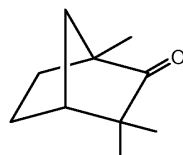
2,5-dimethylpyrazine



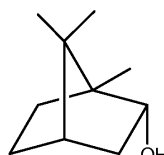
Isobutylamine



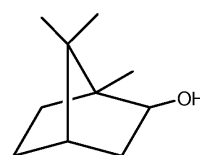
Eucalyptol



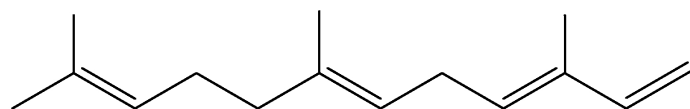
Fenchone



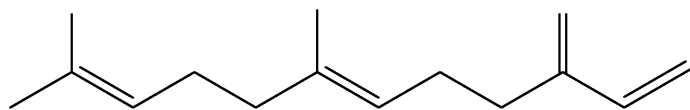
Borneol



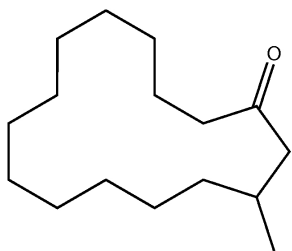
Isoborneol



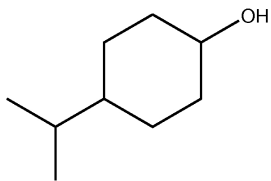
α -farnesene



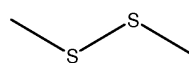
β -farnesene



Muscone



Patchone



Dimethyl disulfide

Fig. S2. Structures of additional synthetic compounds tested.