

1 **Supporting information for**
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3 **Structural identification of in vitro metabolites for 23-**
4 **nordeoxycholic acid by structural analogue matching**

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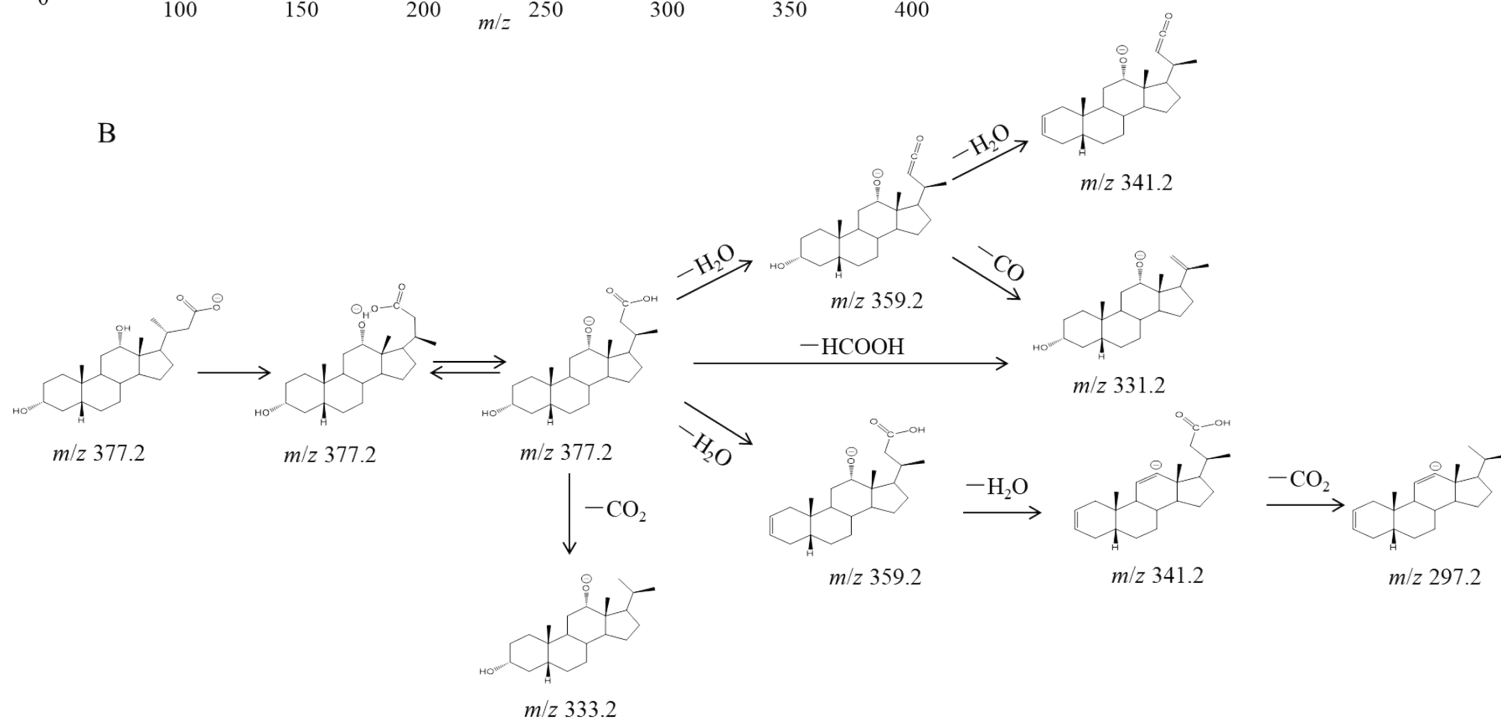
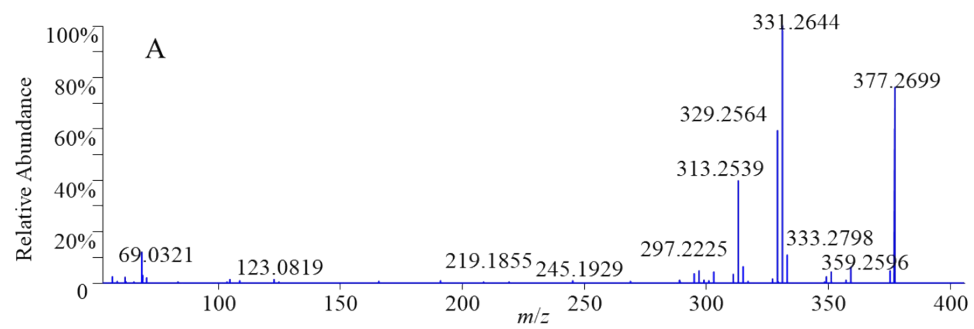
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21 **Supplementary data includes the following items:**

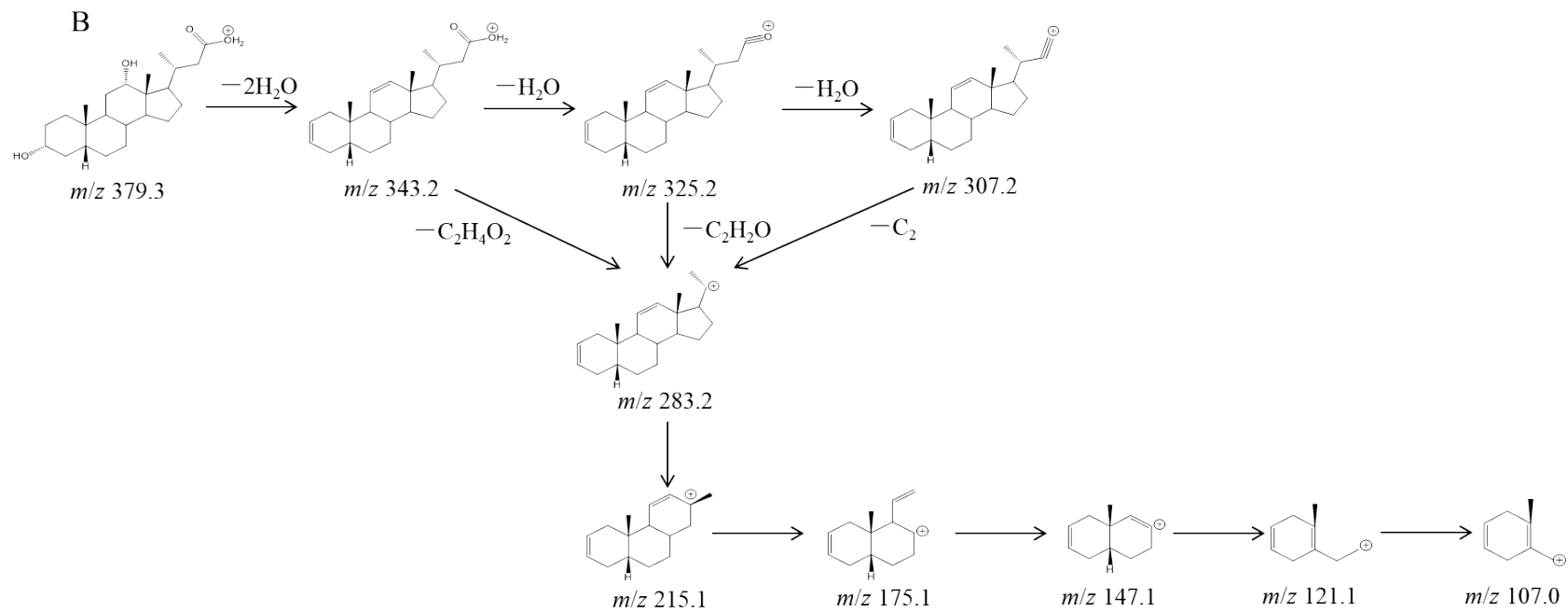
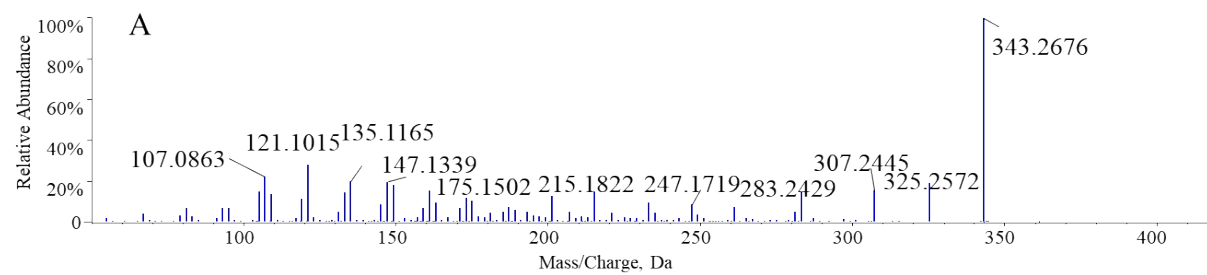
P_{S2}	Table S1. The predefined metabolic pathways, ion transitions, and compound-dependent mass parameters of all targeted analytes.
P_{S3}	Fig. S1 MS/MS spectrum (A) and proposed fragmentation pathways (B) of norDCA in the negative ion mode.
P_{S4}	Fig. S2 MS/MS spectrum (A) and proposed fragmentation pathways (B) of norDCA in the positive ion mode.
P_{S5}	Fig. S3 MS ² spectrum comparison between deprotonated molecular ions of norCA (A, m/z 393.3 [M-H] ⁻) and CA (B, m/z 407.3 [M-H] ⁻).
P_{S6}	Fig. S4 Representative LC-MRM chromatograms for incubation of norDCA with HLMs (A), with MLMs (B), with RLMs (C), without protein (D), and without NADPH-regenerating system (E).
P_{S7}	Fig. S5 Representative LC-MRM chromatograms for incubation of norDCA with HLMs and PAPS, with human recombinant SULT2A1 and PAPS, and without protein. without PAPS.
P_{S7}	Fig. S6 Representative LC-MRM chromatograms for incubation of norDCA with HLMs and UDPGA, without protein, and without UDPGA.

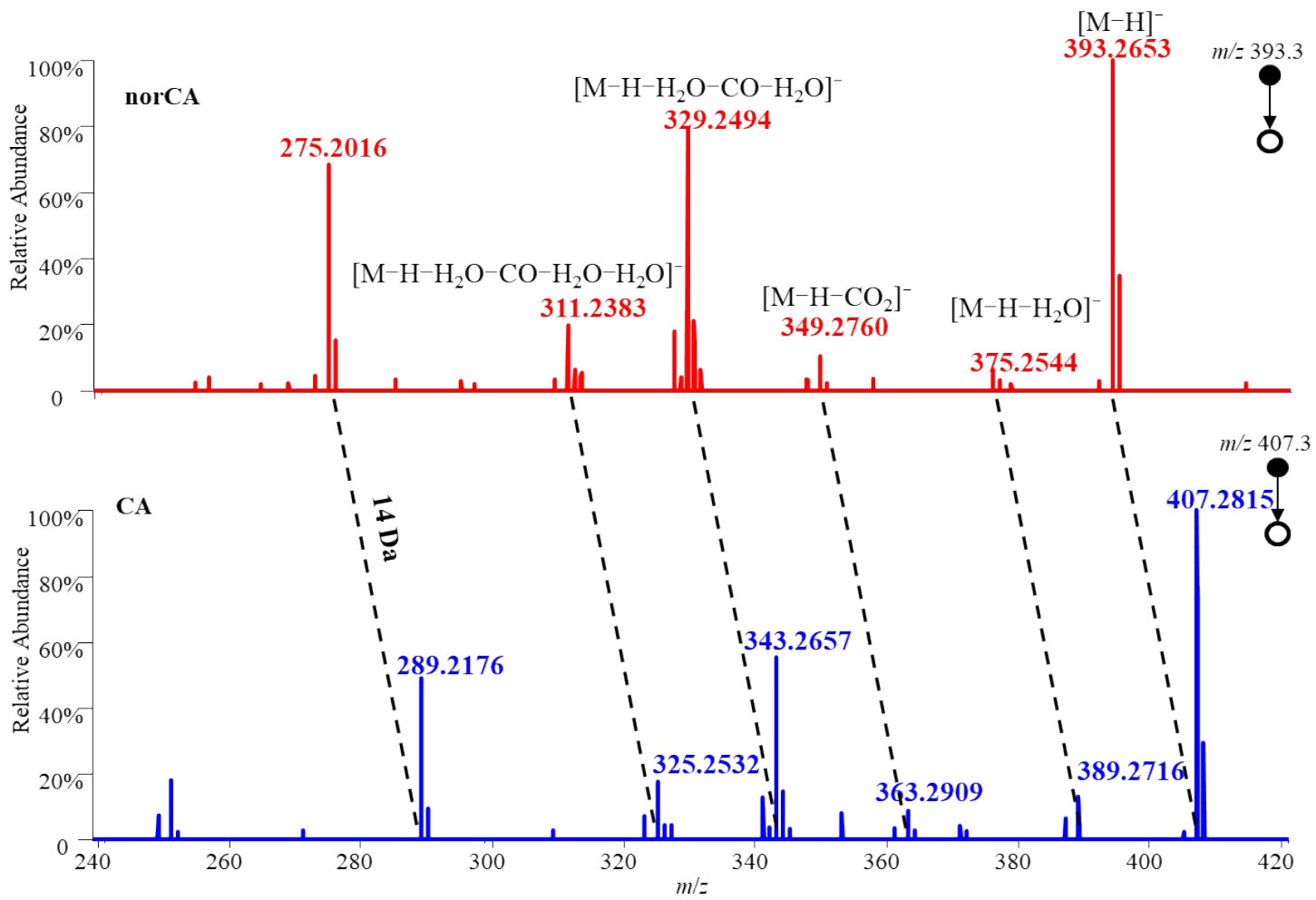
23 **Table S1 The predefined metabolic pathways, ion transitions, and compound-dependent**
 24 **mass parameters of all possible metabolites.**

Metabolic type	Q1	Q3	CE (eV)	DP (V)
Parent compound	377.3	377.3	-20	-120
Oxidation	375.3	375.3	-20	-120
Oxidation	373.3	373.3	-20	-120
Hydroxylation	393.3	393.3	-20	-120
Oxidation	391.3	391.3	-20	-120
Oxidation	389.3	389.3	-20	-120
Sulfation	457.3	96.9	-120	-120
Glucuronidation	553.3	377.3	-50	-120



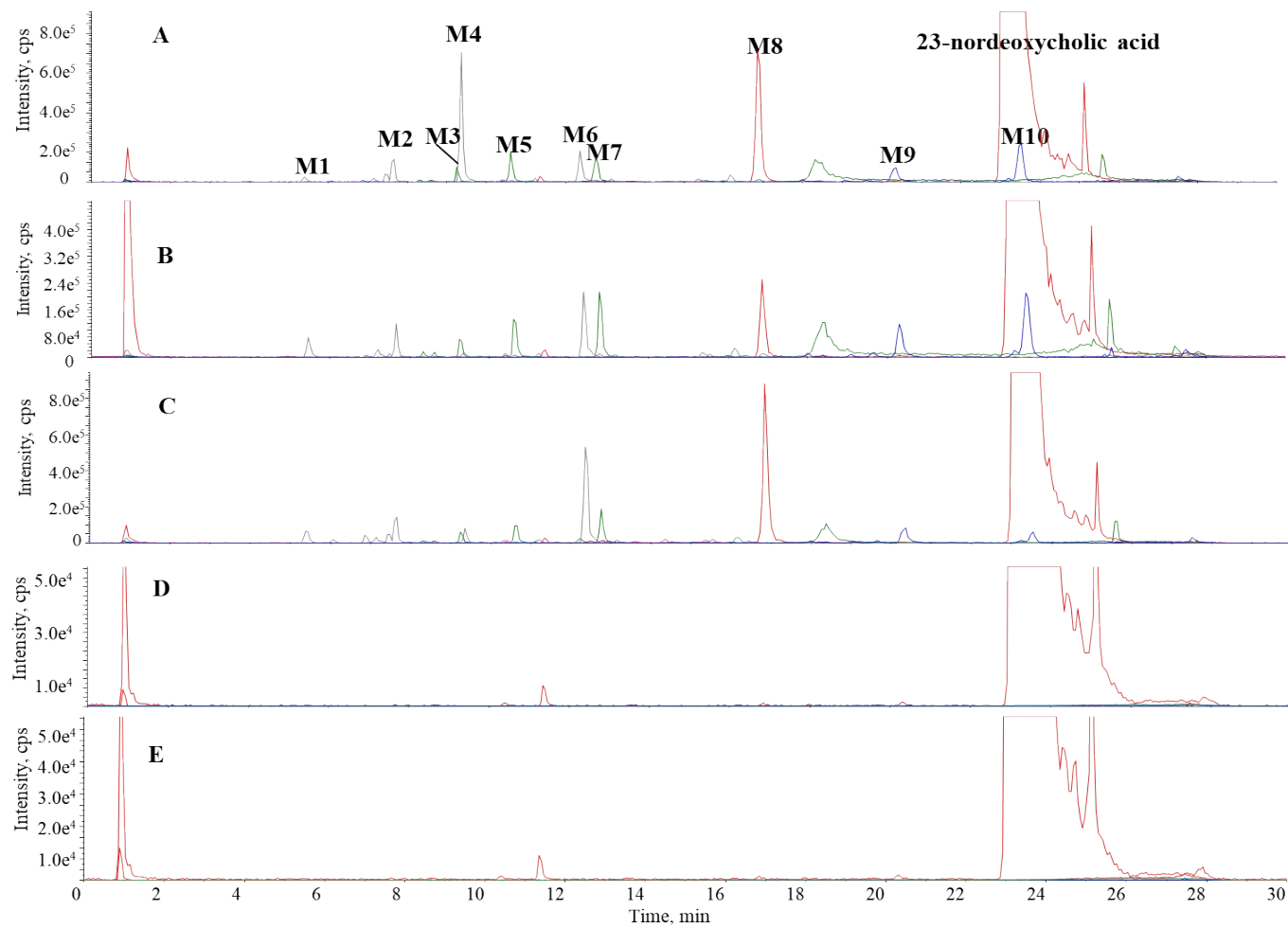
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27 **Fig. S1**



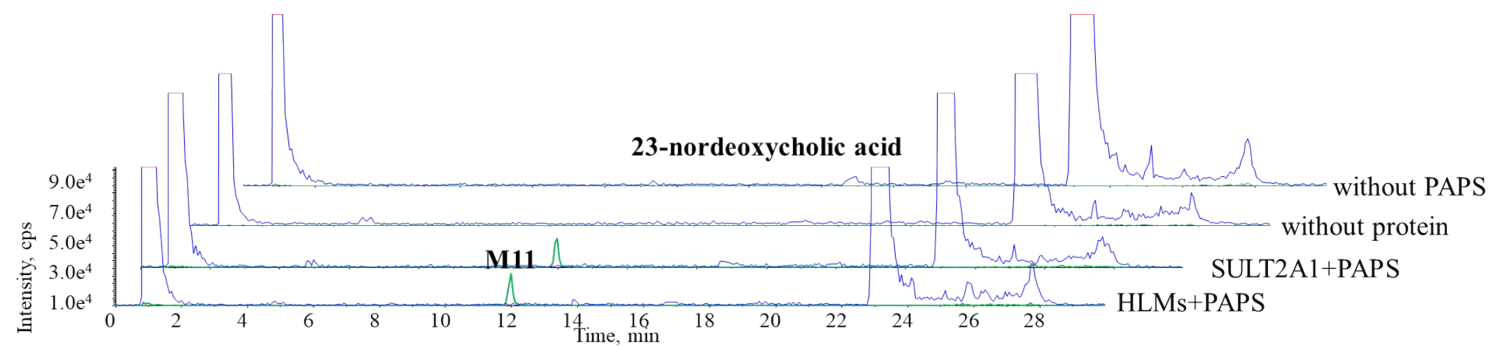


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32 **Fig. S3**



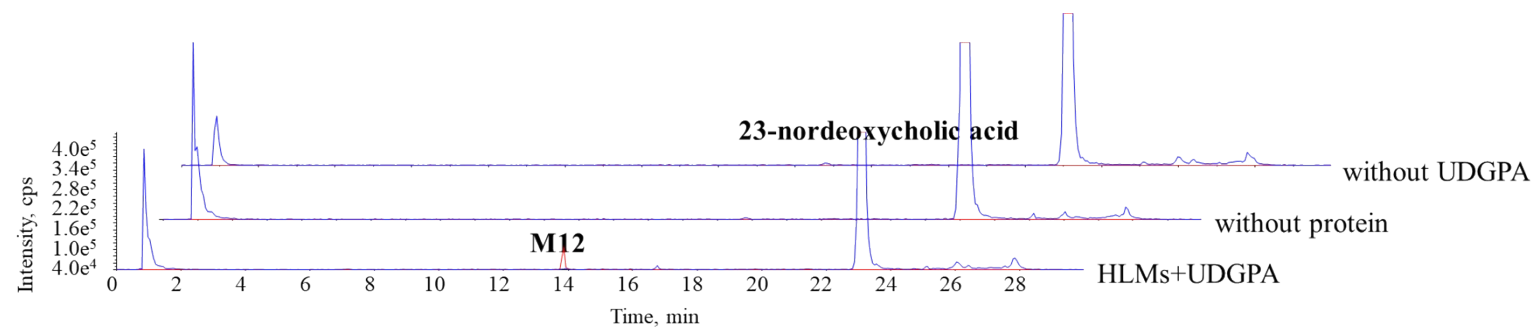
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38 **Fig. S5**

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41 **Fig. S6**

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