

Supplementary Materials

Figure Captions

Fig. S1. HPLC diagram of 9 standard substances

Fig. S2. UPLC-MS/MS diagram of potential XOD inhibitors in ASTE/FASTE

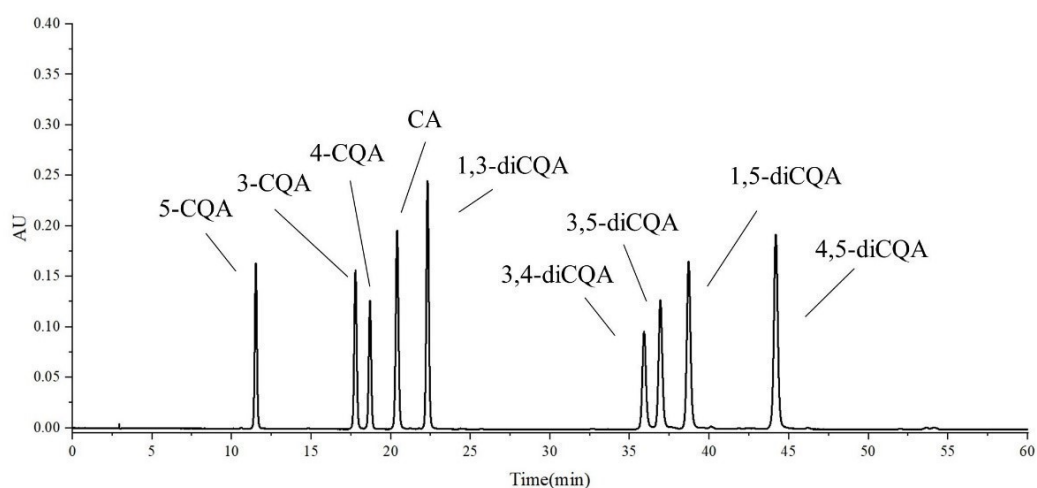


Fig. S1.

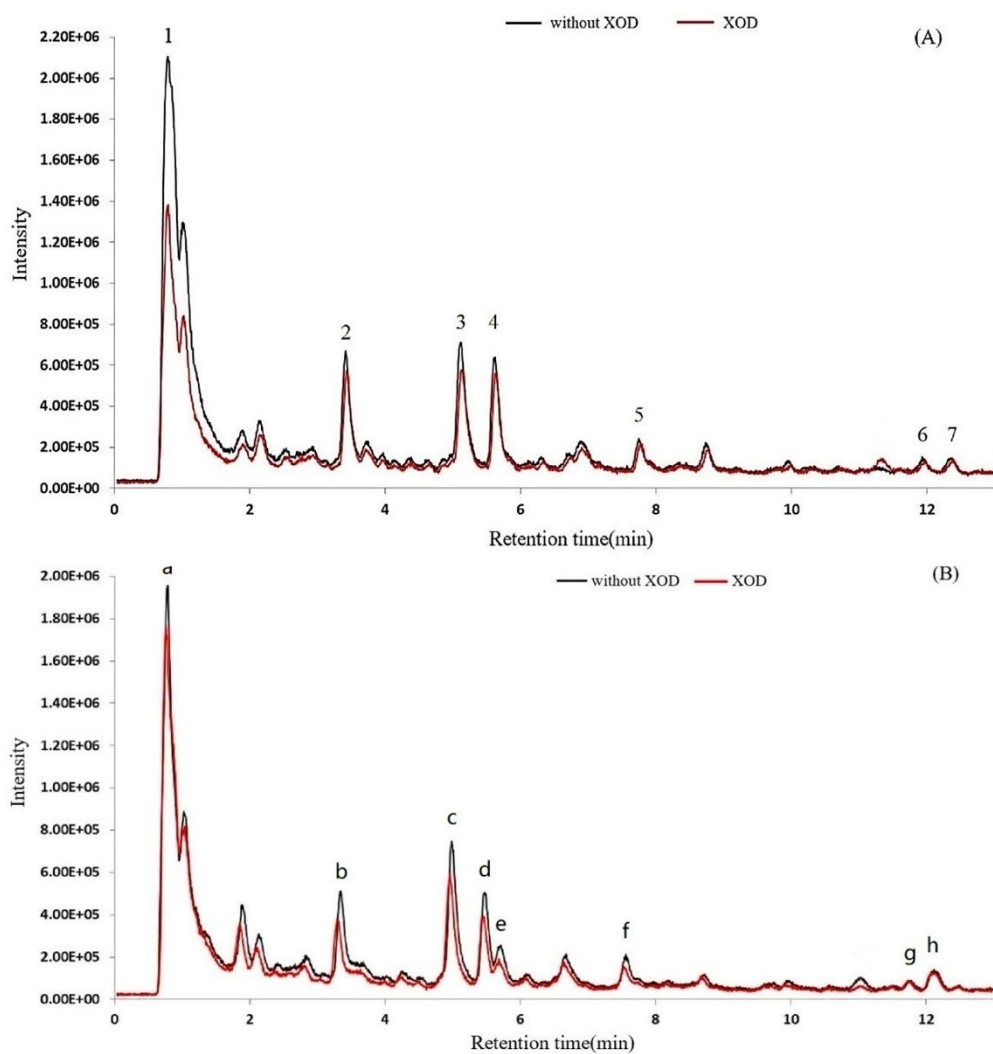


Fig. S2.

Table S1. Identification of XOD inhibitors in ASTE by UPLC-MS/MS

Peak	RT/min	MS[M-H] ⁻	MS ²	Molecular	Compound
1	0.83	191.0567	173.0517, 127.0457, 93.0397, 85.0345, 73.0343, 59.0179	C ₇ H ₁₂ O ₆	Quinic acid
2	3.35	353.0900	191.0638, 179.0419, 173.0314, 161.0314, 135.0512	C ₁₆ H ₁₈ O ₉	5-CQA
3	4.98	353.0897	191.0638	C ₁₆ H ₁₈ O ₉	3-CQA and (or) 4-CQA
4	5.51	353.0901	191.0636, 179.0418, 173.0525, 161.0316, 135.1511, 111.0505, 93.0397, 85.0348	C ₁₆ H ₁₈ O ₉	1-CQA
5	7.61	515.1216	353.0978, 191.0635, 179.0421, 161.0307, 135.0512	C ₂₅ H ₂₄ O ₁₂	3,4-diCQA
6	11.83	515.1216	353.0970, 335.0860, 191.0618, 179.0413, 173.0508	C ₂₅ H ₂₄ O ₁₂	3,5-diCQA and (or) 1,5-diCQA
7	12.24	515.1208	353.0970, 191.0619, 179.0405, 135.0488	C ₂₅ H ₂₄ O ₁₂	4,5-diCQA

Table S2. Identification of XOD inhibitors in FASTE by UPLC-MS/MS

peak	RT/min	MS[M-H] ⁻	MS ²	Molecular	Compound
a	0.82	191.0408	93.0366, 87.01081, 85.0316, 67.0210, 59.0157	C ₇ H ₁₂ O ₆	Quinic acid
b	3.35	353.0865	191.0589, 179.0376, 173.0483, 161.0267, 135.0474	C ₁₆ H ₁₈ O ₉	5-CQA
c	5.02	353.0864	191.0591	C ₁₆ H ₁₈ O ₉	3-CQA and 4-CQA
d	5.53	351.0861	191.0586, 179.0378, 173.0483, 135.0473, 93.0367, 59.0154	C ₁₆ H ₁₈ O ₉	1-CQA
e	5.72	179.0958	135.0474, 134.0394, 89.0415	C ₉ H ₈ O ₄	CA
f	7.57	515.1177	353.0918, 335.0823, 191.0591, 179.0377, 173.0483, 161.0267, 135.0471	C ₂₅ H ₂₄ O ₁₂	3,4-diCQA
g	11.80	515.1174	353.0920, 191.0591, 179.0378, 173.0481, 161.0264, 155.0362, 135.0476	C ₂₅ H ₂₄ O ₁₂	3,5-diCQA and (or) 1,5-diCQA
h	12.05	515.1177	353.0915, 191.0595, 179.0390	C ₂₅ H ₂₄ O ₁₂	4,5-diCQA