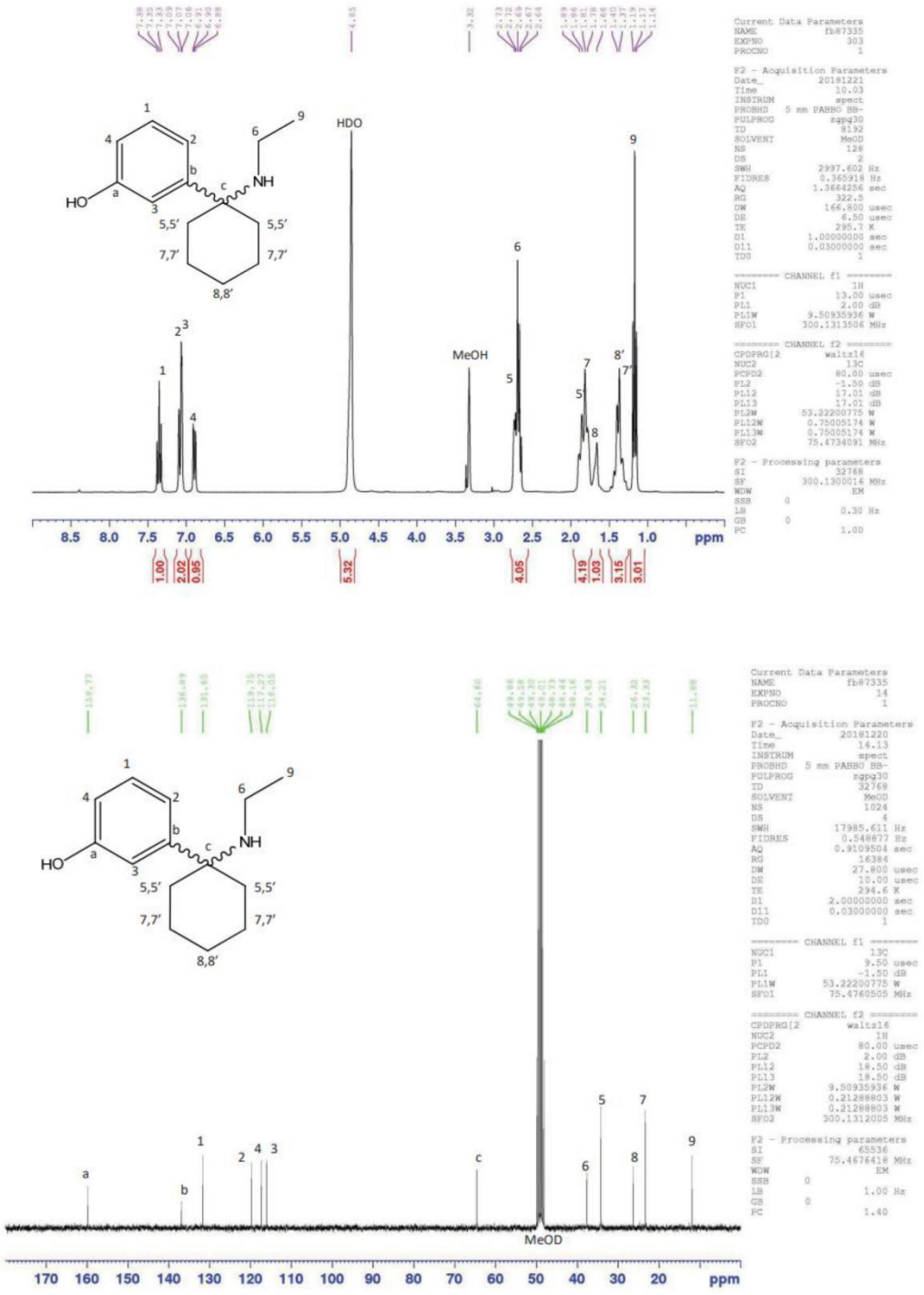
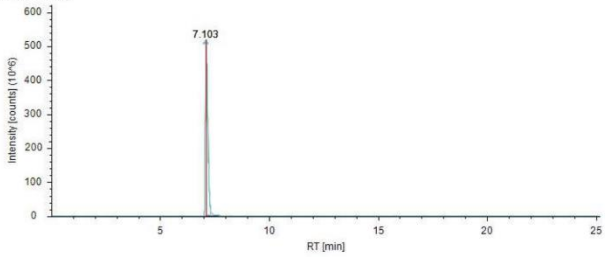
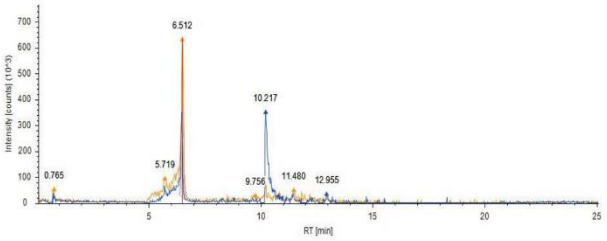


Figure S1. [1]H NMR (top) and [13]C NMR (bottom) spectra of 3-HO-PCE.

3-HO-PCE



M1



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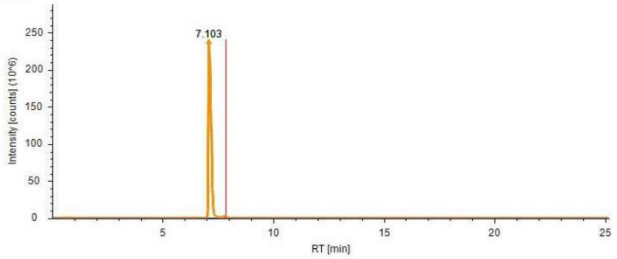

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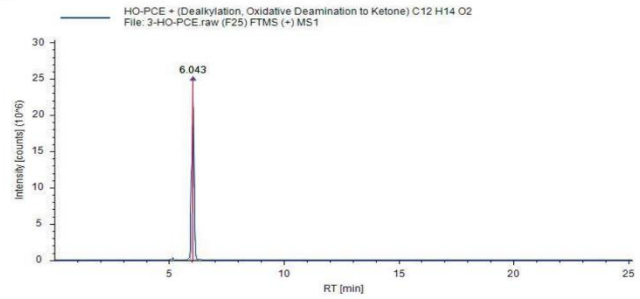

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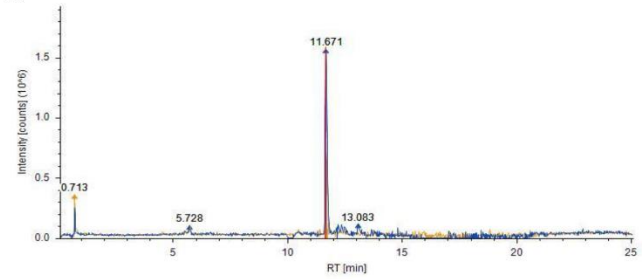

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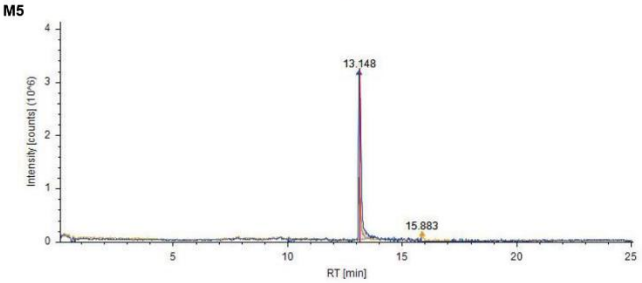
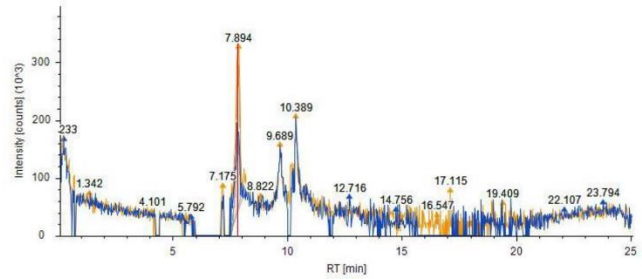
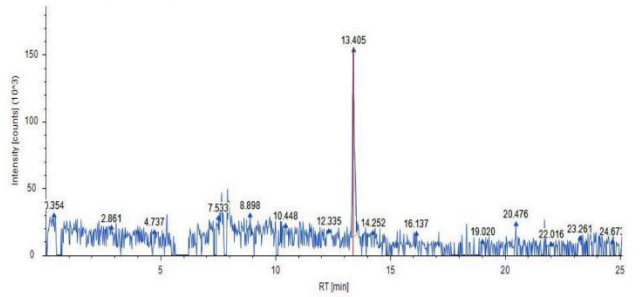


M6a



M6b



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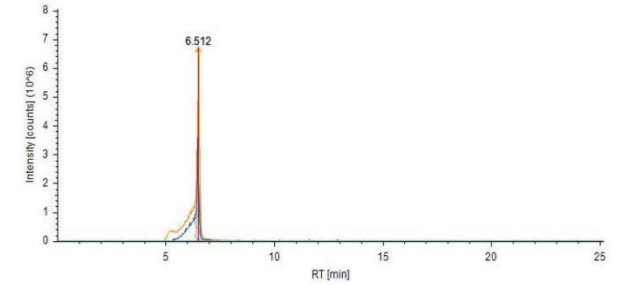

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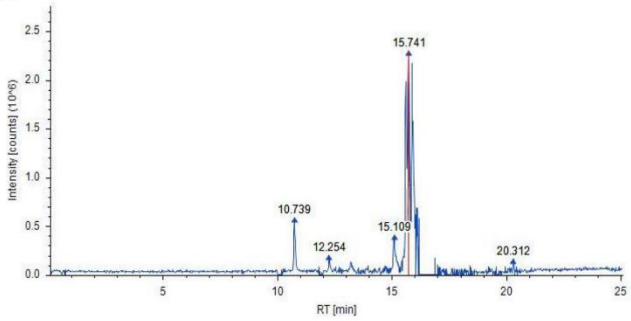
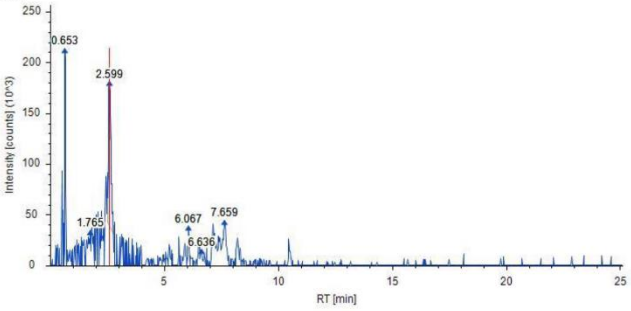


M9a



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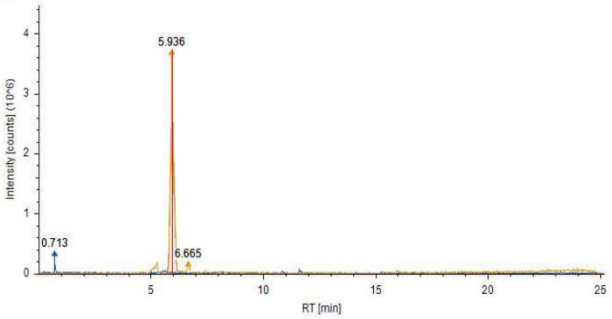

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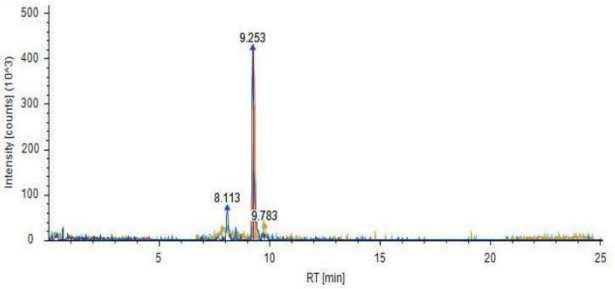
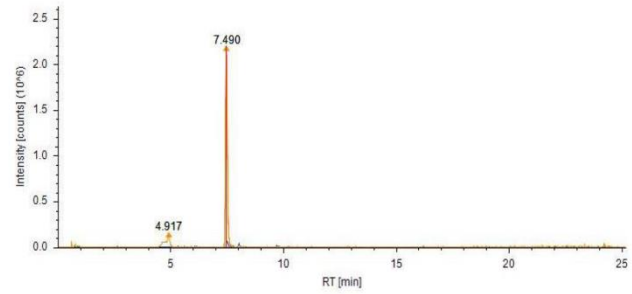
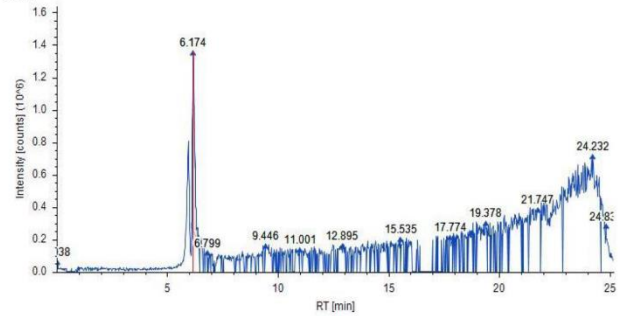


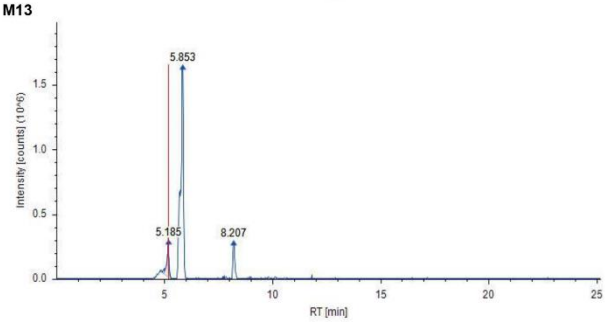
M11



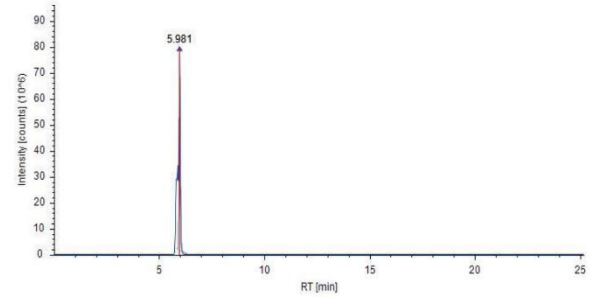
M12



M13



M14



M15

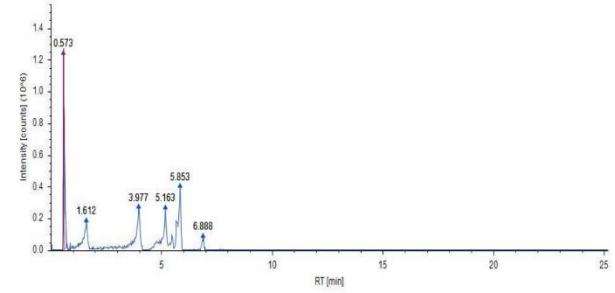


Figure S2. Extracted chromatograms of 3-HO-PCE and its potential metabolites from HLM, urine or hair.

Putative structure elucidation proposed by Compound Discoverer software on each ddMS2 spectra was consulted but not used to build the metabolic profile of 3-HO-PCE, and is provided here for informational purposes only.M6b did not trigger a ddMS2 fragmentation due its low abundance.

3-HO-CPE

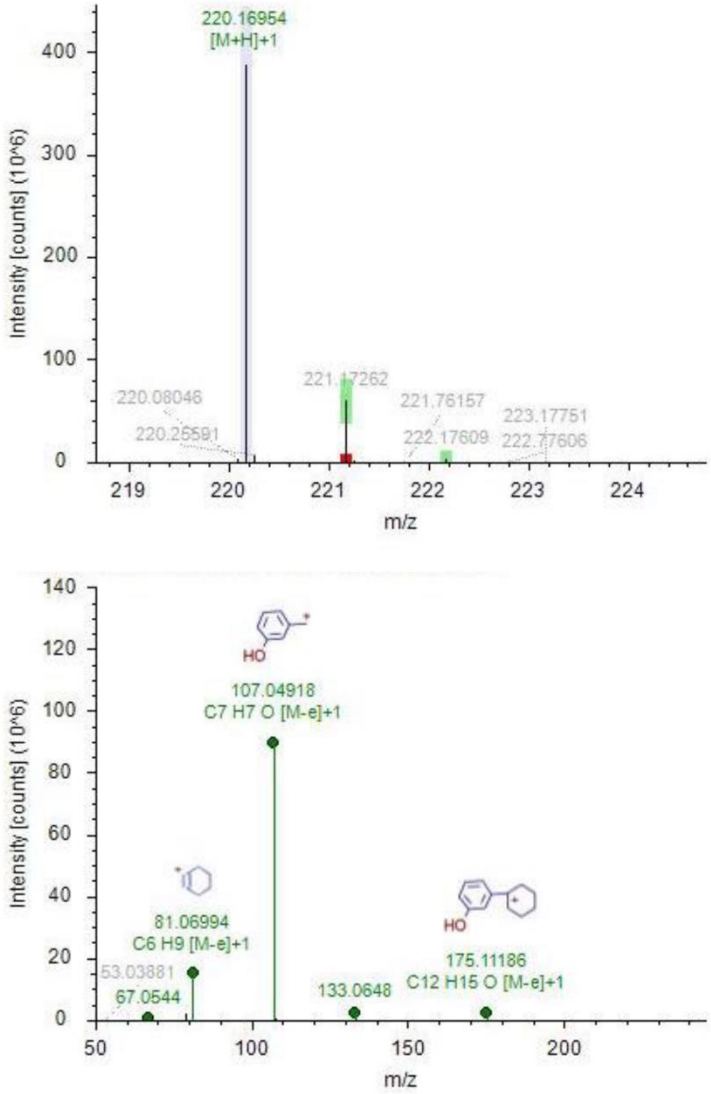


Figure S3. Full scan (Top) and ddM2 (Bottom) High resolution mass spectra of 3-HO-PCE and its putative metabolites.