Electronic Supplementary Material (ESI) for Food & Function.


# Supplement Data

# for

## A pilot study on clinical pharmacokinetics and preclinical pharmacodynamics of (+)-epicatechin on cardiometabolic endpoints

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Abbreviated Title: (+)-Epicatechin pharmacokinetics

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**Supplemental Table S1**. Mass accuracy measurements of (+)-epicatechin ((+)-Epi) and metabolites by HPLC-HR-MS

| Compound | Composition $[M-H]^-$ | Theoretical mass $[M-H]^-$ | Measured mass $[M-H]^-$ | Mass error (ppm) |
|---|---|---|---|---|
| **(+)-Epi** | $C_{15}H_{13}O_6$ | 289.0717 | 289.0718 | 0.3 |
| **M1a** | $C_{15}H_{13}O_9S$ | 369.0286 | 369.0277 | -2.4 |
| **M1b** | $C_{15}H_{13}O_9S$ | 369.0286 | 369.0281 | -1.4 |
| **M2a** | $C_{16}H_{15}O_9S$ | 383.0442 | 383.0440 | -0.5 |
| **M2b** | $C_{16}H_{15}O_9S$ | 383.0442 | 383.0440 | -0.5 |
| **M2c** | $C_{16}H_{15}O_9S$ | 383.0442 | 383.0438 | -1.0 |
| **M3a** | $C_{21}H_{21}O_{12}$ | 465.1038 | 465.1034 | -0.9 |
| **M3b** | $C_{21}H_{21}O_{12}$ | 465.1038 | 465.1032 | -1.3 |
| **Taxifolin (IS)** | $C_{15}H_{11}O_7$ | 303.05103 | 303.0510 | -0.1 |

M1 are sulfate metabolites; M2 are methyl sulfate metabolites; M3 are glucuronide metabolites.