

## Description of Additional Supplementary Files

File Name: Supplementary Data 1

Description: Caffeine table quantification for 7-day caffeine diary

File Name: Supplementary Data 2a

Description: Baseline Dietary Food Group Comparison (CD vs NCD)

File Name: Supplementary Data 2b

Description: Dietary Food Group by Timepoint for Coffee Drinkers (Caffeinated vs Decaffeinated)

File Name: Supplementary Data 2c

Description: Baseline Diet Macro and Micronutrients (CD vs NCD)

File Name: Supplementary Data 2d

Description: Macronutrients and Micronutrients by timepoint for Coffee Drinkers (Caffeinated vs Decaffeinated)

File Name: Supplementary Data 2e

Description: Statistical Information for Supplementary Data 2d

File Name: Supplementary Data 3

Description: Anthropometric measurements and self-reported questionnaires at the baseline of non-coffee drinker and coffee drinkers.

File Name: Supplementary Data 4

Description: Reduction in anthropometric measurements and self-reported cognitive assessments following a 2-week period of coffee abstinence.

File Name: Supplementary Data 5

Description: Caffeine specific and non-caffeine specific alterations in anthropometric measurements, self-reported questionnaires following a caffeinated and decaffeinated coffee intervention.

File Name: Supplementary Data 6

Description: Caffeine and non-caffeine specific reductions in anthropometric measurements and self-reported questionnaires between the initial study visit and the final study visit following an intervention with either caffeinated or decaffeinate coffee.

File Name: Supplementary Data 7

Description: Similar Cognitive task output between non-coffee drinkers and coffee drinkers at baseline visit.

File Name: Supplementary Data 8

Description: Coffee and decaffeinated coffee specific changes in cognitive task responses between baseline visit and post intervention.

File Name: Supplementary Data 9

Description: Similar response to self-reported questionnaires relevant to stress, during SECPT at the baseline (Visit 2) of non-coffee drinker and coffee drinker participants

File Name: Supplementary Data 10

Description: Self-reported questionnaires during SECPT at the baseline (Visit 2) compared to post-intervention (Visit 4) in habitual coffee drinkers.

File Name: Supplementary Data 11

Description: Reduced expression of inflammatory mediators and increase in anti-inflammatory cytokines in plasma and in LPS-stimulated whole blood at baseline in habitual coffee and non-coffee drinkers.

File Name: Supplementary Data 12

Description: Increased concentration of inflammatory mediators in the plasma and in LPS-stimulated whole blood following a 2-week period of coffee abstinence.

File Name: Supplementary Data 13

Description: Reduction of cytokine expression in the plasma and in whole blood following caffeinated and decaffeinate coffee consumption.

File Name: Supplementary Data 14

Description: Concentration of inflammatory markers in the plasma and in LPS-stimulated whole blood at the baseline (Visit 2) compared to post-intervention (Visit 4) in habitual coffee drinkers.

File Name: Supplementary Data 15

Description: Demographic characteristics of caffeinated and decaffeinated groups of CDs that underwent a 3-week coffee intervention.

File Name: Supplementary Data 16

Description: Alpha-diversity metrics across all study timepoints.

File Name: Supplementary Data 17a

Description: (Poly)phenols content obtained from the 7-day food diary of non-coffee drinkers and coffee drinkers.

File Name: Supplementary Data 17b

Description: (Poly)phenols content obtained from the 7-day food diary comparing baseline with pre-intervention (post 2-week abstinence).

File Name: Supplementary Data 17c

Description: (Poly)phenols content obtained from the 7-day food diary comparing post-abstinent period with post intervention with caffeine or decaffeinated coffee.

File Name: Supplementary Data 17d

(Poly)phenols content obtained from the 7-day food diary comparing the baseline visit to the post-intervention with caffeine or decaffeinated coffee.

File Name: Supplementary Data 18a

The three highest food group sources (% contribution to phenolic intake) of total (poly)phenols and (poly)phenol subclasses obtained from the 7-day food diary of non-coffee drinkers and coffee drinkers.

File Name: Supplementary Data 18b

The three highest food group sources (% contribution to phenolic intake) of total (poly)phenols and (poly)phenol subclasses obtained from the 7-day food diary comparing baseline with pre-intervention (post 2-week abstinence).

File Name: Supplementary Data 18c

The three highest food group sources (% contribution to phenolic intake) of total (poly)phenols and (poly)phenol subclasses obtained from the 7-day food diary comparing post-abstinent period with post intervention with caffeine or decaffeinated coffee.

File Name: Supplementary Data 18d

The three highest food group sources (% contribution to phenolic intake) of total (poly)phenols and (poly)phenol subclasses obtained from the 7-day food diary comparing the baseline visit to the post-intervention with caffeine or decaffeinated coffee.

File Name: Supplementary Data 19

Total (Poly)phenol intake from 7-day food diary prior to Visit 2

File Name: Supplementary Data 20

Total (Poly)phenol intake from 7-day food diary prior to Visit 3

File Name: Supplementary Data 21

Total (Poly)phenol intake from 7-day food diary prior to Visit 4

File Name: Supplementary Data 22

LC/MS Information Urine

File Name: Supplementary Data 23

LC/MS Information Faeces