



Supplementary material

## Climate and Processing Effects on Tea (*Camellia sinensis* L. Kuntze) Metabolome: Accurate Profiling and Fingerprinting by Comprehensive Two-Dimensional Gas Chromatography/Time-of-Flight Mass Spectrometry

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The supplementary material comprises four Supplementary Figures:

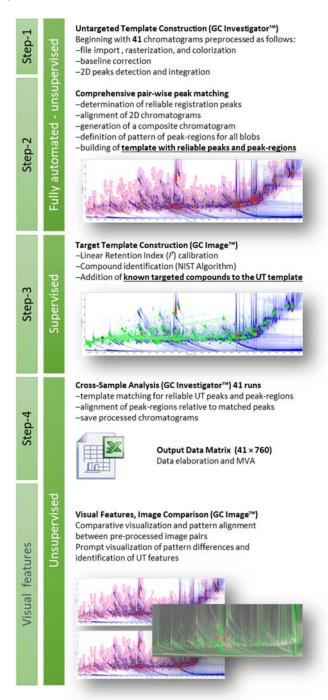
**Figure S1**: 2D data elaboration work-flow adopted to comprehensively map tea primary metabolites signatures, by adopting a combined Untargeted and Targeted UT template matching approach.

Figure S2: schematic diagram of the extraction and derivatization procedure.

Figure S3: experimental results on targeted primary metabolites extraction yields.

**Figure S4**: method repeatability is indicated in terms of % relative standard deviation (%RSD) for both chromatographic dimensions (1tR and 2tR) and for % response, collected from UT peak-regions.

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**Figure S1.** 2D data elaboration work-flow adopted to comprehensively map tea primary metabolites signatures, by adopting a combined Untargeted and Targeted UT template matching approach.

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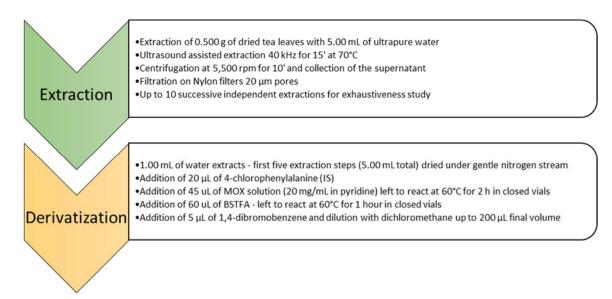
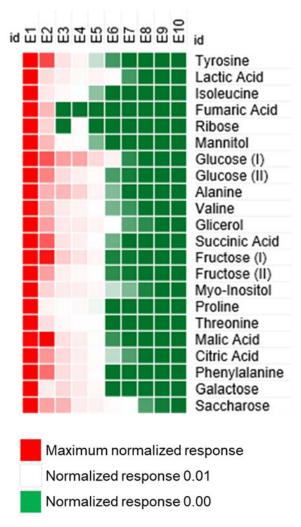


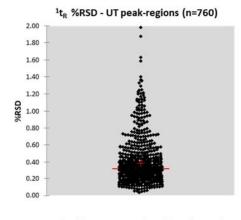
Figure S2. schematic diagram of the extraction and derivatization procedure.

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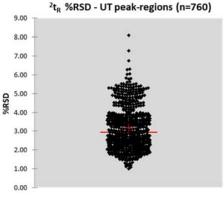


**Figure S3.** extraction yield results according to Figure S2 process; rows indicate relative metabolite concentration, while each column shows the relative amount by extraction step (from 1 to 10). All targeted compounds were extracted completely by step #9.

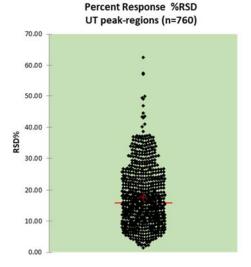
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Statistic	%RSD
No. of observations	760
Minimum	0.0341
Maximum	1.9794
1st Quartile	0.2243
Median	0.3174
3rd Quartile	0.4492
Mean	0.3889
Variance (n-1)	0.0696
Standard deviation (n-1)	0.2638



Statistic	%RSD
No. of observations	760
Minimum	0.9833
Maximum	8.0914
1st Quartile	2.2486
Median	2.9435
3rd Quartile	3.7709
Mean	3.1534
Variance (n-1)	1.2623
Standard deviation (n-1)	1.1235



Statistic	RSD%
No. of observations	760
Minimum	1.4134
Maximum	62.4575
1st Quartile	10.6071
Median	15.8763
3rd Quartile	23.3992
Mean	17.6463
Variance (n-1)	88.3691
Standard deviation (n-1)	9.4005

**Figure S4.** method repeatability is indicated in terms of % relative standard deviation (%RSD) for both chromatographic dimensions (1tR and 2tR) and for % response, collected from UT peak-regions.



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