**DECLARATION**

The file “METABOLiGA-app.R” code is the original work of Martina Stoycheva in The University of Manchester.

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The program code in the file “Francesco\_code\_modified.R” is a modified version of the code written by Francesco Del Carratore and is freely available at GitHub (<https://github.com/francescodc87/iterative-Group-Analysis> ).

The supplementary data files provided are adapted versions of the supplementary files provided by Abraham et al. (2016) with annotations downloaded from PubChem (Wheeler et al., 2005) and KEGG.

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