**Supplementary Information**

**Identification and Quantification of Bioactive Molecules Inhibiting Pro-inflammatory Cytokine Production in Spent Coffee Grounds Using Metabolomics Analyses**

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**Supplementary Table 1**. Putative metabolites with known to produce anti-inflammatory activities in the methanolic extracts of spent coffee grounds identified via an untargeted metabolomics approach

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| **No.** | **Putatively identified compound** | **Anti-inflammatory activity** |
| 1 | 3-Caffeoylquinic acid | Hwang et al. (2014) |
| 2 | 5-Caffeoylquinic acid | Kim et al. (2015) |
| 3 | 3,5-Caffeoylquinic acid  | Hong et al. (2015) |
| 4 | Caffeic acid | Chao et al. (2009) |
| 5 | Caffeine | Köroğlu et al. (2014) |
| 6 | Catechin | Nakanishi et al. (2010) |
| 7 | Chrysin | Ahad et al. (2014) |
| 8 | Daidzein | Liu et al. (2009) |
| 9 | Epicatechin | Morrison et al. (2014) |
| 10 | Eugenol | Yogalakshmi et al. (2010) |
| 11 | Ferulic acid | Zhu et al. (2014) |
| 12 | Gallic acid | Kim et al. (2005) |
| 13 | Naringenin | Pinho-Ribeiro et al. (2016) |
| 14 | Naringin | Sahu et al. (2014) |
| 15 | Oxyresveratrol | Wei et al. (2017) |
| 16 | p-Coumaric acid | Pragasam et al. (2013) |
| 17 | p-Hydroxybenzoic acid | Manuja et al. (2013) |
| 18 | Pectolinarin | Lim et al. (2008) |
| 19 | Quercetin | Guardia et al. (2001) |
| 20 | Quinic acid | Åkesson et al. (2005) |
| 21 | Resveratrol | Nunes et al. (2018) |
| 22 | Rutin | Guardia et al. (2001) |
| 23 | Tectochrysin | Hou et al. (2018) |
| 24 | Theaflavin | Zu et al. (2012) |
| 25 | Vanillic acid | Kim et al. (2011) |
| 26 | Vitexin rhamnoside | Tadić et al. (2008) |

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