

# SUPPORTING INFORMATION

## **Metabolomics of breast milk: the importance of phenotypes**

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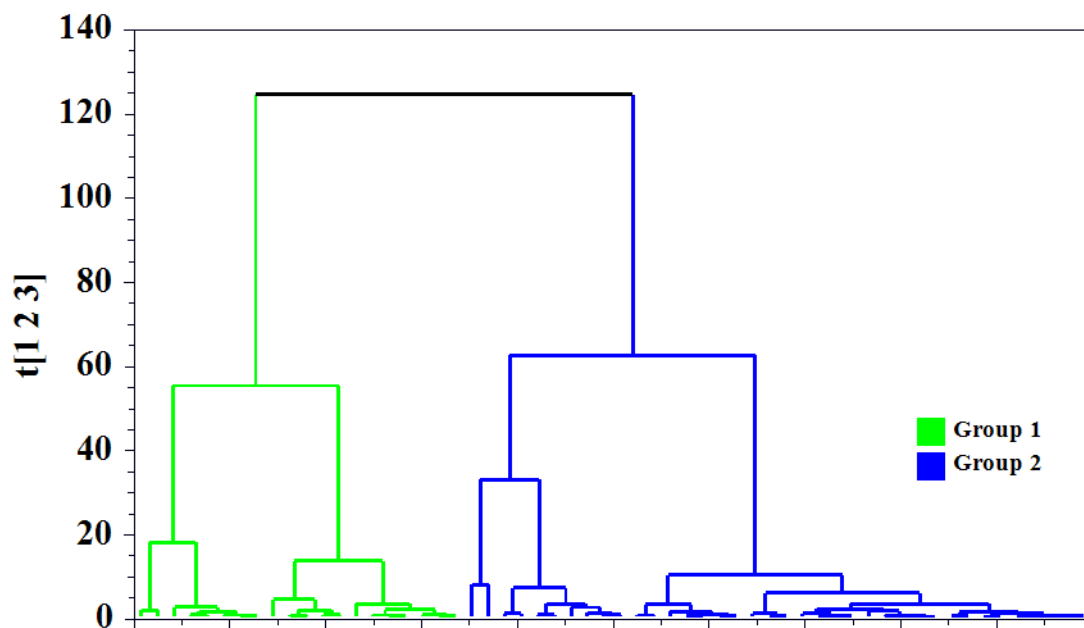
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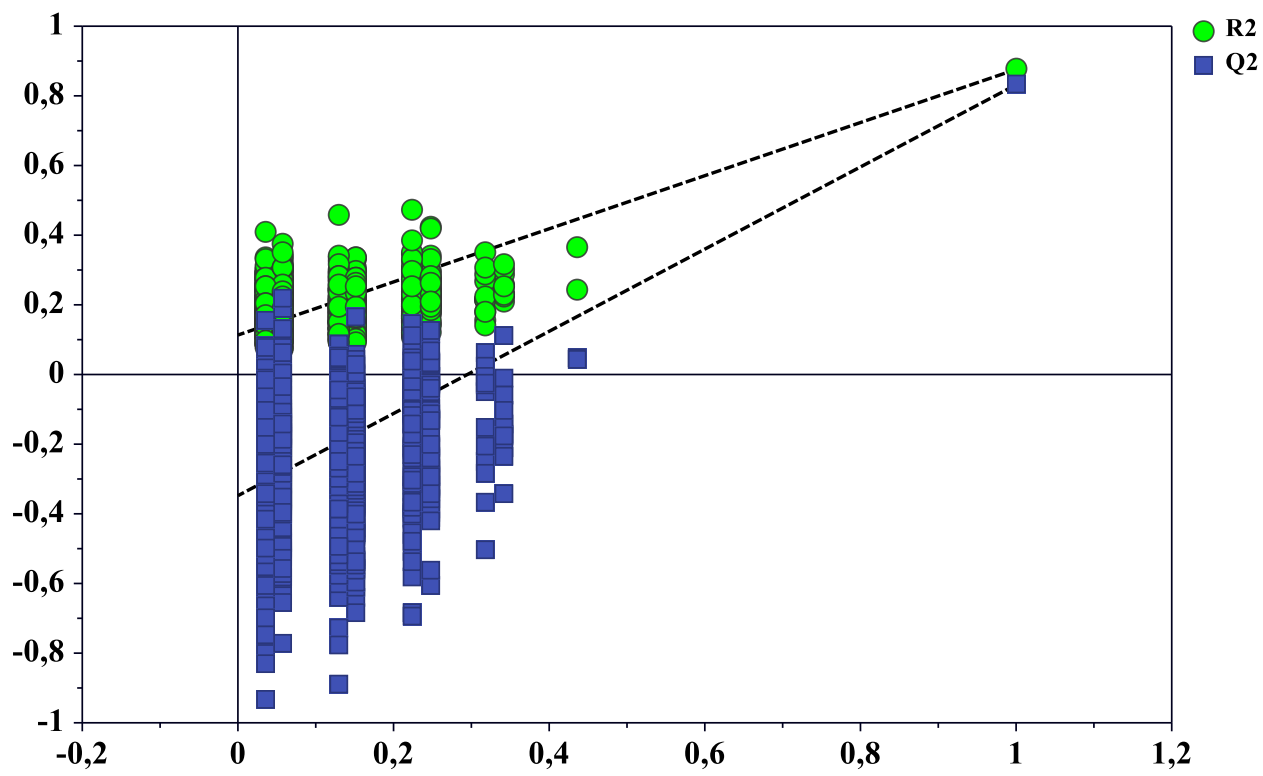
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**Figure S1.** Dendrogram of the hierarchical clustering analysis (HCA) performed on the 3D PCA model



**Figure S2.** Permutation test with 999 permutations of OPLS-DA model:  $R^2Y$  intercept = 0,113;  $Q^2Y$  intercept = -0,348.

**Table 1.** Characteristics of study population

| Sample code  | Mother      |                          |                             |                              |                  | Newborn |         |
|--------------|-------------|--------------------------|-----------------------------|------------------------------|------------------|---------|---------|
|              | Age (years) | BMI (Kg/m <sup>2</sup> ) | Milk phenotype <sup>1</sup> | Gestational age (weeks+days) | Mode of delivery | Gender  | Centile |
| <b>AGA</b>   |             |                          |                             |                              |                  |         |         |
| <b>HBM1</b>  | 19          | 15.8                     | <i>Secretor</i>             | 37+1                         | C                | F       | 20      |
| <b>HBM2</b>  | 20          | 19.7                     | <i>Secretor</i>             | 39+1                         | V                | M       | 15      |
| <b>HBM3</b>  | 21          | 26.4                     | <i>Secretor</i>             | 40+1                         | V                | M       | 15      |
| <b>HBM4</b>  | 21          | 18.6                     | <i>Secretor</i>             | 39                           | V                | F       | 20      |
| <b>HBM5</b>  | 24          | 26.8                     | <i>Secretor</i>             | 35+3                         | C                | F       | 27      |
| <b>HBM6</b>  | 24          | 33                       | <i>Secretor</i>             | 39+1                         | C                | F       | 40      |
| <b>HBM7</b>  | 26          | 22.2                     | <i>Secretor</i>             | 39+4                         | V                | M       | 37      |
| <b>HBM8</b>  | 26          | 33.2                     | <i>Non secretor</i>         | 39+2                         | V                | F       | 40      |
| <b>HBM9</b>  | 26          | 21.3                     | <i>Non secretor</i>         | 39+1                         | V                | F       | 52      |
| <b>HBM10</b> | 26          | 29.6                     | <i>Non secretor</i>         | 38+6                         | C                | F       | 72      |
| <b>HBM11</b> | 27          | 25.4                     | <i>Secretor</i>             | 39+5                         | V                | M       | 35      |
| <b>HBM12</b> | 27          | 33                       | <i>Secretor</i>             | 38+5                         | V                | M       | 42      |
| <b>HBM13</b> | 27          | 21.1                     | <i>Secretor</i>             | 39+5                         | C                | M       | 59      |
| <b>HBM14</b> | 28          | 20                       | <i>Secretor</i>             | 39+1                         | V                | M       | 26      |
| <b>HBM15</b> | 28          | 21                       | <i>Secretor</i>             | 39+1                         | V                | M       | 56      |
| <b>HBM16</b> | 29          | 23                       | <i>Secretor</i>             | 40                           | V                | F       | 18      |
| <b>HBM17</b> | 29          | 25                       | <i>Secretor</i>             | 40+5                         | C                | F       | 67      |
| <b>HBM18</b> | 29          | 20.4                     | <i>Secretor</i>             | 40+1                         | V                | F       | 75      |
| <b>HBM19</b> | 30          | 20.4                     | <i>Secretor</i>             | 38+3                         | C                | M       | 44      |
| <b>HBM20</b> | 30          | 20                       | <i>Secretor</i>             | 40+3                         | C                | M       | 45      |
| <b>HBM21</b> | 31          | 24.1                     | <i>Secretor</i>             | 38+6                         | C                | M       | 40      |
| <b>HBM22</b> | 32          | 26                       | <i>Secretor</i>             | 37                           | V                | F       | 21      |
| <b>HBM23</b> | 32          | 22                       | <i>Secretor</i>             | 38+5                         | C                | M       | 33      |
| <b>HBM24</b> | 32          | 20                       | <i>Non secretor</i>         | 38+6                         | C                | M       | 39      |
| <b>HBM25</b> | 32          | 22                       | <i>Non secretor</i>         | 40                           | V                | F       | 57      |
| <b>HBM26</b> | 32          | 32                       | <i>Secretor</i>             | 38+6                         | V                | M       | 75      |
| <b>HBM27</b> | 33          | 21.5                     | <i>Secretor</i>             | 40+1                         | C                | M       | 44      |
| <b>HBM28</b> | 33          | 23.4                     | <i>Secretor</i>             | 38+6                         | C                | M       | 54      |
| <b>HBM29</b> | 34          | 33                       | <i>Secretor</i>             | 40                           | V                | F       | 20      |
| <b>HBM30</b> | 34          | 25.9                     | <i>Secretor</i>             | 38+4                         | V                | M       | 40      |

|              |    |      |                     |      |   |   |    |
|--------------|----|------|---------------------|------|---|---|----|
| <b>HBM31</b> | 34 | 19.3 | <i>Non secretor</i> | 38+6 | C | M | 43 |
| <b>HBM32</b> | 34 | 26   | <i>Secretor</i>     | 38   | C | F | 72 |
| <b>HBM33</b> | 35 | 23.1 | <i>Secretor</i>     | 38+3 | C | F | 44 |
| <b>HBM34</b> | 36 | 32   | <i>Secretor</i>     | 39+6 | C | F | 17 |
| <b>HBM35</b> | 36 | 21.4 | <i>Secretor</i>     | 40+1 | V | M | 30 |
| <b>HBM36</b> | 36 | 22   | <i>Secretor</i>     | 38+5 | C | M | 32 |
| <b>HBM37</b> | 36 | 20.6 | <i>Secretor</i>     | 39+2 | C | M | 45 |
| <b>HBM38</b> | 36 | 20.9 | <i>Secretor</i>     | 38+6 | V | M | 65 |
| <b>HBM39</b> | 36 | 30   | <i>Secretor</i>     | 39+5 | V | M | 69 |
| <b>HBM40</b> | 36 | 22.2 | <i>Non secretor</i> | 38+6 | C | F | 75 |
| <b>HBM41</b> | 37 | 30.8 | <i>Secretor</i>     | 40+2 | V | F | 49 |
| <b>HBM42</b> | 37 | 21   | <i>Non secretor</i> | 36+1 | C | F | 50 |
| <b>HBM43</b> | 38 | 23.2 | <i>Secretor</i>     | 41   | V | M | 23 |
| <b>HBM44</b> | 39 | 35.4 | <i>Secretor</i>     | 40   | V | M | 25 |
| <b>HBM45</b> | 39 | 26.9 | <i>Secretor</i>     | 38+6 | C | F | 40 |
| <b>HBM46</b> | 42 | 21.4 | <i>Non secretor</i> | 40   | V | F | 70 |

#### SGA

|              |    |      |                     |      |   |   |    |
|--------------|----|------|---------------------|------|---|---|----|
| <b>HBM47</b> | 23 | 21   | <i>Secretor</i>     | 37+1 | C | F | 5  |
| <b>HBM48</b> | 25 | 34   | <i>Non secretor</i> | 40   | V | M | 2  |
| <b>HBM49</b> | 26 | 21   | <i>Secretor</i>     | 39   | V | F | 4  |
| <b>HBM50</b> | 32 | 22.2 | <i>Secretor</i>     | 38+4 | V | F | 1  |
| <b>HBM51</b> | 33 | 19.6 | <i>Non secretor</i> | 39+1 | V | F | 1  |
| <b>HBM52</b> | 33 | 23.6 | <i>Secretor</i>     | 38+5 | V | M | 7  |
| <b>HBM53</b> | 34 | 23.4 | <i>Non secretor</i> | 39   | V | M | 4  |
| <b>HBM54</b> | 36 | 20   | <i>Non secretor</i> | 39+6 | V | F | 5  |
| <b>HBM55</b> | 36 | 23.6 | <i>Secretor</i>     | 39+2 | C | F | 9  |
| <b>HBM56</b> | 36 | 18.5 | <i>Non secretor</i> | 39   | V | F | 10 |

#### LGA

|              |    |      |                 |      |   |   |    |
|--------------|----|------|-----------------|------|---|---|----|
| <b>HBM57</b> | 37 | 19   | <i>Secretor</i> | 38+5 | C | M | 92 |
| <b>HBM58</b> | 32 | 21.4 | <i>Secretor</i> | 39   | V | M | 91 |

**Abbreviations:** AGA: adequate for gestational age; SGA: small for gestational age; LGA: large for gestational age; BMI: body mass index; C: cesarean section; V: vaginal delivery; F: female; M: male.

<sup>1</sup>Milk phenotype established according to NMR spectra analysis.