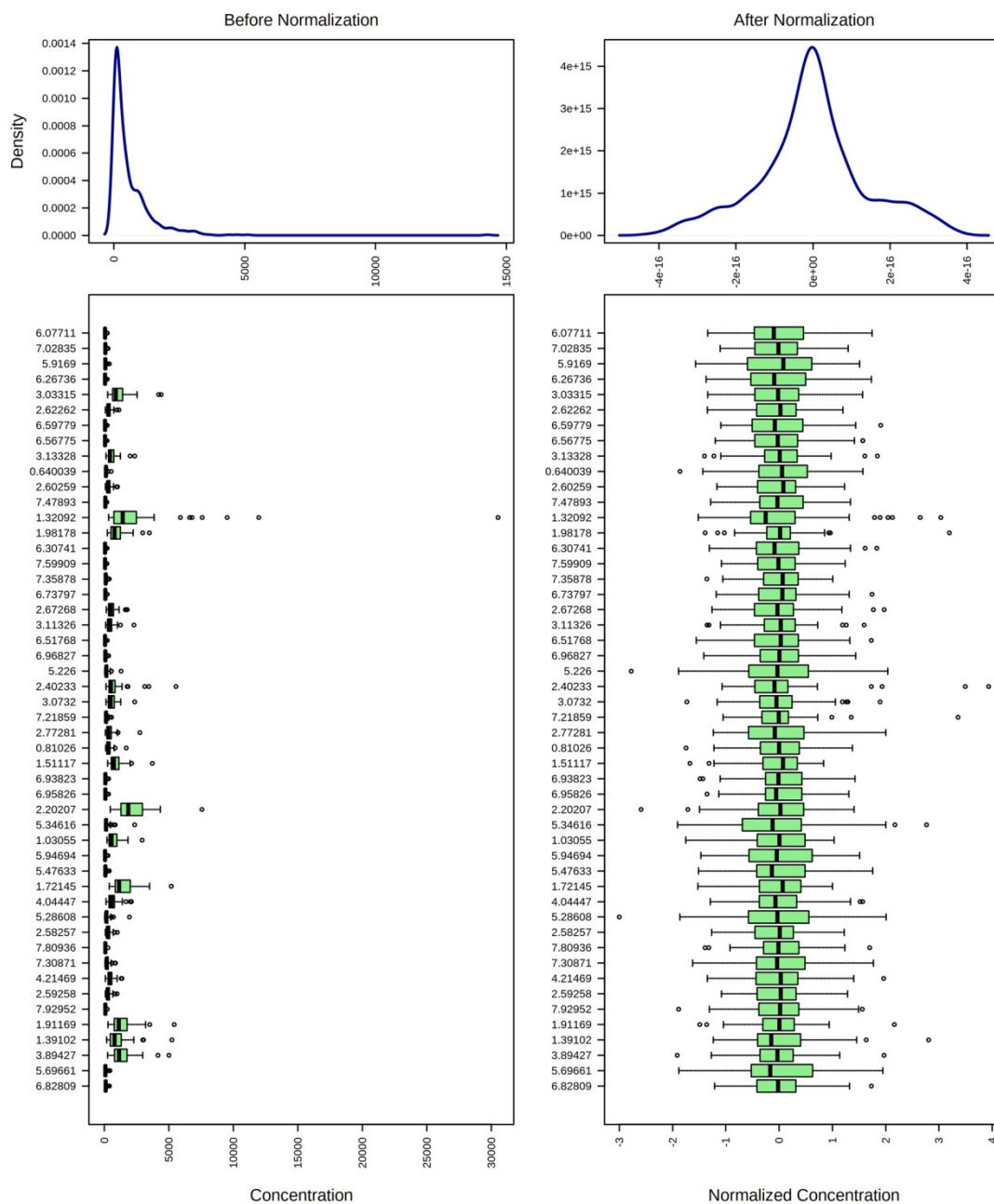


- 1 **Figure S1. The distribution of the input metabolomic data values before (left)**
- 2 **and after (right) normalization.** The input metabolomic data was normalized by
- 3 sum peak area, transformed with log transformation, and scaled with Pareto scaling.



4

5

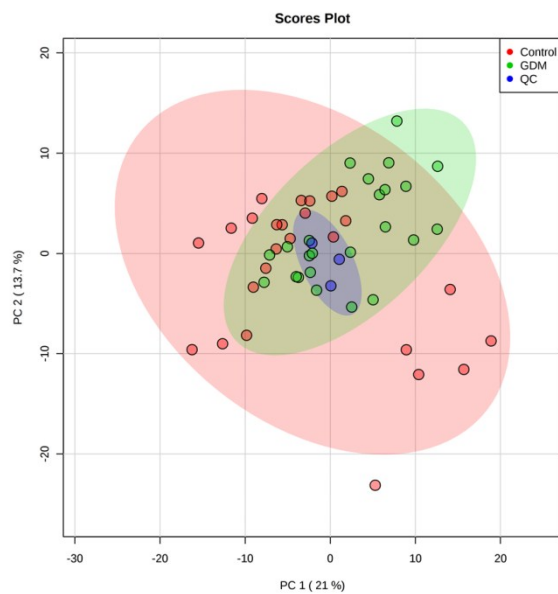
6

7

8

9

10



11

12

13

14 **Figure S2. PCA score plot based on the ¹H-NMR data of clinical samples and**
15 **quality control samples.** Red oval represents the 95% CI of score calculated from the
16 NDM control samples. Green oval represents the 95% CI of score calculated from the
17 GDM samples. Purple oval represents the 95% CI of score calculated from the quality
18 control samples.

19

20

21

22

23

24

25

26

27

28

29

30

31

32

33

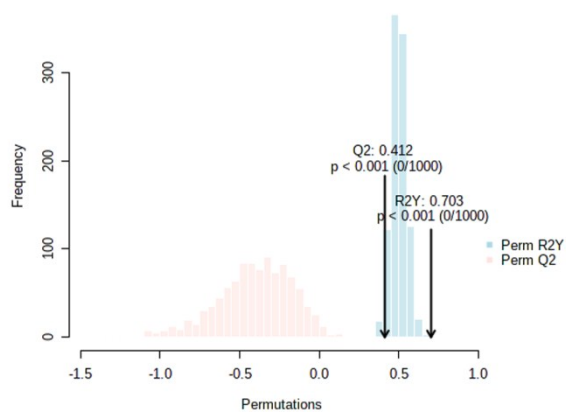
34

35

36

37

38



39 **Figure S3. Permutation tests of the OPLS-DA models.** R2Y represents multiple
40 correlation coefficient. Q2 represents the cross-validated R2. Both of the parameters
41 were used for assessment of the fitting validity and predictive ability of the OPLS-DA
42 models.

