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| **Supplemental Table 1.** Protocol for measurement of serum amino acids metabolites |
| 1. Amino acids and their metabolites were quantified using liquid chromatography-mass spectrometry (LC-MS) based on previous publication methods1,2. Briefly, 10 μL of 13C-tryptophan (5 μM), as the internal standard (IS), was added to 100 μL of serum and standard solution in 4% bovine serum albumin solution and diluted with 20 μL of water containing 0.1% formic acid (v/v). Subsequently, 400 μL of cold acetonitrile for protein precipitation was added, vortexed, and centrifuged at 10,000 x g at 4 °C for 10 min. Next, 400 μl of the supernatant was dried using a speed vacuum evaporator and reconstituted in 0.1% formic acid in water/acetonitrile (9/1, v/v) solution. Then, 10 μL of the samples was injected into an HPLC-MS/MS system (Agilent 1200 HPLC equipped with AB SCIex 3200 Mass analyzer) equipped with the Waters Atlantis T3 (4.6×150 mm i.d., 3 μm) column at 30 °C. 2. Ions of each analyzed compound, except the IS, were detected in a positive ionization mode using the multiple reaction monitoring mode. Liquid chromatographic separation was performed with mobile phases A (0.1% formic acid in water, v/v) and B (0.1% formic acid in acetonitrile, v/v) at 0.5 mL/min flow rate under the following conditions: 5% for the first gradient starting at 5% B to 40% B in 6 min, to 90% B in 5 min, staying at 90% B for 5 min, then to 5% B in 1 min. The column equilibration was performed for 8 min before each analysis under the 5% B condition. 3. In terms of the MS conditions, the ion source temperature was set to 600 °C. The curtain and nebulizer gas were set at 20 psi and 50 psi, respectively. The MS capillary voltage was 4.5 kV for the positive mode or -4.5 kV for the negative mode. The acquired data were analyzed using Analyst software (v1.6.3, SCIex, USA). |
| 1 Zhu W, Stevens AP, Dettmer K, et al. Quantitative profiling of tryptophan metabolites in serum, urine, and cell culture supernatants by liquid chromatography-tandem mass spectrometry. Anal Bioanal Chem 2011;401:3249-3261.  2 Choi JM, Park WS, Song KY, et al. Development of simultaneous analysis of tryptophan metabolites in serum and gastric juice - an investigation towards establishing a biomarker test for gastric cancer diagnosis. Biomed Chromatogr2016;30:1963-1974 |

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| **Supplemental Table 2.** Chromatographic retention time (RT), selected MRM parameters, DP, EP, CE, and CXP for each analyte measured | | | | | | | | | |
| Compounds | Exact Mass | RT | Ion mode | [MH+] or [M-H]- | Product Ion Mass | DP | EP | CE | CXP |
| Leucine (C6H13NO2) | 131.095 | 6.5 | Pos | 132.1 | **43.2** | 21 | 7.5 | 31. | 10 |
| 86.1 | 21 | 7.5 | 31.0 | 10 |
| Isoleucine (C6H13NO2) | 131.095 | 6.2 | Pos | 132.0 | **86.1** | 26 | 5.5 | 21.0 | 10 |
| Valine (C5H11NO2) | 117.0789 | 4.1 | Pos | 118.1 | **72.1** | 26 | 5.0 | 19.0 | 10 |
| Phenylalanine (C9H11NO2) | 165.079 | 7.3 | Pos | 166.2 | 103.2 | 21 | 3.0 | 33.0 | 10 |
| **120.2** | 21 | 3.0 | 19.0 | 10 |
| Tyrosine (C9H11NO3) | 181.074 | 6.3 | Pos | 181.9 | **91.2** | 26 | 6.0 | 35.0 | 14 |
| 136.1 | 26 | 5.5 | 35.0 | 14 |
| Tryptophan (C11H12N2O2) | 204.09 | 8.1 | Pos | 205.0 | **117.9** | 26 | 6.0 | 33.0 | 12 |
| 158.8 | 26 | 6.0 | 33.0 | 12 |
| Kynurenine (C10H12N2O3) | 208.0848 | 7.4 | Pos | 209.1 | 94.0 | 26 | 5.0 | 19.0 | 10 |
| **192.200** | 26 | 5.0 | 13.0 | 10.0 |
| Kynurenic acid (C10H7NO3) | 189.043 | 9.2 | Pos | 189.900 | **116.000** | 31 | 3.0 | 39.0 | 12.0 |
| 143.900 | 21 | 3.0 | 39.0 | 12.0 |
| Anthranilic acid (C7H7NO2) | 137.048 | 11.4 | Pos | 138.106 | 92.100 | 16 | 3.0 | 27.0 | 14.0 |
| **119.900** | 16 | 3.0 | 15.0 | 14.0 |
| Xanthurenic acid (C10H7NO4) | 205.0375 | 8.1 | Pos | 206.071 | **132.200** | 51 | 10.5 | 41.0 | 12.0 |
| 159.900 | 51 | 10.5 | 23.0 | 12.0 |
| 3-Hydroxykynurenine (C10H12N2O4) | 224.0797 | 6.2 | Pos | 225.061 | 110.100 | 26 | 8.5 | 23.0 | 20.0 |
| **208.100** | 26 | 8.5 | 13.0 | 20.0 |
| 3-Hydroxyanthranilic acid (C7H7NO3) | 153.043 | 9.0 | Pos | 154.000 | 108.100 | 26 | 2.5 | 25.0 | 10.0 |
| **136.200** | 21 | 2.0 | 25.0 | 10.0 |
| 5-hydroxyindoleacetic acid (C10H9NO3) | 191.058 | 9.6 | Pos | 192.100 | **146.100** | 26.0 | 5.5 | 29.0 | 10.0 |
| 5-Hydroxytryptophan (C11H12N2O3) | 220.084 | 6.9 | Pos | 221.100 | **175.000** | 26.0 | 5.5 | 23.0 | 12.0 |
| L-Dihydroxyphenylalanine (C9H11NO4) | 197.069 | 5.0 | Pos | 197.934 | 107.200 | 36.0 | 4.0 | 29.0 | 14.0 |
| **152.000** | 36.0 | 4.0 | 21.0 | 14.0 |
| IS(13C-Tryptophan) (C11H12N2O2) | 215.09 | 8.3 | Pos | 216.100 | 126.100 | 26.0 | 5.5 | 33.0 | 12.0 |
| Neg | 214.000 | 124.100 | -50.0 | -10.0 | -24.0 | -12.0 |
| MRM: multiple reaction mode, DP: declustering potential, EP: entrance potential, CE: collision energy, CXP: collision cell exit potential, IS: internal standard, [MH+]: positive ion mode, [M-H]-: negative ion mode | | | | | | | | | |

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| **Supplemental Table 3.** Prognostic performance of amino acid metabolites to predict diabetes remission 12 months after bariatric surgery | | |
| Amino acid metabolites [abbreviations] | Area under ROC curve (SE) | 95% CI |
| BCAAs |  |  |
| Leucine [Leu] | 0.60 (0.17) | 0.28 to 0.92 |
| Isoleucine [Iso] | 0.41 (0.17) | 0.08 to 0.75 |
| Valine [Val] | 0.65 (0.14) | 0.38 to 0.93 |
| Sum of BCAAs | 0.64 (0.16) | 0.33 to 0.95 |
| AAAs |  |  |
| Phenylalanine [Phe] | 0.64 (0.18) | 0.28 to 0.99 |
| Tyrosine [Tyr] | 0.77 (0.14) | 0.51 to 1.00 |
| Tryptophan [Trp] | 0.76 (0.13) | 0.51 to 1.00 |
| Sum of BCAAs and AAAs | 0.68 (0.14) | 0.40 to 0.96 |
| Metabolites from the kynurenine pathway |  |  |
| Kynurenine [Kyn] | 0.59 (0.17) | 0.26 to 0.91 |
| Anthranilic acid [AA] | 0.49 (0.17) | 0.16 to 0.81 |
| 3-hydroxykynurenine [3-HK] | 0.76 (0.11) | 0.54 to 0.99 |
| 3-hydroxyanthranilic acid [3-HAA] | 0.85 (0.09) | 0.67 to 1.00 |
| Kynurenic acid [KA] | 0.57 (0.16) | 0.27 to 0.88 |
| Xanthurenic acid [XA] | 0.60 (0.16) | 0.28 to 0.91 |
| Metabolites from the serotonin pathway |  |  |
| 5-hydroxytryptophan [5-HTP] | 0.63 (0.18) | 0.28 to 0.98 |
| Serotonin [Ser] | 0.70 (0.15) | 0.41 to 1.00 |
| 5-hydroxyindoleacetic acid [5-HIAA] | 0.73 (0.13) | 0.47 to 0.98 |
| Metabolites from the tyrosine pathway |  |  |
| L-dihydroxyphenylalanine [L-DOPA] | 0.92 (0.09) | 0.75 to 1.00 |
| Abbreviations: ROC, receiver operating characteristic; SE, standard error; CI, confidence interval; BCAA, branched-chain amino acid; AAA, aromatic amino acid | | |

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| **Supplemental Table 4.** Prognostic performance of existing prediction models and clinical parameters to predict diabetes remission 12 months after bariatric surgery | | |
| Variables | Area under ROC curve (SE) | 95% CI |
| Age | 0.14 (0.10) | 0.00 to 0.33 |
| Body mass index | 0.74 (0.12) | 0.49 to 0.98 |
| Waist circumference | 0.57 (0.13) | 0.31 to 0.83 |
| Waist-to-hip ratio | 0.13 (0.08) | 0.00 to 0.29 |
| Duration of diabetes | 0.27 (0.17) | 0.00 to 0.61 |
| Glycated hemoglobin | 0.19 (0.11) | 0.00 to 0.40 |
| Fasting plasma glucose | 0.45 (0.16) | 0.14 to 0.77 |
| ABCD score | 0.81 (0.14) | 0.54 to 1.00 |
| DiaRem score | 0.10 (0.07) | 0.00 to 0.24 |
| IMS score | 0.11 (0.07) | 0.00 to 0.25 |
| Abbreviations: ROC, receiver operating characteristic; SE, standard error; CI, confidence interval | | |

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| **Supplemental Table 5.** Longitudinal changes of serum metabolites after bariatric surgery | | | | | | | | | |
| Metabolites (μmol/L) | Remission | | | Non-remission | | | *P* value for baseline | *P* value for 3 months | *P* value for 12 months |
| Baseline (n=14) | 3 months (n=14) | 12 months (n=14) | Baseline (n=10) | 3 months (n=10) | 12 months (n=10) |
| L-DOPA | 0.042 (0.004) | 0.037 (0.003) | 0.031 (0.002) | 0.022 (0.002) | 0.018 (0.001) | 0.029 (0.005) | 0.014 | 0.004 | 0.771 |
| 3-HAA | 0.059 (0.006) | 0.045 (0.003) | 0.055 (0.002) | 0.027 (0.003) | 0.029 (0.005) | 0.041 (0.008) | 0.005 | 0.030 | 0.083 |
| Numbers represent mean (standard error).  Abbreviations: L-DOPA, L-dihydroxyphenylalanine; 3-HAA, 3-hydroxyanthranilic acid | | | | | | | | | |

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**Figure S2.** Diabetes-related amino acid metabolites.

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