Supplementary File 1. Chromatography gradient method for untargeted metabolomics

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| **Time (min)** | **% Solvent A** | **% Solvent B** |
| 0 | 90 | 10 |
| 5 | 60 | 40 |
| 7 | 5 | 95 |
| 9 | 5 | 95 |
| 9.1 | 90 | 10 |
| 13 | 90 | 10 |

Solvent A: 0.1% (v/v) formic acid solution in water. Solvent B was a 0.1% (v/v) formic acid solution in methanol. The flow rate was 0.4 mL/min.