Figure S1. Patient flow diagram. Among the biological samples deposited at SHINGEN, a total of 20 plasma samples from patients with GC and 16 plasma samples from control patients were analyzed in the present study, excluding postoperative and clinically early stage, as well as metastatic GC. GC, gastric cancer; SHINGEN, Yamanashi Biobank of Gastroenterological Cancers.


Figure S2. Graphic explanation of the data acquisition and leave-one-out cross validation performed in the present study. Machine learning was performed using normalized data of lipid molecule expression levels excluding one blinded sample. Subsequently, the cancer probability for the blinded sample was evaluated using the unique algorithm. This procedure was repeated for all samples ( 16 control and 20 gastric cancer samples). MS, mass spectrometry.


Figure S3. Comparison of intended molecules among three groups. Each molecule investigated in the present study exhibited various expression levels in the HV group, compared with those in the control and GC groups. Each bracket shows the number of carbon and double bonds included. A.U., arbitrary unit; Con, control; GC, gastric cancer; HV, healthy volunteer; LPC, lysophosphatidylcholine; PC, phosphatidylcholine; SM, sphingomyelin; PE, phosphatidylethanolamine.

## Dominant in Control



Dominant in GC


Figure S4. Plot of the PLS regression. PLS analysis for the three groups (control, GC and HV) showed different characteristics for each group. PLS, partial least squares; Con, control; Gas, gastric cancer; HV, healthy volunteer.


Table SI. Cancer probability of discriminant analysis.

| Sample | Cancer probability |
| :---: | :---: |
| Control |  |
| 1 | 0.0262 |
| 2 | 0.0458 |
| 3 | 0.0199 |
| 4 | 0.0816 |
| 5 | 0.0015 |
| 6 | 0.1187 |
| 7 | 0.2787 |
| 8 | 0.2948 |
| 9 | 0.1284 |
| 10 | 0.0738 |
| 11 | 0.0258 |
| 12 | 0.1400 |
| 13 | 0.0012 |
| 14 | 0.3747 |
| 15 | 0.9925 |
| 16 | 0.0132 |
| Gastric cancer |  |
| 1 | 0.9680 |
| 2 | 0.7218 |
| 3 | 0.9575 |
| 4 | 0.9449 |
| 5 | 0.9601 |
| 6 | 0.9609 |
| 7 | 0.8701 |
| 8 | 0.8992 |
| 9 | 0.9596 |
| 11 | 0.8163 |
| 12 | 0.9504 |
| 13 | 0.8526 |
| 14 | 0.2003 |
| 16 | 0.9096 |
| 17 | 0.9633 |
| 18 | 0.8223 |
|  | 0.9688 |

