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 post-operative and clinically early stage, as well as metastatic GC. GC, gastric cancer; SHINGEN, Yamanashi Biobank of Gastroenterological Cancers.

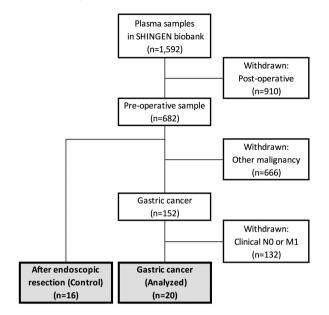


Figure S2. Graphic explanation of the data acquisition and leave-one-out cross validation performed in the present study. Machine learning was performed using normalized data of lipid molecule expression levels excluding one blinded sample. Subsequently, the cancer probability for the blinded sample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

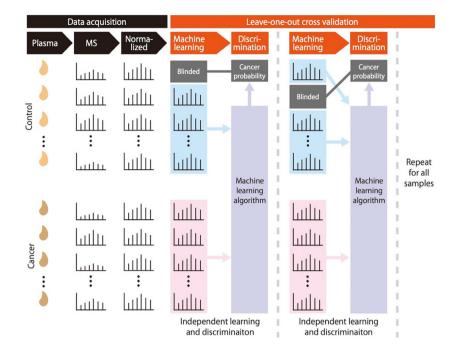


Figure S3. Comparison of intended molecules among three groups. Each molecule investigated in the present study exhibited various expression levels in the HV group, compared with those in the control and GC groups. Each bracket shows the number of carbon and double bonds included. A.U., arbitrary unit;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



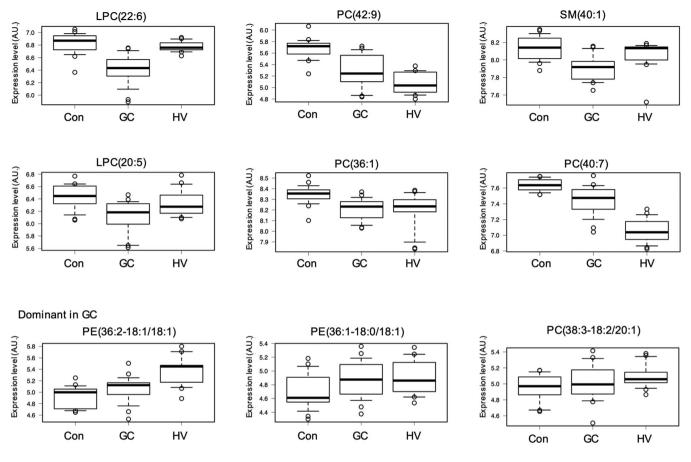


Figure S4. Plot of the PLS regression. PLS analysis for the three groups (control, GC and HV) showed different characteristics for each group. PLS, partial least squares; Con, control; Gas, gastric cancer; HV, healthy volunteer.

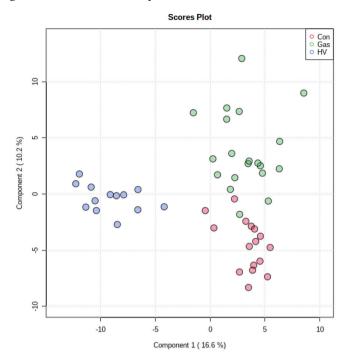


Table SI. Cancer probability of discriminant analysis.

Control   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     1   0.9680     2   0.7218     3   0.9575     4   0.9449     5   0.9601     6   0.9609     7   0.8701	
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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   1 0.9680   2 0.7218   3 0.9575   4 0.9449   5 0.9601   6 0.9609	
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 0.9680   2 0.7218   3 0.9575   4 0.9449   5 0.9601   6 0.9609	
$\begin{array}{ccccccc} 6 & 0.1187 \\ 7 & 0.2787 \\ 8 & 0.2948 \\ 9 & 0.1284 \\ 10 & 0.0738 \\ 11 & 0.0258 \\ 12 & 0.1400 \\ 13 & 0.0012 \\ 14 & 0.3747 \\ 15 & 0.9925 \\ 16 & 0.0132 \\ \hline Gastric cancer \\ 1 & 0.9680 \\ 2 & 0.7218 \\ 3 & 0.9575 \\ 4 & 0.9449 \\ 5 & 0.9601 \\ 6 & 0.9609 \\ \end{array}$	
$\begin{array}{ccccccc} 7 & 0.2787 \\ 8 & 0.2948 \\ 9 & 0.1284 \\ 10 & 0.0738 \\ 11 & 0.0258 \\ 12 & 0.1400 \\ 13 & 0.0012 \\ 14 & 0.3747 \\ 15 & 0.9925 \\ 16 & 0.0132 \\ \hline \\ Gastric cancer \\ \hline 1 & 0.9680 \\ 2 & 0.7218 \\ 3 & 0.9575 \\ 4 & 0.9449 \\ 5 & 0.9601 \\ 6 & 0.9609 \\ \end{array}$	
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   1 0.9680   2 0.7218   3 0.9575   4 0.9449   5 0.9601   6 0.9609	
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$\begin{array}{ccccccc} 10 & 0.0738 \\ 11 & 0.0258 \\ 12 & 0.1400 \\ 13 & 0.0012 \\ 14 & 0.3747 \\ 15 & 0.9925 \\ 16 & 0.0132 \\ \hline & & & & \\ Gastric cancer \\ 1 & 0.9680 \\ 2 & 0.7218 \\ 3 & 0.9575 \\ 4 & 0.9449 \\ 5 & 0.9601 \\ 6 & 0.9609 \\ \end{array}$	
$\begin{array}{ccccccc} 11 & & 0.0258 \\ 12 & & 0.1400 \\ 13 & & 0.0012 \\ 14 & & 0.3747 \\ 15 & & 0.9925 \\ 16 & & 0.0132 \\ \hline & & & & & \\ Gastric cancer & & & \\ 1 & & & 0.9680 \\ 2 & & & 0.7218 \\ 3 & & & 0.9575 \\ 4 & & & 0.9449 \\ 5 & & & 0.9601 \\ 6 & & & 0.9609 \\ \end{array}$	
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9 0.9596	
10 0.8163	
11 0.9504	
12 0.8526	
13 0.2003	
14 0.9096	
15 0.9633	
16 0.8223	
17 0.9688	
18 0.9766	
19 0.8905	
20 0.9240	