We thank the reviewers for their constructive feedback.

### Reviewer #1

This Reviewer assessed the paper and was supportive of publication, but provided no specific comments.

# Reviewer #2

**Comment:** The title doesn't accurately describe the data generated. In order for others to utilize that data and search for the dataset the title should be revised.

**Response:** We revised the title to specify the types of data generated.

# Reviewer #3

Comment: This is a great dataset that can be reused by other researchers who are interested in gut microbiome in immunocompromised patients. I appreciate the efforts to compile such a beautiful dataset very much. Great job! Therefore, I recommend for publication of the manuscript. However, I have some questions that need to be addressed. Most of these questions are clarifications. One exception is the column "quality" in StoolSamplesTable. If there is any possibility, I strongly suggest the authors report the raw 16S qPCR data (16S copies per g feces or in similar units), instead of a binary adequate/inadequate. The 16S qPCR data can be used to convert relative abundance to absolute abundance, which may alter the results of associations between microbiome and metabolomics or other clinical outcomes. This will also facilitate the studies of the difference between relative microbiome profiling and absolute microbiome profiling.

**Response:** Thank you very much for your detailed review and comments. We address your questions below.

**Comment:** StoolSamplesTable:

1. As I mentioned above, is it possible to show the numeric values of 16S data?

**Response:** We added this data to the table.

**Comment:** SerumMetabolomicsTable:

- 1. Some metabolites have missing values. What do they represent? Unknown values or zero or something else?
- 2. Metabolite levels were normalized by median. This is ok but researchers may have their own preferred normalization approach. One way is to report the unnormalized metabolite levels. Another way is to give two tables, one with normalized (by median) and the other unnormalized. It would be great to give some flexibility to users on how they perform data normalization.

**Response:** Metabolites with no values listed were undetectable. We added this information in the heading of the revised table. We also added another table showing unnormalized values.

**Comment:** PatientMetadata:

- 1. What is "7+3" in Chemotherapy? I do not see a legend.
- 2. Diarrhea: Each diarrhea is defined by a start and an end date. Does it mean that the patient has only diarrhea without any normal poop during this period? If the end date is None, does it mean that the patient still had diarrhea at the time of discharge?

3. Neutropenic fever: This is out of my curiosity. What's the typical neutropenia period for these patients? This information will be helpful for the readers to understand the immune system's status during the treatment.

**Response:** We added the full name for 7+3 in the table's heading where we had listed the full name of all other chemotherapy agents. During the periods designated by start and end dates, patients did not have normal bowel movements. Patients with "None" listed as end date also have "None" for start date, meaning they did not have diarrhea. Neutropenia typically starts during week 1 and ends in week 4 (if patients achieve a remission). We added this to the revised manuscript (paragraph 1 of main text).

# **Comment:** MetabolitesIDTable:

1. I do not understand the following technical statement

"Compounds in column B for which no authentic standards were available for confirmation are marked with \* after the compound name to designate these as Metabolomics Standards Initiative level 2/3". What does "Metabolomics Standards Initiative level 2/3" mean? Could you better explain metabolites with \*?

Response: We added a detailed description under Data Records in the main text.

# **Comment:** AntibioticsTable:

1. The dataset includes 69 AML patients. However, the antibiotic table has 67 patients. Why 2 patients have missing antibiotic data? Is it because their data are unavailable or they have not received any antibiotics (very unlikely)? Regardless of the case, please specify.

**Response:** Thank you for pointing out this error. As seen in the patient metadata table, there were 68 patients. This is correct, but in the text we had incorrectly mentioned 69 patients. We have now corrected the text. As the reviewer mentioned, the antibiotic table only showed data for 67 patients. We fixed the table by adding data for the missing patient.

**Comment:** One final question, the authors made all dates relative to the first day of Chemotherapy. Was chemo only given on a single day or spanned over multiple days or spanned over multiple periods? This might be an important covariant in statistical analysis. I would expect some information in the revised manuscript about when and how many days chemotherapy was given.

**Response:** Most chemotherapy regimens for AML are 5-10 days long. We added chemotherapy duration for each regimen in the heading of the patient metadata table.