

To referee #2

1/ In Line 62, I noticed that the reference Wang et al., 2021 appears to be misplaced in the text. It would be more appropriate to include it within the next citation bracket.

Reply #1: Thanks. It is now revised as suggested.

2/ I recommend incorporating more recent literature to support the discussion, particularly in line 70, where a reference from 2006 is cited.

Reply #2: Thanks. We have now cited a literature from 2024.

Liu, S. J., Wang, Y. Q., Zhang, S., Chen, Y. B., Wu, C., Zhang, G. Q., and Wang, G. H.: The synergistic effect of NO_x and SO₂ on the formation and light absorption of secondary organic aerosols from o-xylene photooxidation, *Atmos. Res.*, 304, <https://doi.org/10.1016/j.atmosres.2024.107387>, 2024.

3/ In Line 304-305, "Note both light absorption and organic molecules are for MSOA.", Should this term be "WSOA" instead of "MSOA"? In your conclusion part, i saw one limitation of this paper is that no source apportionment was conducted on MSOA due to technical difficulties, please check for this.

Reply #3: Sorry that we did not state it clearly, it is indeed “MSOA” not “WSOA”. Here we want to clarify that since the molecular characterization of OA was conducted on methanol-soluble OA (MSOA) not WSOA, therefore the light absorption data was also for MSOA. The source apportionment was conducted on WSOA not MSOA due to technical difficulties, but the source apportionment results were not used for ML analysis therefore do not affect the ML results. We change the sentence to “Note since molecular characterization was conducted on MSOA (not WSOA), therefore light absorption of MSOA were used here for consistency.”

4/ I would suggest expanding the discussion of the machine learning results in the conclusion section, as this represents a significant innovation of your work. Specifically, it would be valuable to highlight which findings were uniquely discovered or validated through the machine learning approach. Providing more detailed insights into these aspects would strengthen the impact of your study and better emphasize its contributions to the field.

Reply #4: Thanks for the suggestion. We have now expanded our discussion on the ML results, it now reads, “Nevertheless, the ML approach has demonstrated its great potential in identifying new key BrC species (such as 4-methylcoumarin, urocanate, etc here) as well as reaffirming the important role of known key BrC molecules (such as the nitrogen-containing aromatic molecules; such ML-identified list can be a useful reference for future studies. Of course, since there are multiple types of ML algorithms (such as supervised, unsupervised, semisupervised and reinforcement learning) with differing performances as well as advantages/pitfalls used in environmental research (Zhu et al., 2023), the rigorous, accurate, robust and also practicable ML analysis requires more research efforts and should be an active and important topic in the future. The ML approach can be a powerful and promising tool to achieve a quantitative closure between the BrC molecules and its total light absorption. ”