



Modeling of Glyphosate Speciation in Rumen Fluid of Cattle



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Introduction

Several publications, such as (1), hypothesize that glyphosate is a chelator, it was patented as one, and it limits absorption of minerals from the gastrointestinal tract. Glyphosate was never patented as a chelator (2) and these claims ignore the fact that there are several chemicals, including amino acids, that compete for formation of these bonds. Formation constants measure the strength of complexation between metal ions and ligands and can be used to model the speciation in mixtures of minerals, amino acids, VFAs, and glyphosate as they exist in the rumen.

Methods

Modeling of the various ion-ligand combinations was done at three pH values (5.8, 6.3 and 6.8) using published formation constants and concentrations of reported substances in rumen fluid:

- Ligands:
 - 19 amino acids
 - 4 fermentation endproducts (NH₃, acetate, butyrate, propionate)
 - Glyphosate (1X and 10X)
- Ions:
 - 6 minerals (trivalent and divalent)

References

1. Mertens, M., S. Höss, G. Neumann, J. Afzal, and W. Reichenbecher. 2018. Glyphosate, a chelating agent—relevant for ecological risk assessment? Environ. Sci. Pollut. Res. Int. 25:5298-5317.
2. Swarthout, J. T., M. S. Bleeker, and J. L. Vicini. 2018. Comments for Mertens et al. (2018), Glyphosate, a chelating agent—relevant for ecological risk assessment? Environ. Sci. Pollut. Res. Int. 25:27662-27663

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Results

Data for pH 6.3 are as follows. 99.99% of glyphosate is complexed with a mineral ion (86%) or with H⁺ (14%). But, as an example, 99.98% of Fe is complexed to His (99.975%). Charts of complexes for iron (Fig 1) and Cobalt (Fig 2) are shown for various conditions.

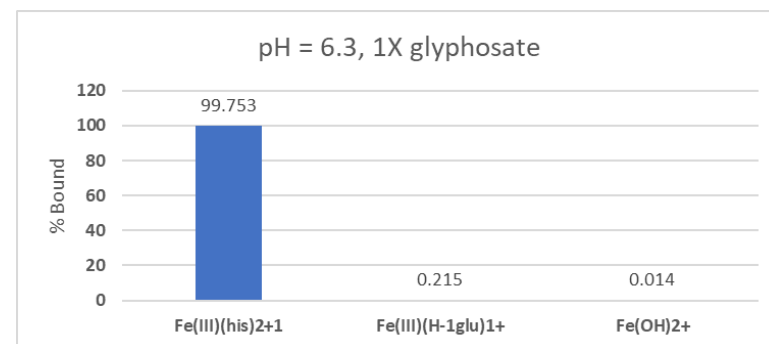


Fig 1. ligand-ion combinations modeled for iron in rumen fluid.

Conflict of Interest

JLV is an employee of Bayer Crop Science, which is a manufacturer of glyphosate based herbicides. WRH was paid for obtaining formation constants and doing the modeling.

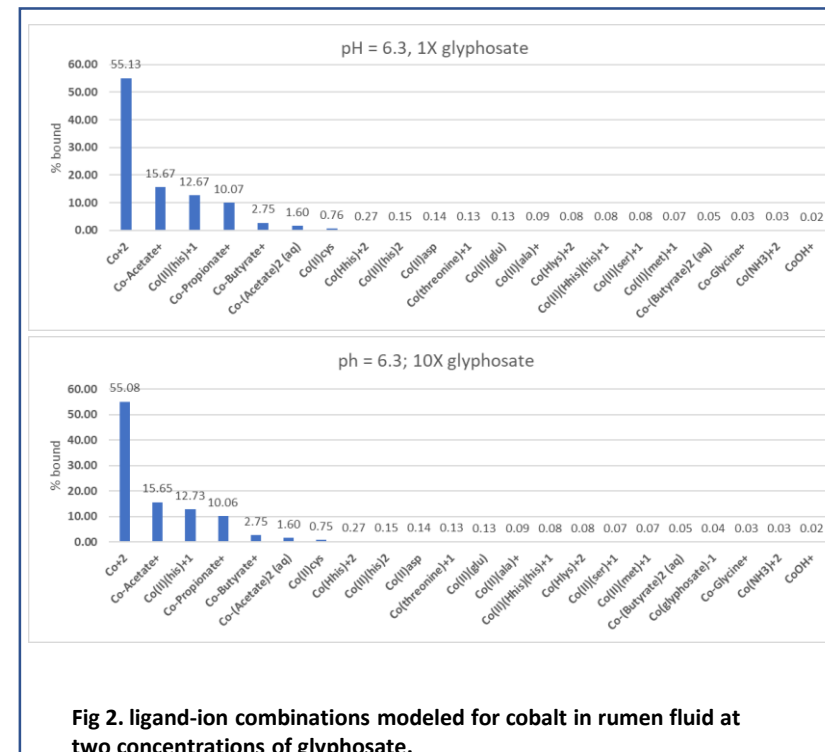


Fig 2. ligand-ion combinations modeled for cobalt in rumen fluid at two concentrations of glyphosate.

Conclusion

- Glyphosate is a chelator, but that by itself is not evidence that glyphosate inhibits absorption of a nutrient.
- Data from these models confirm that glyphosate is a relatively weak chelator compared to other molecules in the rumen such as amino acids and VFAs that should not have deleterious effects in the rumen.

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