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## Catalytic Neutralization of Organophosphate Simulant Over Undercoordinated Fe, Cu, Co, and Zn on SiO<sub>2</sub>

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# Catalytic neutralization of organophosphate simulant over undercoordinated Fe, Cu, Co, and Zn on SiO<sub>2</sub>

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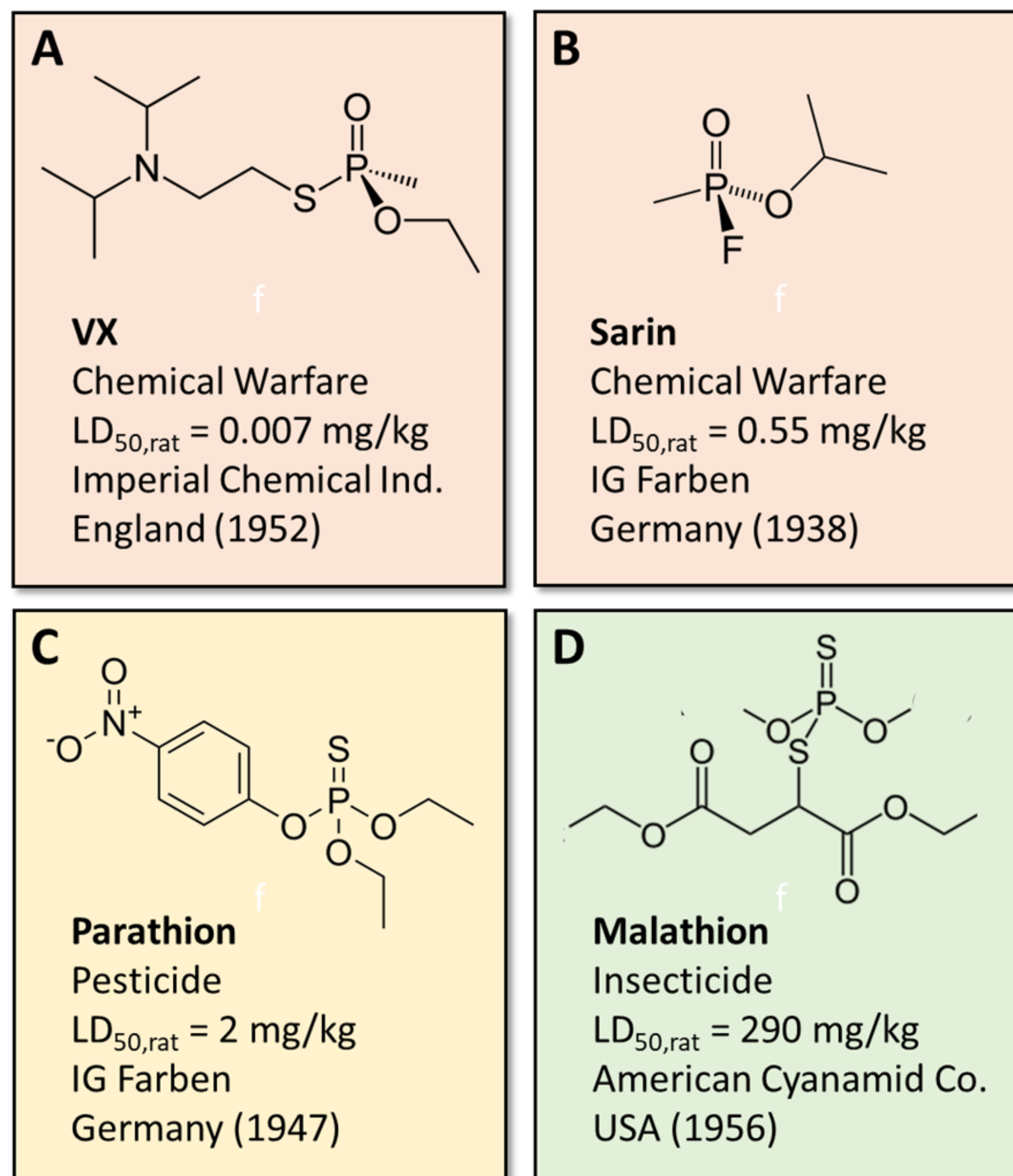
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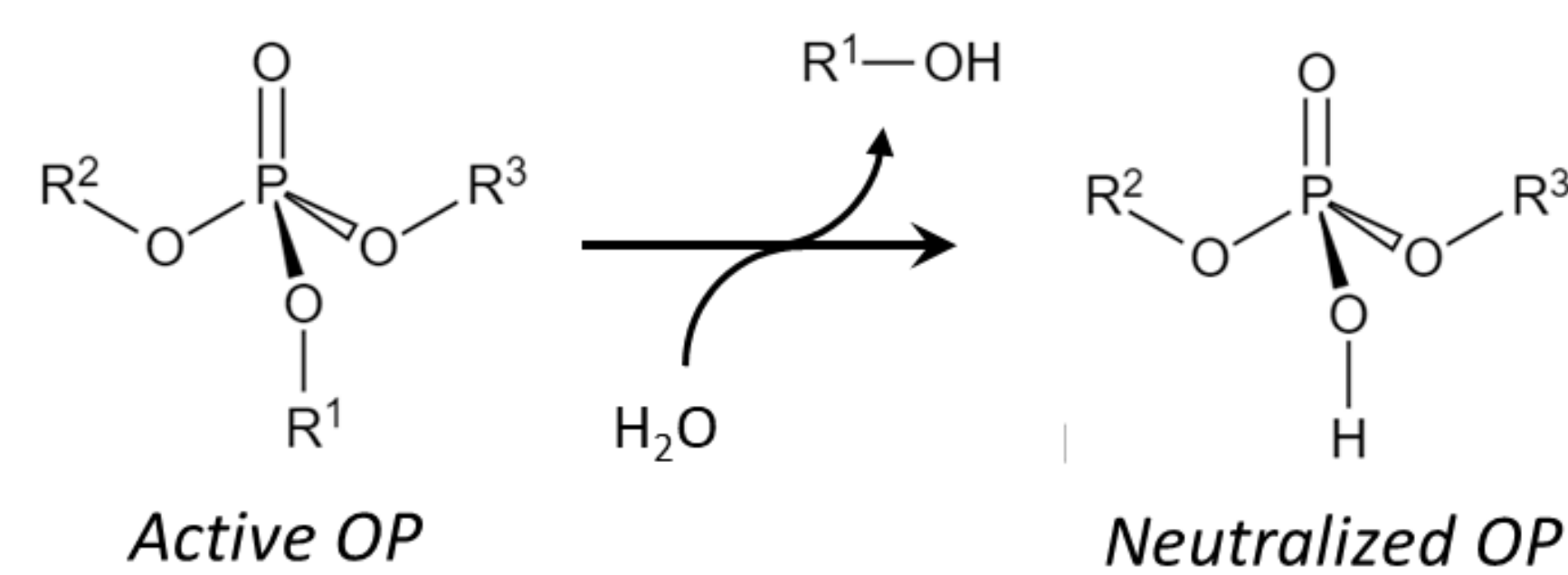


## Background

- Organophosphates (OP) inhibit normal breakdown of neurotransmitters

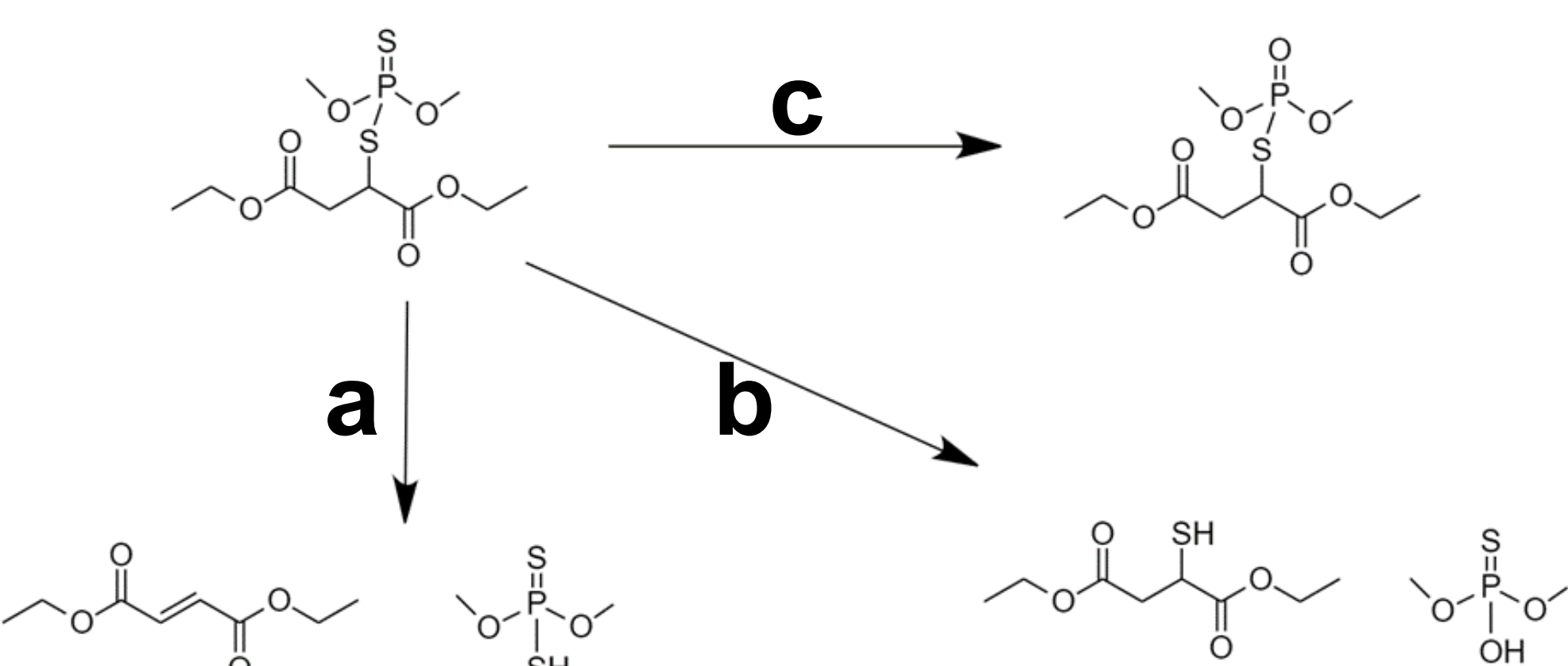


- Zn dimers, Zr clusters neutralize OP by hydrolyzing its best leaving group



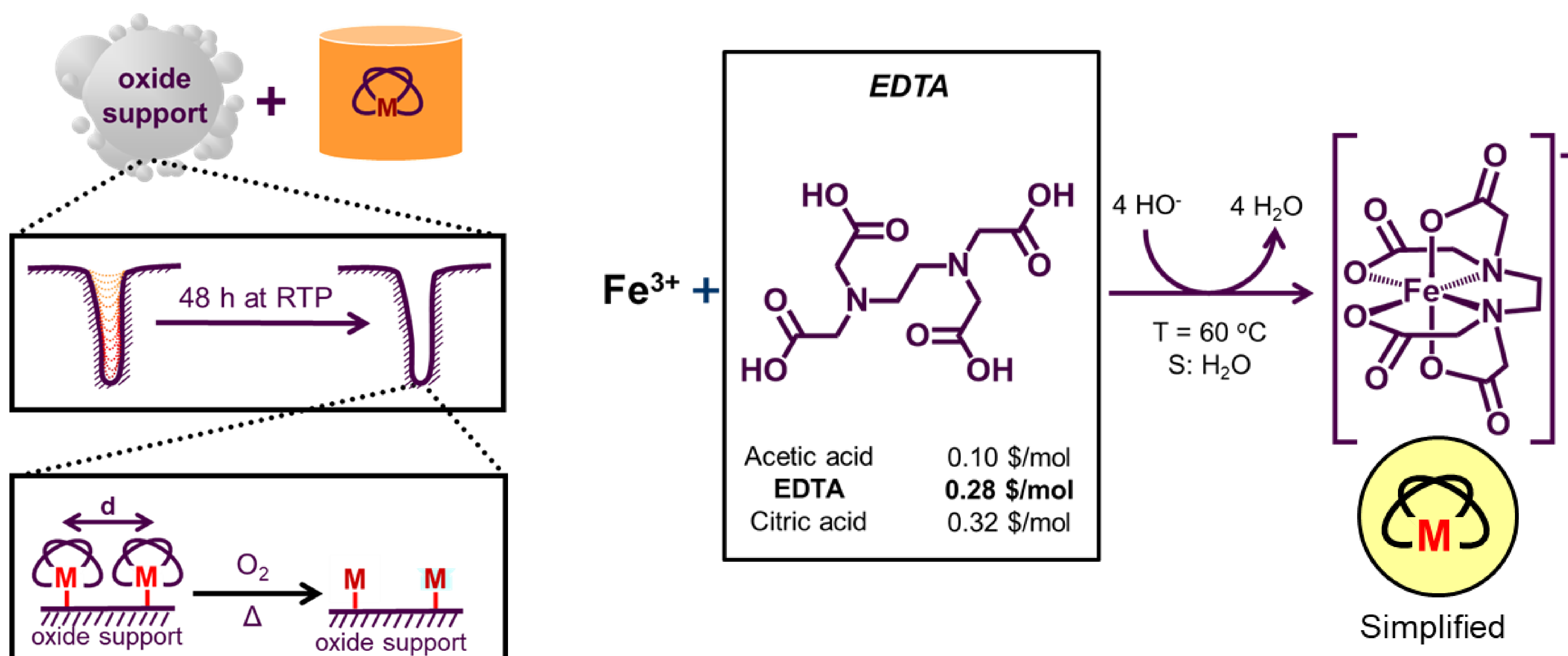
## Hypothesis

Low-coordination transition metals on SiO<sub>2</sub> will catalyze the hydrolysis of OP

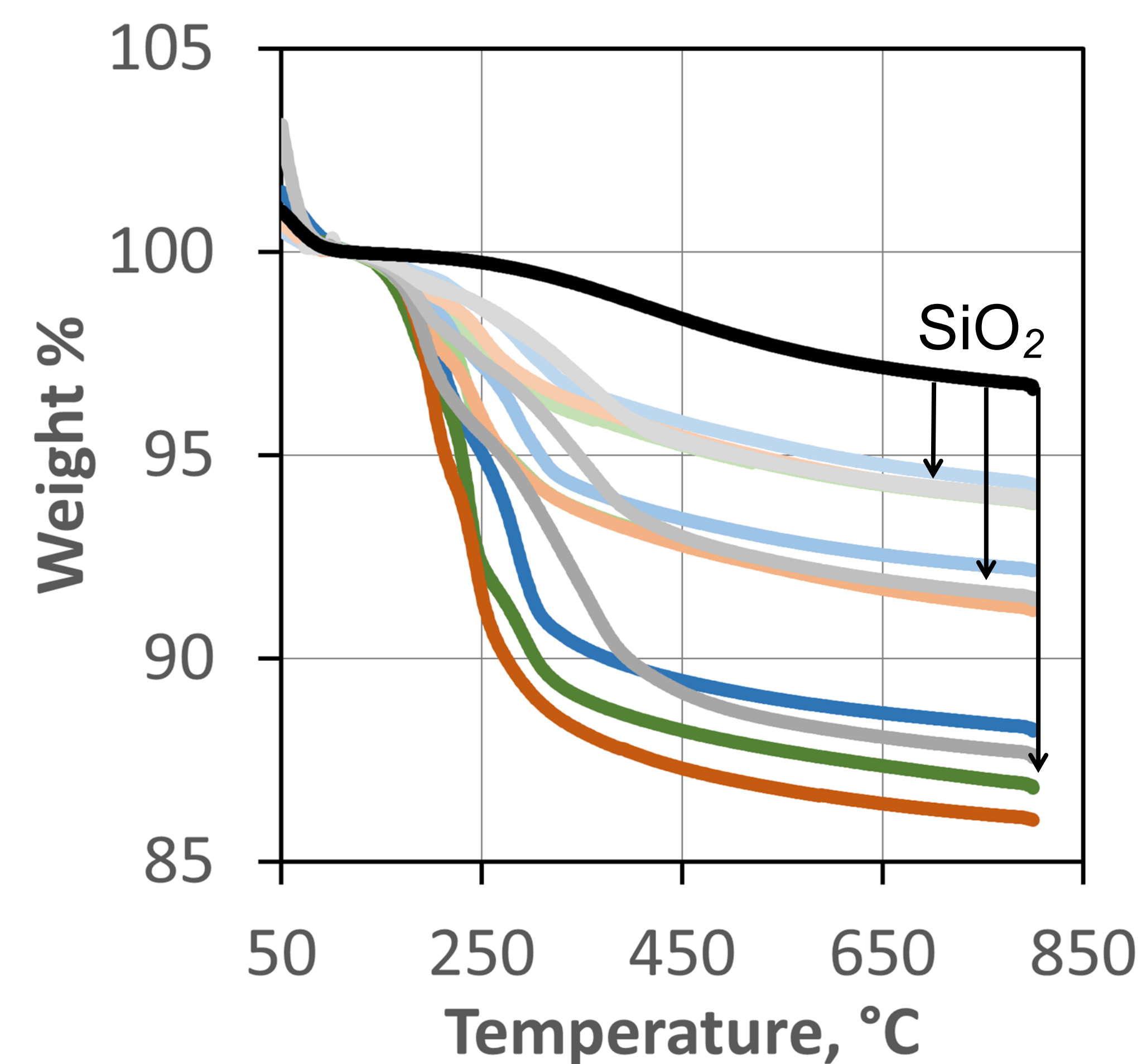


- 3 potential reactions; a & b preferred

## Simple, versatile, and scalable preparation of catalysts and precursors



## EDTA mass loss correlates to loading

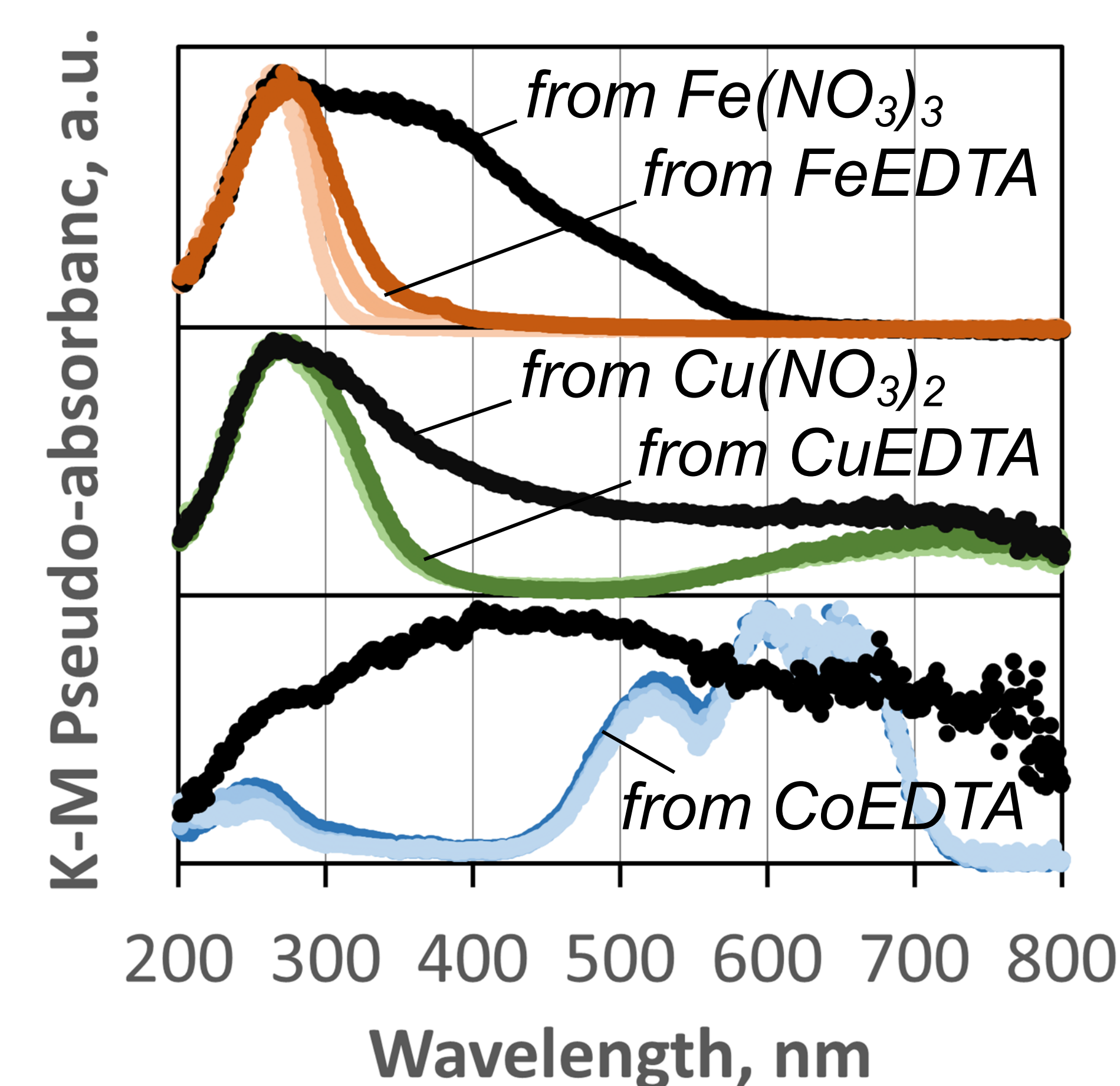


- Ligand mass loss as metal loading proxy
- Metal loadings of 0.6–2.4 wt%
- Surface density of 0.16–0.64 nm<sup>-2</sup>

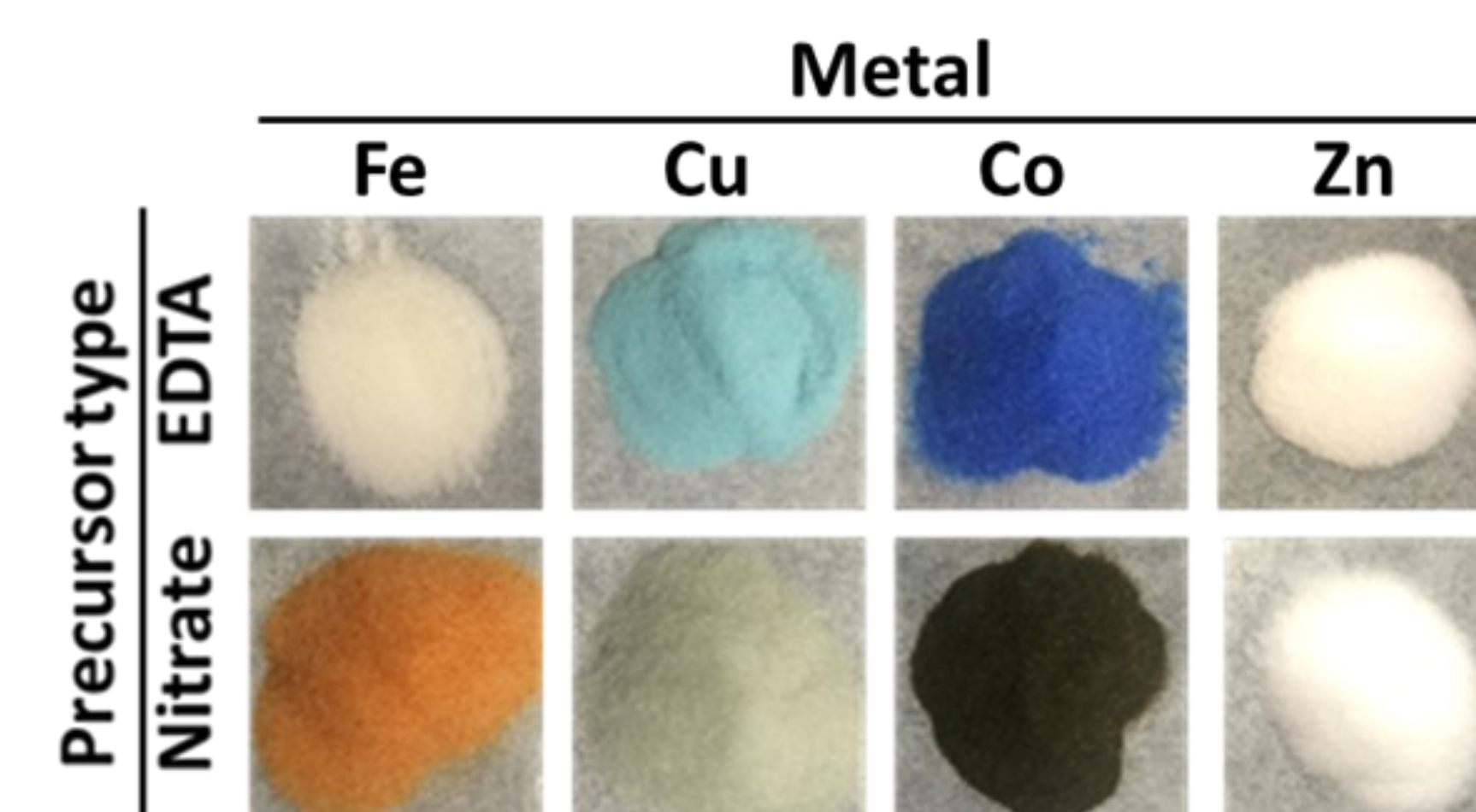
## Instruments

- TA Instruments TA500
- Agilent Cary60 + Pike Tech DiffusIR

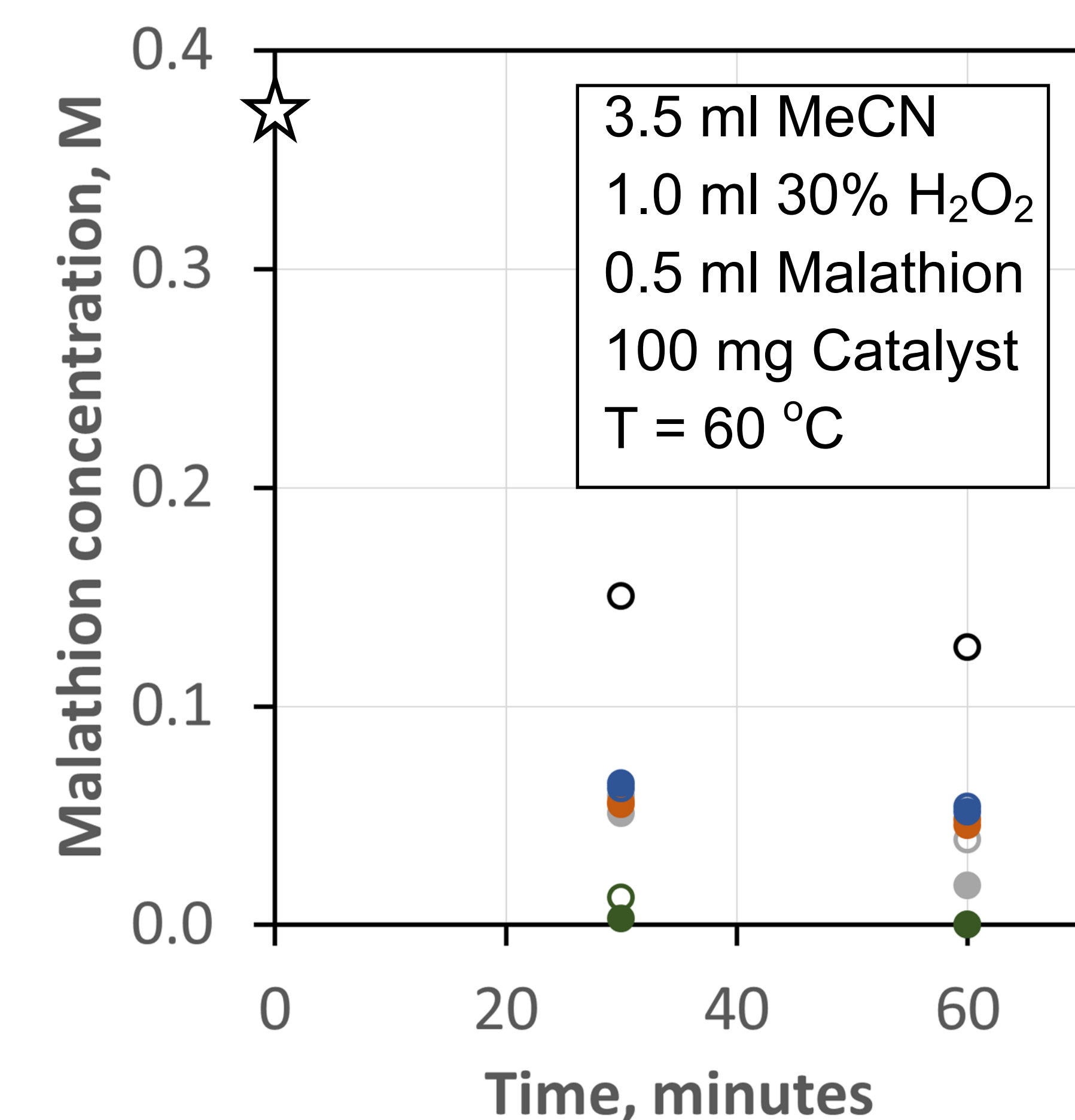
## EDTA promotes metal dispersion



- Higher dispersion relative to M-nitrates



## Catalytic OP neutralization w/ H<sub>2</sub>O<sub>2</sub>



- No reaction without H<sub>2</sub>O<sub>2</sub>
- No activity-precursor relations
- No selectivity-precursor relations
- ~ 1-to-1 reaction a to reaction b
- Activity increases Co = Fe < Zn < Cu

## Homogeneous reaction of OP with •OH

Instrument Shimadzu GC2030-FID/NPD

## References

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