## Supplementary Materials: Modeling of the Bioactivation of an Organic Nitrate by a Thiol to Form a Thionitrate Intermediate

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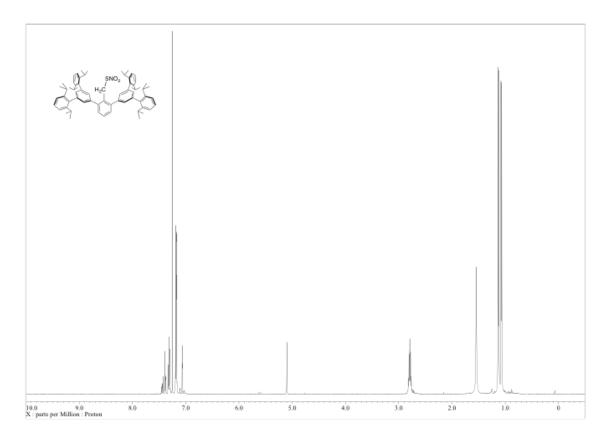


Figure S1. <sup>1</sup>H NMR (500 MHz) spectrum of compound 6 in CDCl<sub>3</sub>.

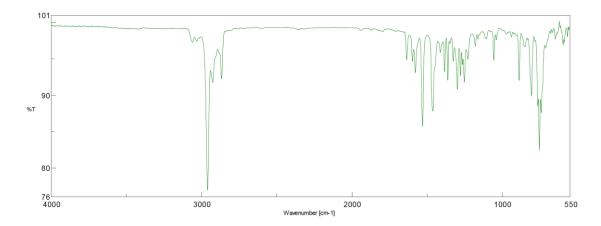


Figure S2. IR (ATR) spectrum of compound 6.