Supporting Information:

Inhibition of Mitochondrial Bioenergetics by Esterase-Triggered COS/H_2S Donors

Andrea K. Steiger,[a] Michela Marcatti,[b] Csaba Szabo,[b] Bartosz Szczesny,[b] Michael D. Pluth[a,*]

[a] Department of Chemistry and Biochemistry
Materials Science Institute
Institute of Molecular Biology
1253 University of Oregon
Eugene, OR 97403-1253.

[b] Department of Anesthesiology
University of Texas Medical Branch
Galveston, TX 77555, USA.

Contact Information:
Michael D. Pluth
pluth@uoregon.edu

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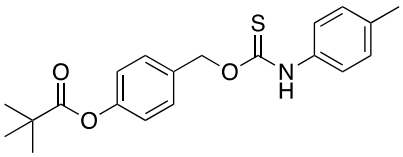
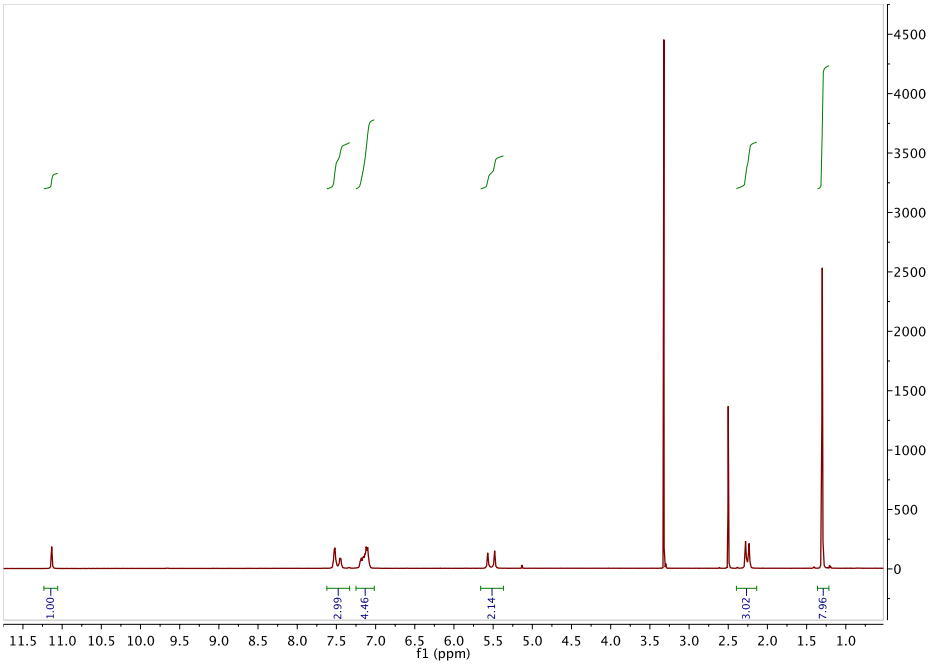
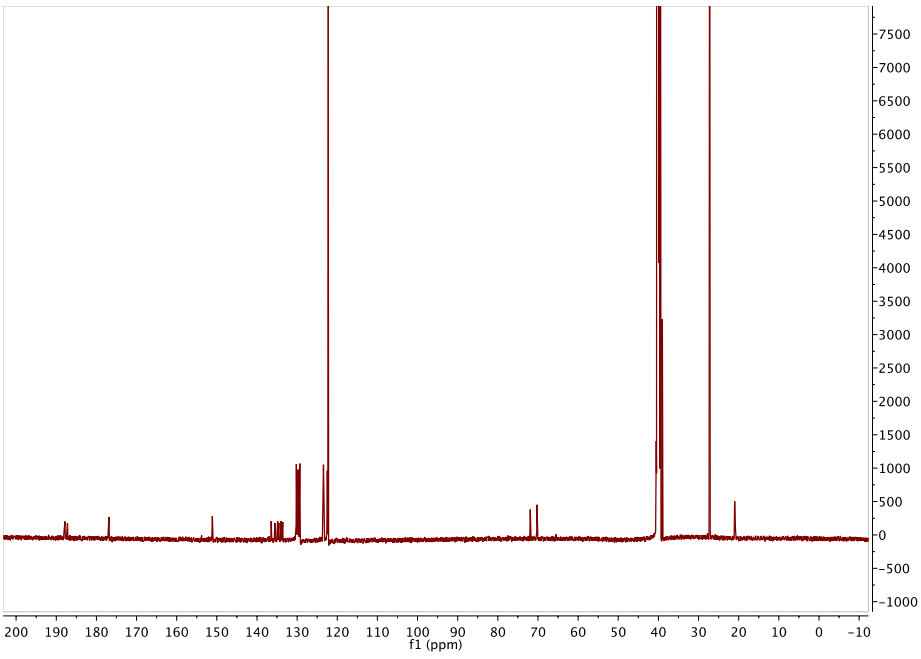
NMR Spectra

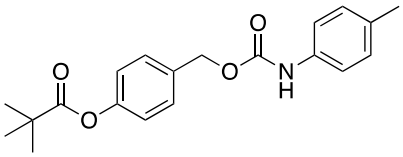
O-(4-pivaloylbenzyl)-*N*-(*p*-tolyl)thiocarbamate (1)

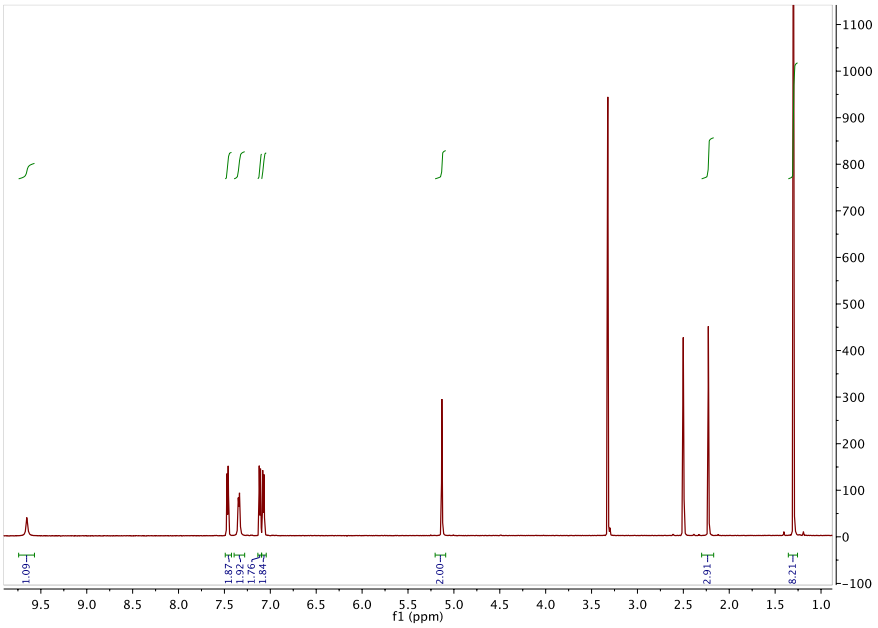


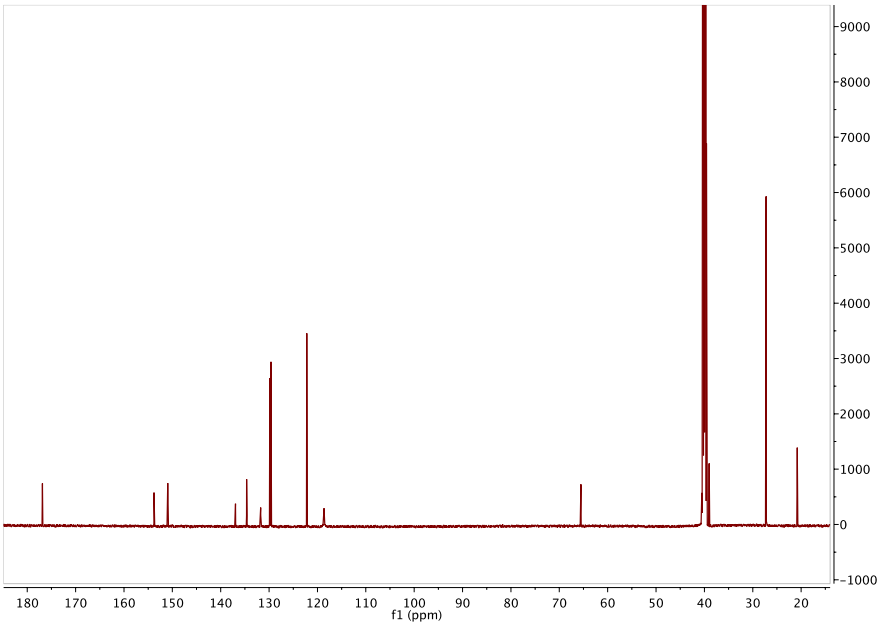




_O_-(4-pivaloylbenzyl)-_N_-(_p_-tolyl)carbamate (2)







Mass Spectrometry Data

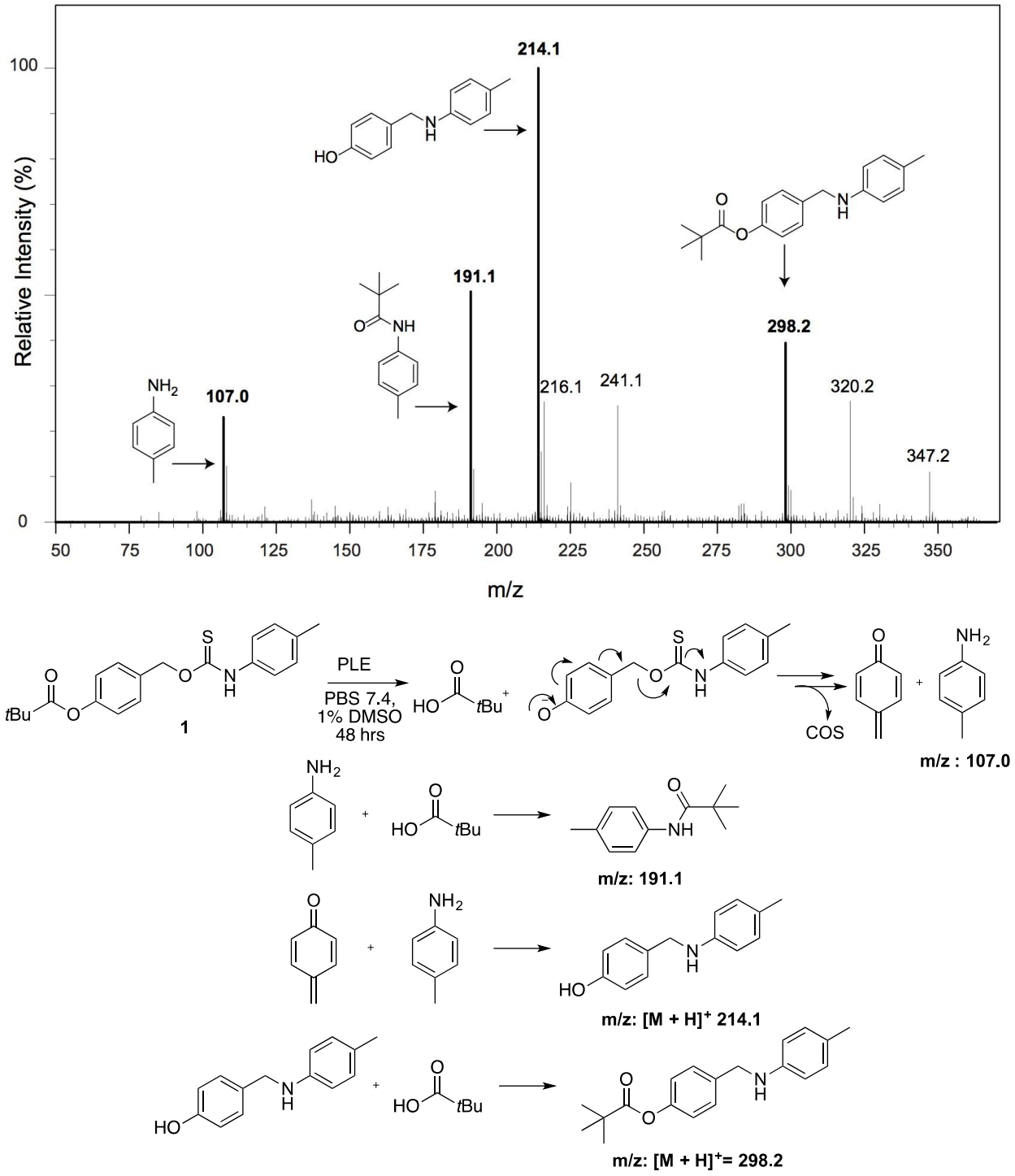


Figure S1. Mass spectrum of the reaction byproducts formed after stirring **1** with PLE in PBS buffer (pH 7.4, 1% DMSO) for 48 hours. Structures of potential byproducts have been labeled with their respective masses and reaction schemes detailing formation of these byproducts are shown.

Cytotoxicity of Na_2S

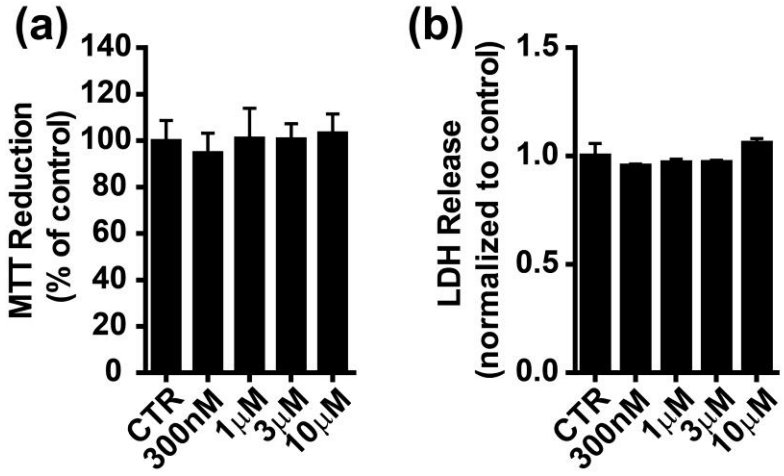


Figure S2. Cell viability studies of Na_2S in BEAS 2B cells using the (a) MTT and (b) LDH cell viability assays.

Cytotoxicity of 1 and 2 in HeLa cells

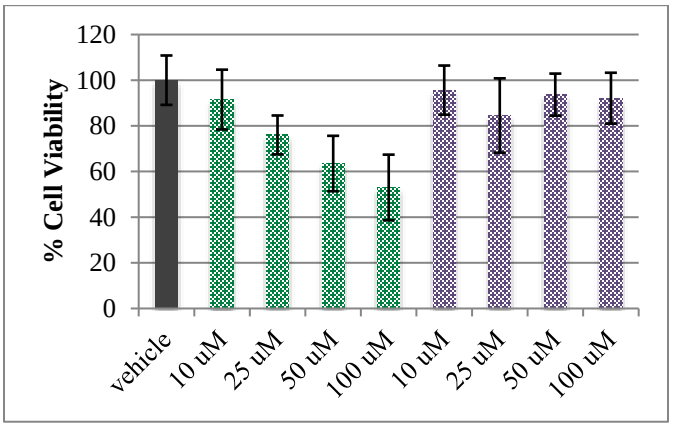


Figure S3. Cytotoxicity assay of donor **1** and control compound **2** in HeLa cells using the CCK-8 assay. HeLa cells were cultured in a 96-well plate overnight in Dulbecco's modified Eagle's medium (DMEM) supplemented with 10% fetal bovine serum (FBS) and 1% penicillin/streptomycin at 37 °C under 5% CO_2 and washed with PBS pH 7.4 prior to incubation in FBS-free DMEM containing vehicle (0.5% DMSO, black bar), **1** (green bars, 10-100 µM), or **2** (purple bars, 10-100 µM) for 1 hour. CCK-8 solution (10% in FBS-free DMEM) was added to each well, and cells were incubated for 3 hours at 37 °C. The absorbance at 450 nm was measured using a microplate reader. The cell viability was measured and normalized to the vehicle group. Results are expressed as mean ± SD (n=6).