OXIDATION OF 3,4-DIHYDROXYPHENYLACETALDEHYDE, A TOXIC DOPAMINERGIC METABOLITE, TO A SEMI-QUINONE RADICAL AND AN *ORTHO*-QUINONE

David G. Anderson[1], S. V. Santhana Mariappan[2], Garry R. Buettner[3], Jonathan A. Doorn[1]*

Division of Medicinal and Natural Products Chemistry, College of Pharmacy, University of Iowa, Iowa City, IA 52242-1112[1], Central High Field NMR Research Facility, Department of Chemistry, University of Iowa, Iowa City, IA 52242-1294[2], and Free Radical and Radiation Biology Program, ESR Facility, Department of Radiation Oncology, College of Medicine, University of Iowa, Iowa City, IA 52242-1101[3]

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Address Correspondence to: Jonathan A. Doorn, Ph. D., 115 So. Grand Ave, College of Pharmacy, Iowa City, IA 52242-1112. Telephone: 319-335-8834. Fax: 319-335-8766. Email: jonathan-doorn@uiowa.edu

Supplementary Tables

Supplementary Table 1. Summary of NMR Correlations and Cross-Peaks.

Experiment	Cross-Peaks Evident
COSY	H1-H2; H2-H4; H7-H8;
NOSEY	H1-H4; H1-H8; H2-H4; H2-H8; H4-H8;
HMQC	H1-C1; H2-C2; H4-C4; H7-C7; H8-C8;
HMBC	H2-C3; H4-C5; H7-C3; H7-C6; H8-C5;

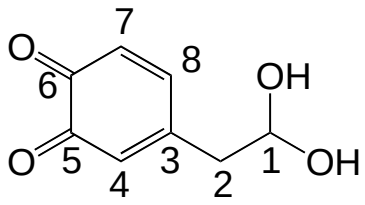
Supplementary Table 2. ^{1}H and ^{13}C Peak Assignments for the DOPAL quinone.

Position	^{1}H Shift	^{13}C Shift
1	5.17	89.8
2	2.65	44.4
3	n/a	152.5
4	6.24	128.8
5	n/a	181.0
6	n/a	180.3
7	7.20	144.1
8	6.28	128.9

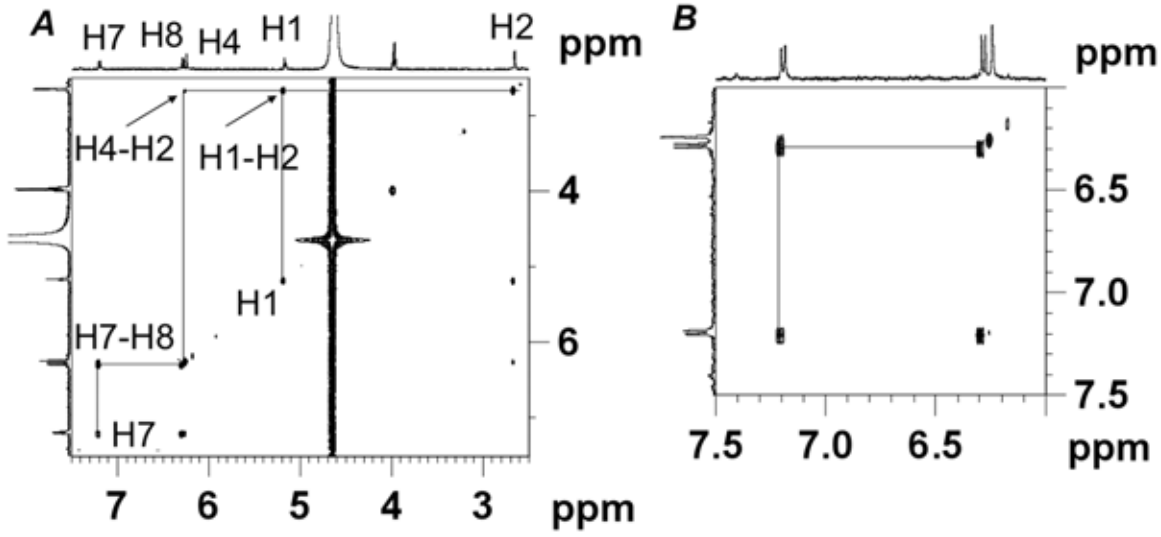
All values reported in ppm.

Supplementary Figures

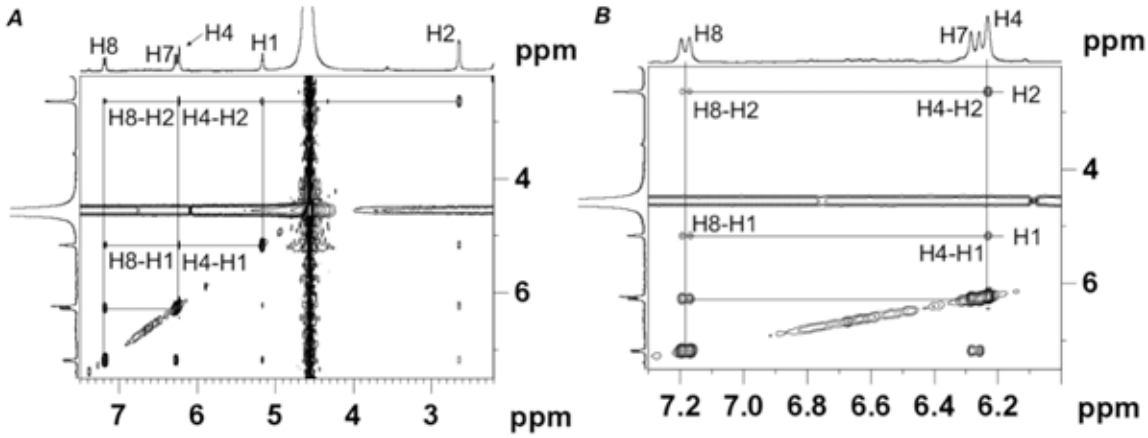
Supplementary Figure 1. Structure of the DOPAL-*ortho*-quinone. The numbered positions indicate atom locations for all supplementary figures.



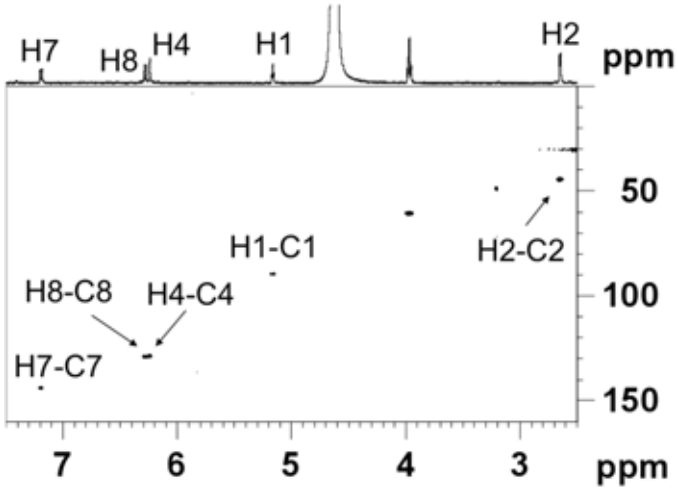
Supplementary Figure 2. ^{1}H-^{1}H COSY NMR Spectrum of Oxidized DOPAL. The figure is annotated to highlight relevant cross-peaks (***A***). The aromatic region is magnified for clarity (***B***). COSY is a homonuclear correlation technique for determining proton couplings in a molecule.



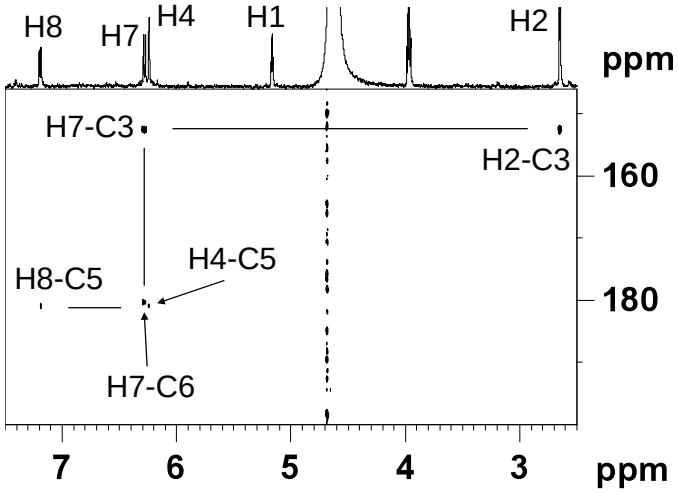
Supplementary Figure 3. ^{1}H-^{1}H NOSEY NMR Spectrum of Oxidized DOPAL. The spectrum is annotated to highlight relevant cross-peaks (***A***). The aromatic region is magnified for clarity (***B***). NOSEY is a homonuclear correlation technique for identifying resonances that are in close spatial proximity within a molecule.



Supplementary Figure 4. ^{1}H-^{13}C HMQC NMR Spectra of Oxidized DOPAL. The spectrum is annotated to highlight relevant cross-peaks. HMQC is a 2D inverse correlation technique for determining direct (single bond) heteronuclear couplings in a molecule.



Supplementary Figure 5. ^{1}H-^{13}C HMBC NMR Spectrum of Oxidized DOPAL. The spectrum is annotated to highlight relevant cross-peaks. HMBC is a 2D inverse correlation technique for determining long range (2-4 bond) heteronuclear couplings in a molecule.



Supplementary Figure 6. Lifetime of the DOPAL Quinone Over Time. The relative intensities of the 8.44 ppm peak (hypothesized polymer) and the quinone are shown over time.