Supplementary Materials: The Metabolic Fate of *Ortho*-Quinones Derived from Catecholamine Metabolites

Α В С D DOPE (1) DOPEG (2) DOPAC (3) DOMA (4) 1 0 min 0.8 0.8 0.8 0 min 0.8 0 min 0 min 2 min 2 min 2 min 2 min Absorbance 0.6 0.6 0.6 0.6 6 min 6 min 6 min 6 min 10 min 10 min 10 min 10 min 0.4 0.4 0.4 0.4 60 min 60 min 60 min 60 min 0.2 0.2 0.2 0.2 0 0 0 200 300 400 500 600 0 200 300 400 500 600 700 200 300 400 500 600 700 700 200 300 400 500 600 Wavelength (nm)

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Figure S1. Time course of the degrada1on of *ortho*-quinone products from catecholamine metabolites at pH 5.3. (**A**) DOPE (**1**); (**B**) DOPEG (**2**); (**C**) DOPAC (**3**); (**D**) DOMA. Each experiment was performed twice with similar results.



Figure S2. HPLC following the degrada1on of *ortho*-quinone products from catecholamine metabolites at pH 5.3. (**A**,**B**) DOPE (**1**); (**C**,**D**) DOPEG (**2**); (**E**,**F**) DOPAC (**3**); (**G**,**H**) DOMA. For **A**, **C**, **E** and **G**, the oxida1on was stopped by the addi1on of NaBH₄; For **B**, **D**, **F** and **H**, the oxida1on was stopped by the addi1on of clarity, the yields of DHBAld (7) were mul1plied by a factor of 5 in (**F**).

700



Figure S3. UV absorpton spectra of DOPEG (2) and 2-oxo-DOPE (5) obtained by oxidation of DOPE (1) and DOPEG (2), respectively. (A) Spectrum of DOPEG (2) obtained from DOPE (1) in comparison with those of DOPE and 6-hydroxydopamine; (B) Spectrum of 2-oxo-DOPE (5) obtained from DOPEG (2) in comparison with those of DOPEG and DHBAld (7). The spectrum of 6-hydroxydopamine was taken with the UV-VIS spectrophotometer, while the others were obtained from HPLC chromatograms analyzed for the wavelength indicated. Maximal absorbance values were normalized to 1.



Figure S4. HPLC chromatograms of (**A**) 2-oxo-DOPE (**5**) and (**B**) DOPEG (**2**) obtained after the NaBH₄ reduc1on of 2-oxo-DOPE. The same molar quan11es were injected for **A** and **B**.



Figure S5. ¹H-NMR spectrum of 2-oxo-DOPE (5). X is a peak derived from impurity.



Figure S6. ESI(+)/MS spectrum of 2-oxo-DOPE (5). X is a peak derived from impurity.