

Supplementary Materials

4-Hydroxybenzoic Acid as an Antiviral Product from Alkaline Autoxidation of Catechinic Acid: A Fact to Be Reviewed

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Table S1. SRM NI transitions (Q1 and Q3 masses), dwell time, retention time (t_R), and mass spectrometry parameters: Q1 Pre Bias, CE (Collision Energy), Q3 Pre Bias. The most three sensitive transitions for each species were monitored.

Analytes	Q1 (<i>m/z</i>)	Q3 (<i>m/z</i>)	Dwell time (ms)	t_R (min)	Q1 pre Bias (V)	CE (V)	Q3 pre Bias (V)
CA	289	245/109/203	43	0.87	11/30/15	15/19/27	11/20/10
4-HBA	137	93/65/137	43	1.86	10/10/10	20/27/10	13/11/14
(+)-catechin	289	245/109/203	43	1.98	14/16/11	16/24/19	11/10/13

Section S1. (+)-Catechin and Catechinic Acid (CA)

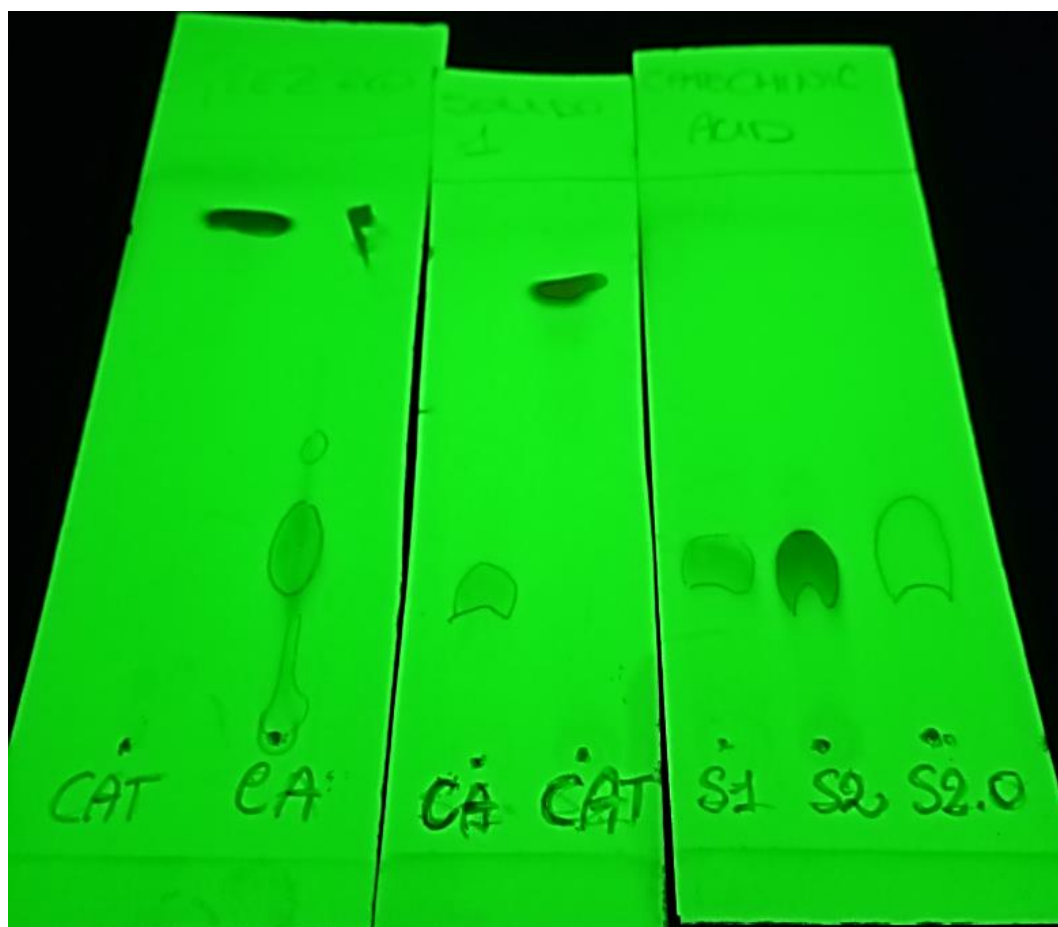


Figure S1. TLCs image observed at 254 nm (eluent ethyl acetate (EtOAc)/methanol (MeOH)/acetic acid (AcOH) 9/1/0.2 v/v/v). From the left: (+)-catechin (Rf. 0.82) and crude CA (Rf. 0.26); isolated CA and (+)-catechin; three samples of CA obtained by three different crystallizations from acetone/ethyl ether.

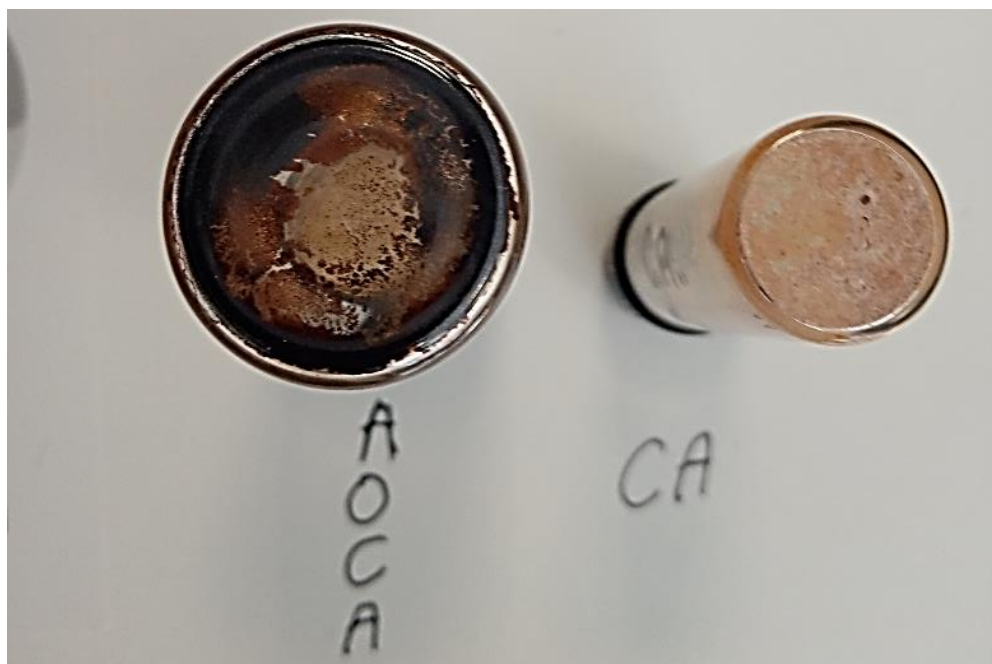


Figure S2. Aspect of the crystallized CA (right) and of the product of alkaline autooxidation of CA (AOCA).

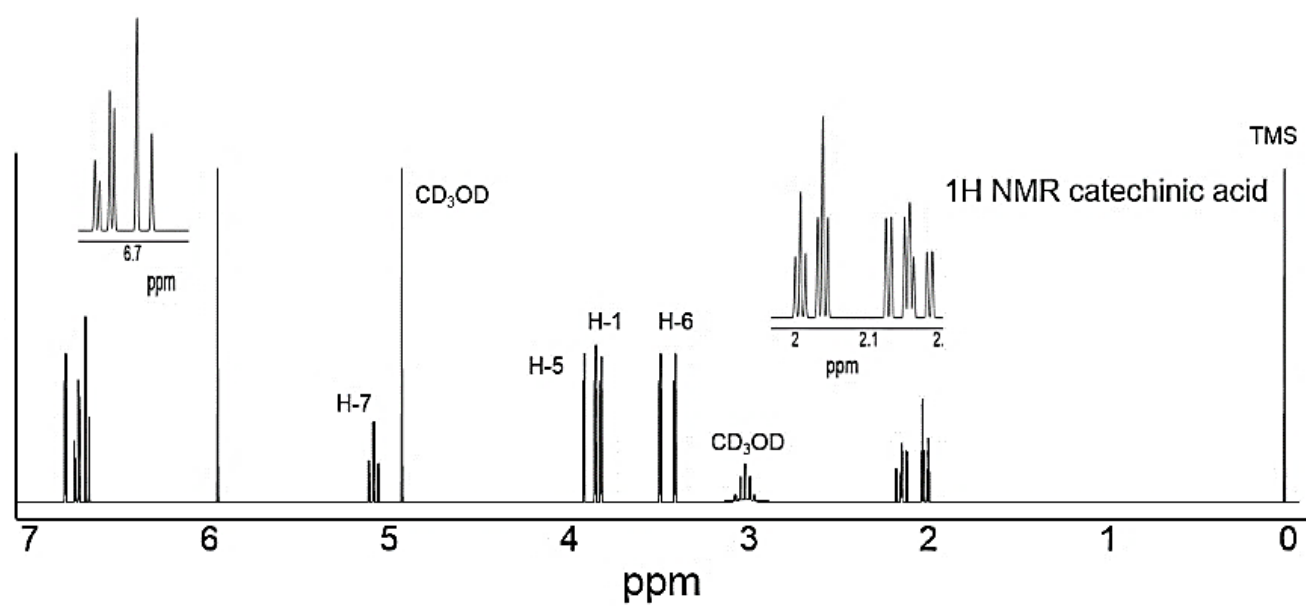


Figure S3. ^1H NMR (CD_3OD , 400 MHz) spectrum of CA.

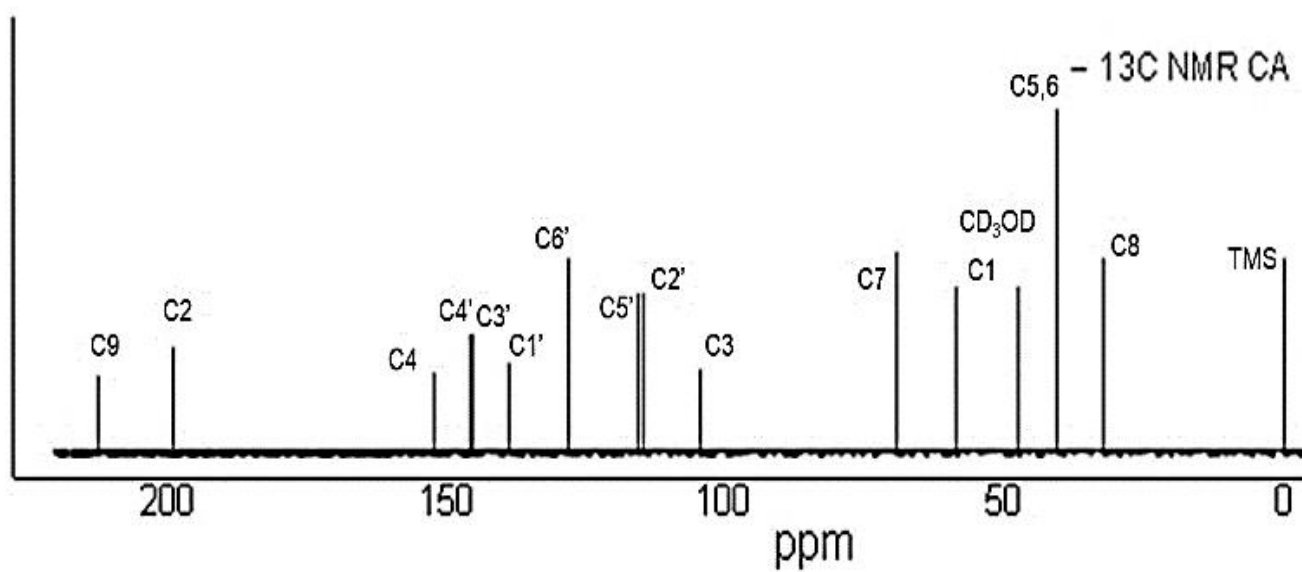


Figure S4. ¹³C NMR (CD₃OD, 100 MHz) spectrum of CA.

Section S2. AOCA vs 4-HBA

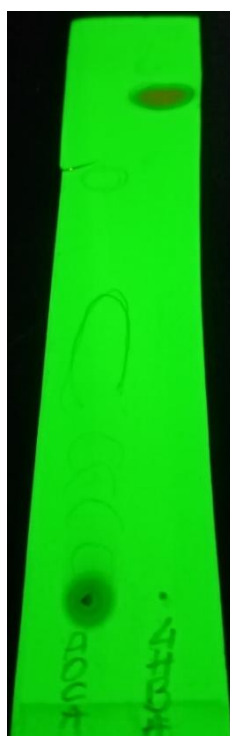


Figure S5. TLC analysis on AOCA and 4-HBA, taken as reference compound (detection at 254 nm) showing the absence of 4-HBA in AOCA.

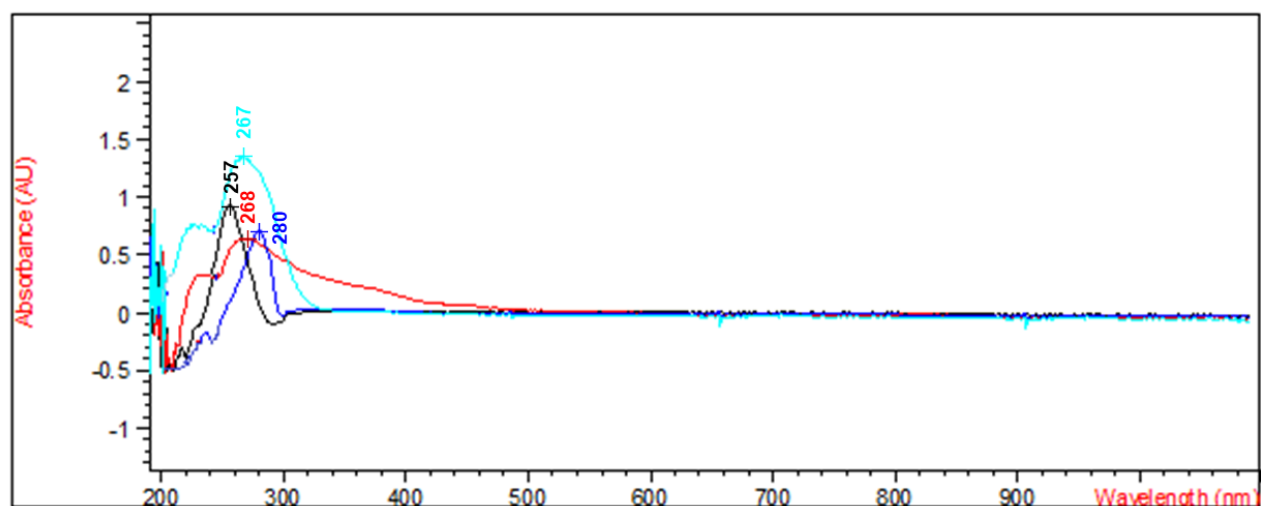


Figure S6. UV-Vis spectra of (+)-catechin (blue line), CA (light-blue line), AOCA (red line) and 4-HBA (black line).

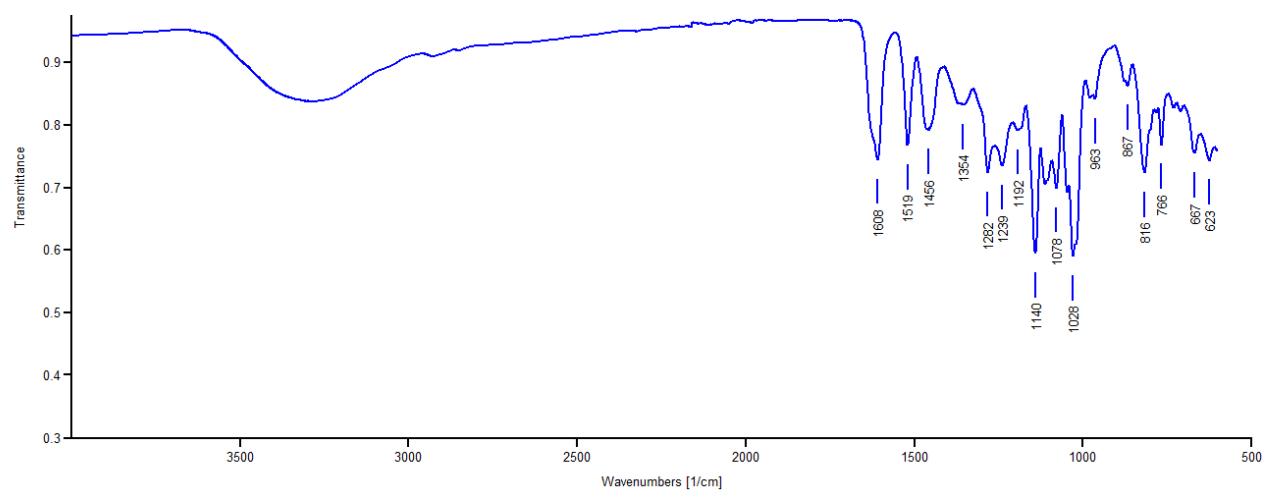


Figure S7. ATR-FTIR spectrum of (+)-catechin.

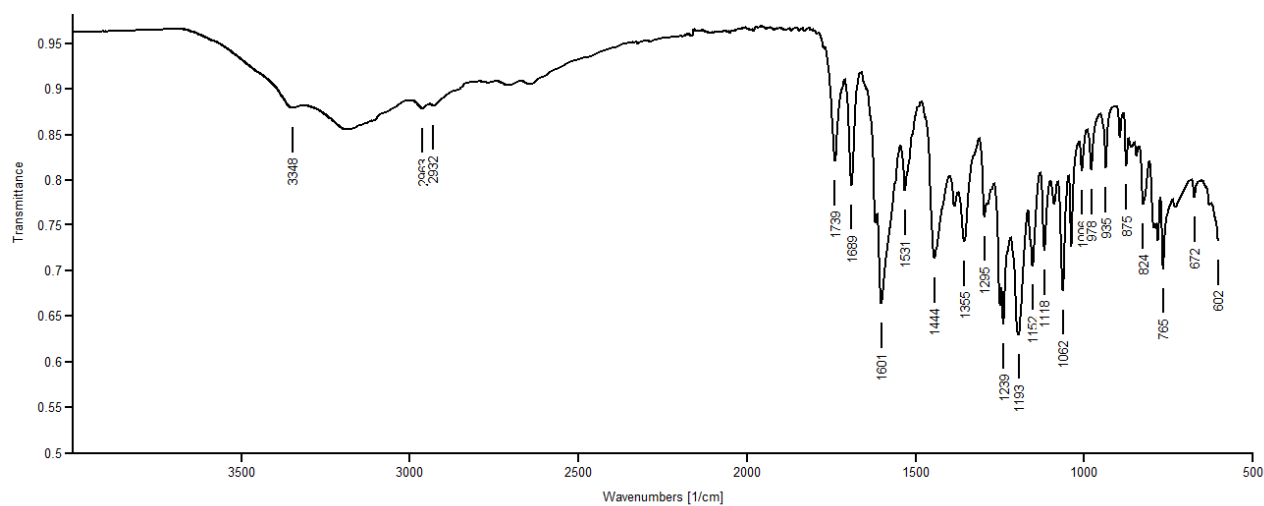


Figure S8. ATR-FTIR spectrum of CA.

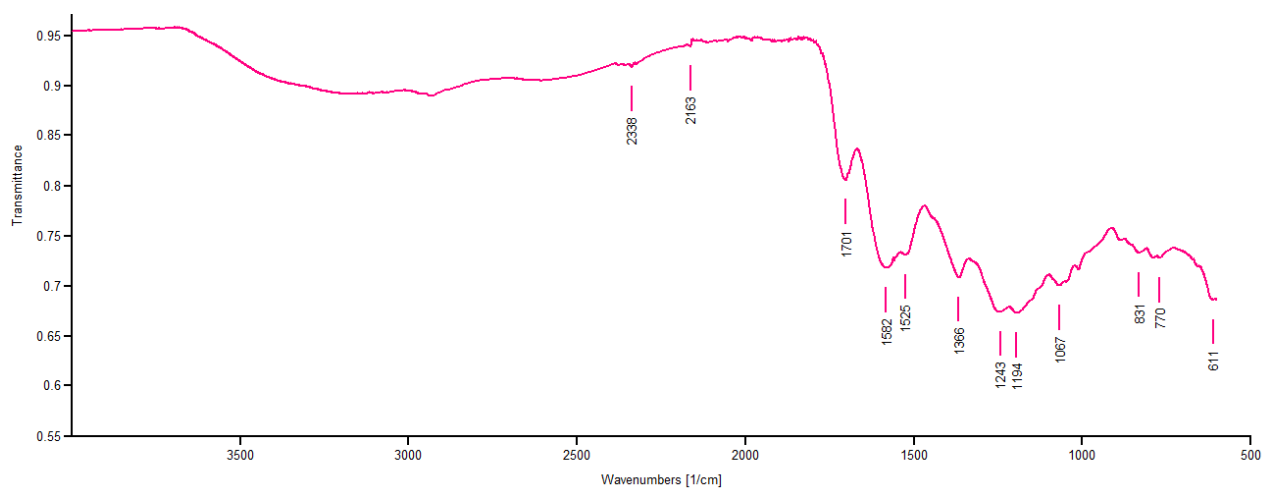


Figure S9. ATR-TFIR spectrum of AOCA.

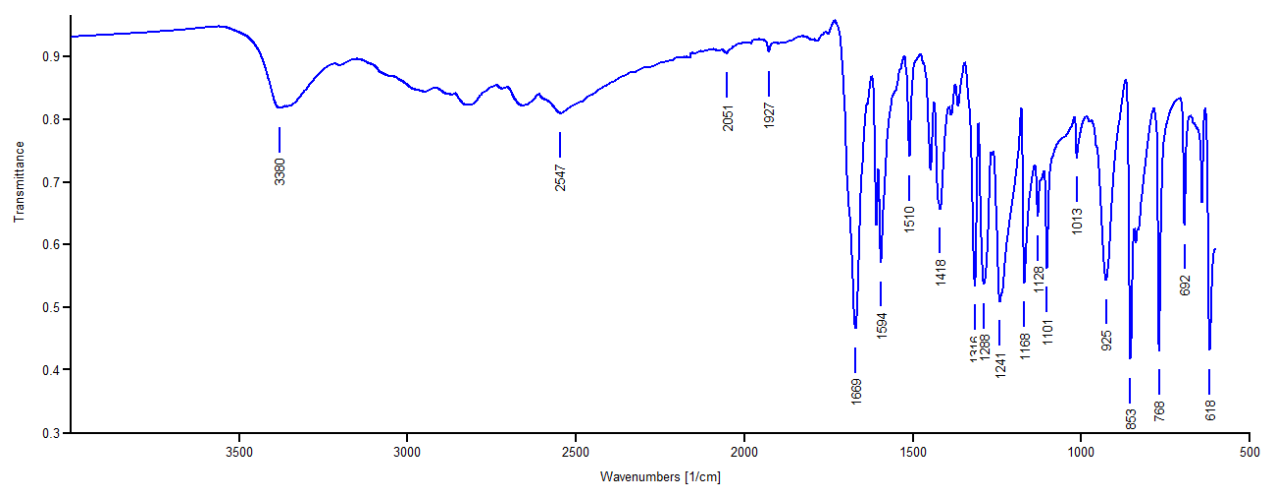


Figure S10. ATR-TFIR spectrum of 4-HBA.