Supporting Information

Corona discharge-induced reduction of quinones in negative electrospray ionization mass spectrometry

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Key word: Quinone reduction, Corona discharge, Negative electrospray ionization

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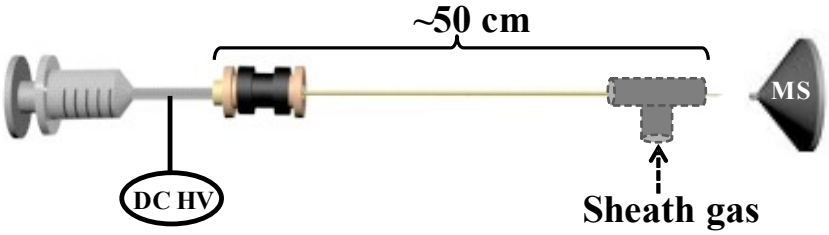

Fig. S1 Setup used in the experiment

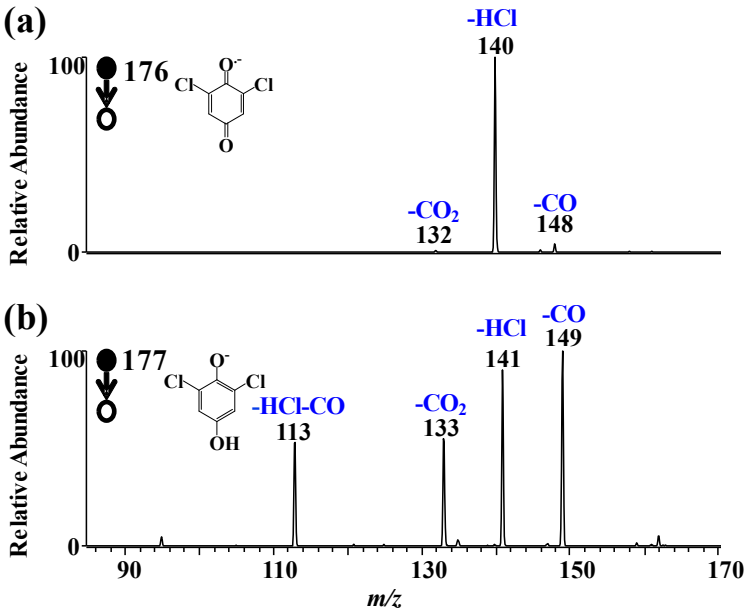

Fig. S2 MS/MS spectra of a) $M^{\cdot -}$ (*m/z* 176) and b) $[M + H]^-$ (*m/z* 177) ions of DCBQ

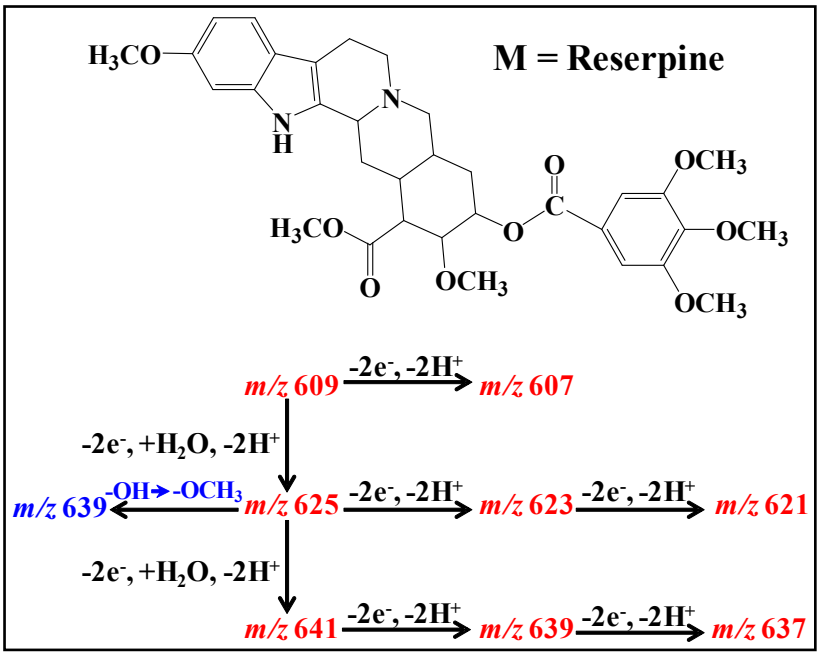

Fig. S3 Oxidation pathway of reserpine

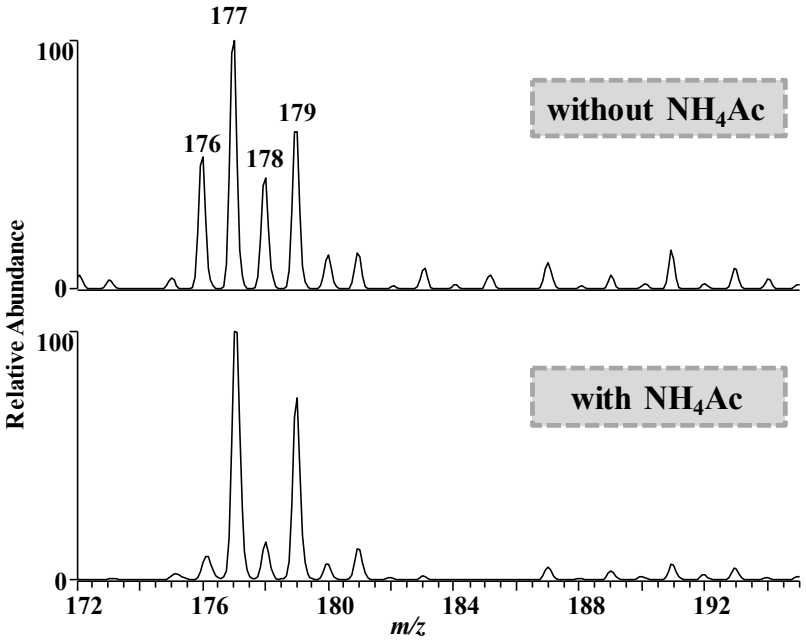

Fig. S4 Effect of NH_4Ac (5 mmol/L) on DCBQ (2 μg/mL in CH_3OH/H_2O (v/v, 1:1)) reduction during negative ESI MS. Spray voltage = 3 kV, flow rate = 2 μL/min.

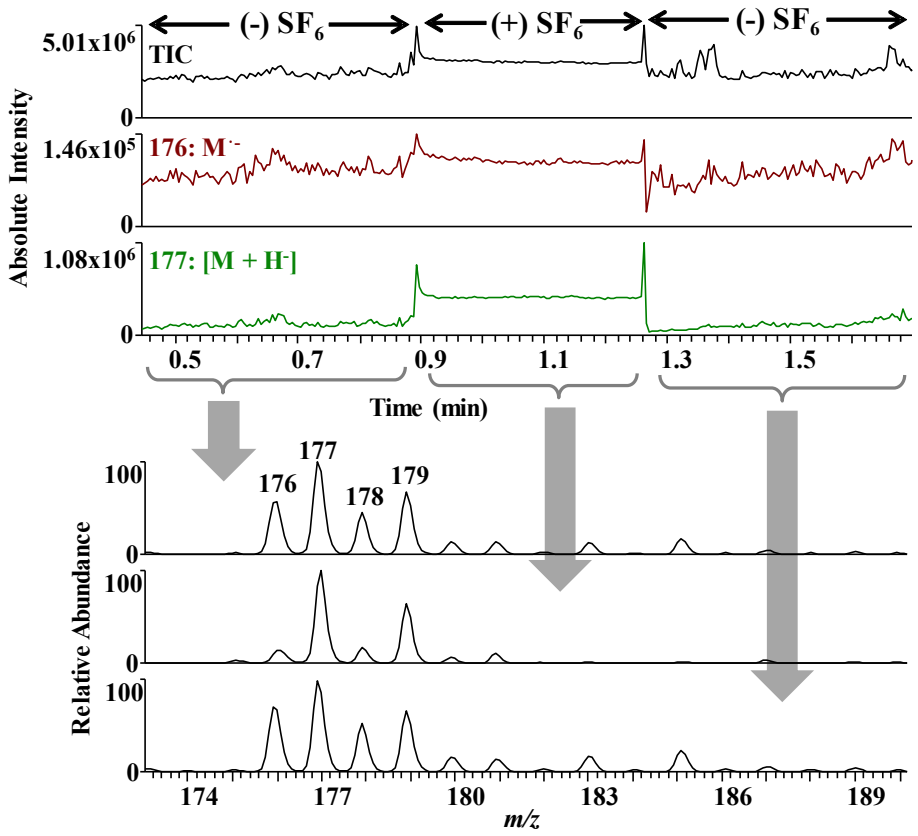

Fig. S5 Effect of sheath gas (SF_6) on DCBQ (2 μg/mL in CH_3OH/H_2O (v/v, 1:1)) reduction during negative ESI MS. Flow rate = 2 μL/min, spray voltage = 3 kV.

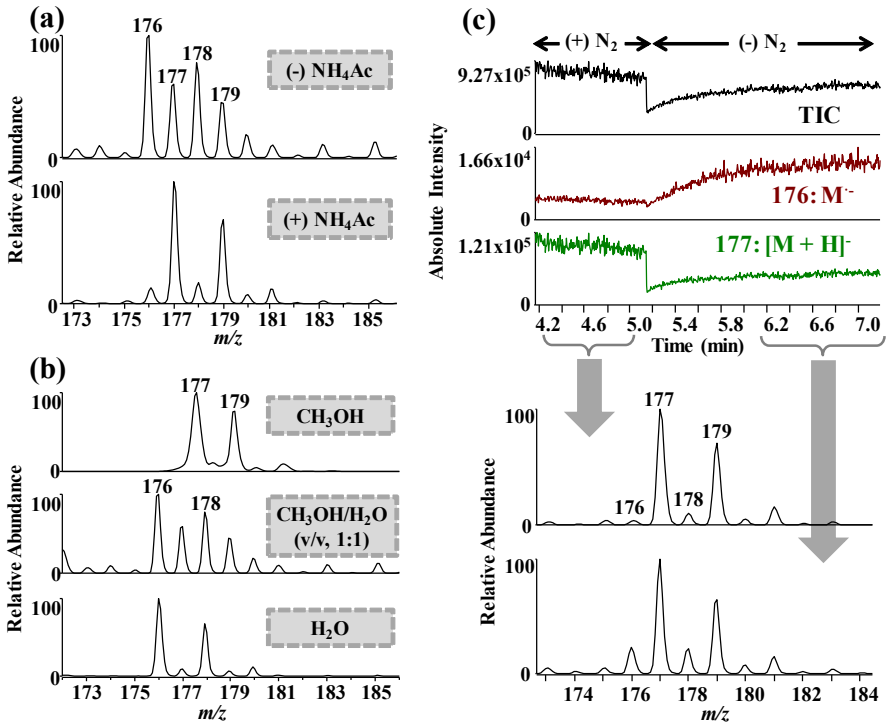

Fig. S6 Effect of a) NH_4Ac, b) solvent composition and c) sheath gas (N_2) on DCBQ (2 μg/mL) reduction during negative ESI MS with a commercial ESI source. Conditions: a) flow rate = 2 μL/min, spray voltage = 3 kV, solvent: CH_3OH/H_2O (v/v, 1:1), N_2 flow rate = 5 arb; b) flow rate = 2 μL/min, spray voltage = 3 kV, N_2 flow rate = 5 arb; c) flow rate = 2 μL/min, spray voltage = 5 kV, solvent: CH_3OH/H_2O (v/v, 1:1), C_{NH4Ac} = 5 mmol/L, N_2 flow rate = 5 arb.

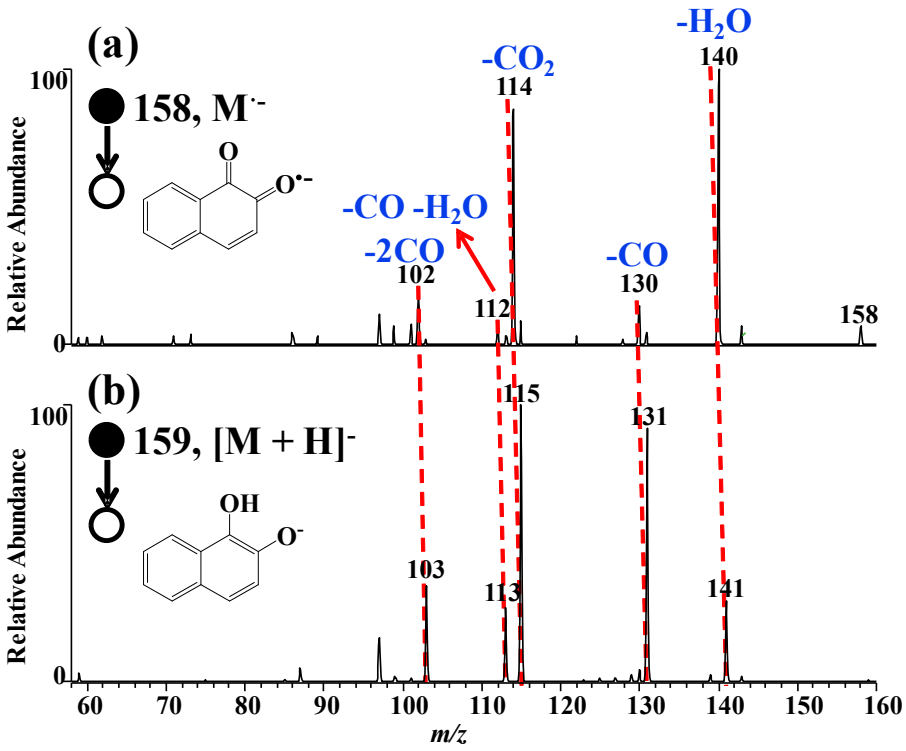

Fig. S7 MS/MS spectra of a) $M^{\cdot -}$ (*m/z* 158) and b) $[M + H]^-$ (*m/z* 159) ions of 1,2-NQ

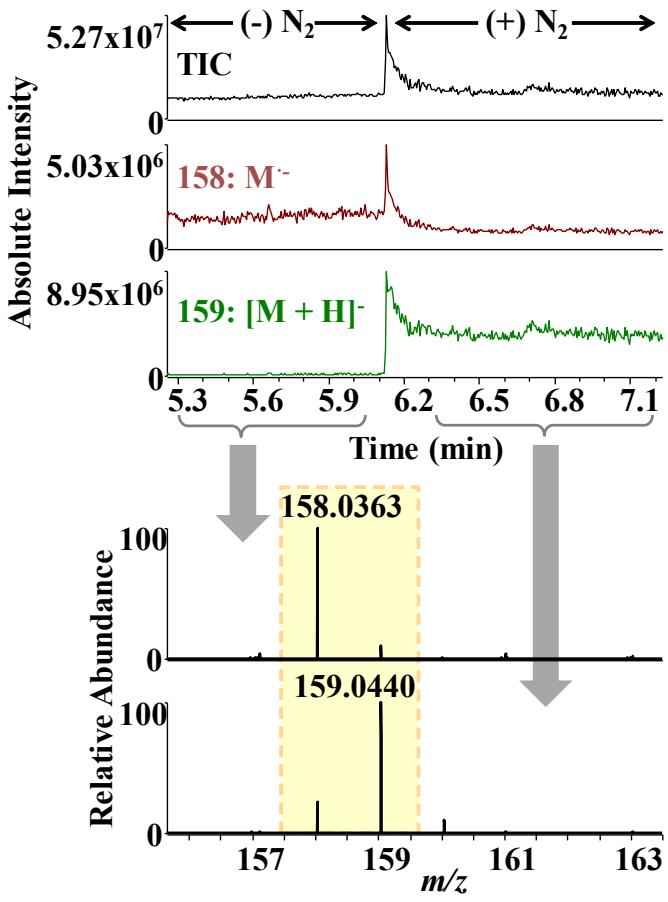

Fig. S8 Effect of sheath gas (N_2) on 1,2-NQ (5 μg/mL) reduction in a commercial ESI source with Orbitrap Exactive Plus mass spectrometer. Flow rate = 2 μL/min, spray voltage = 3 kV, solvent: CH_3OH/H_2O (v/v, 1:1), C_{NH4Ac} = 5 mmol/L.

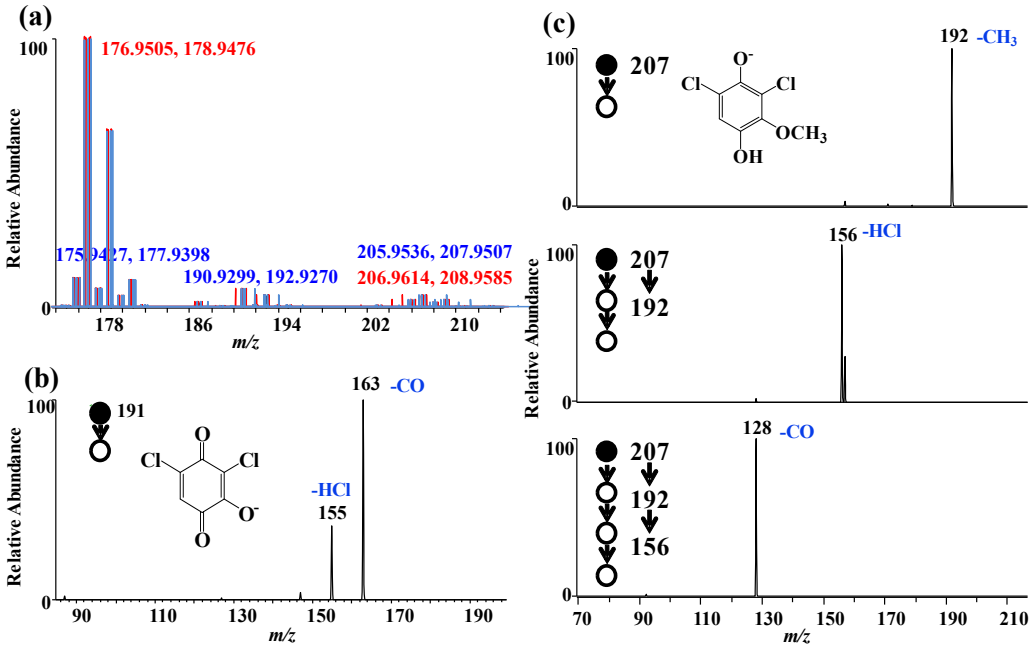

Fig. S9 a) High resolution and (b, c) MS^n mass spectra of DCBQ and the derivatives.