

SUPPORTING INFORMATION for “Desorption Electrospray Ionization Reactions Between Host Crown Ethers and the Influenza Neuraminidase Inhibitor Oseltamivir for the Rapid Screening of Tamiflu[®]”, by Leonard Nyadong, Edward G. Hohenstein, Kristin Johnson, C. David Sherrill, Michael D. Green, and Facundo M. Fernández.

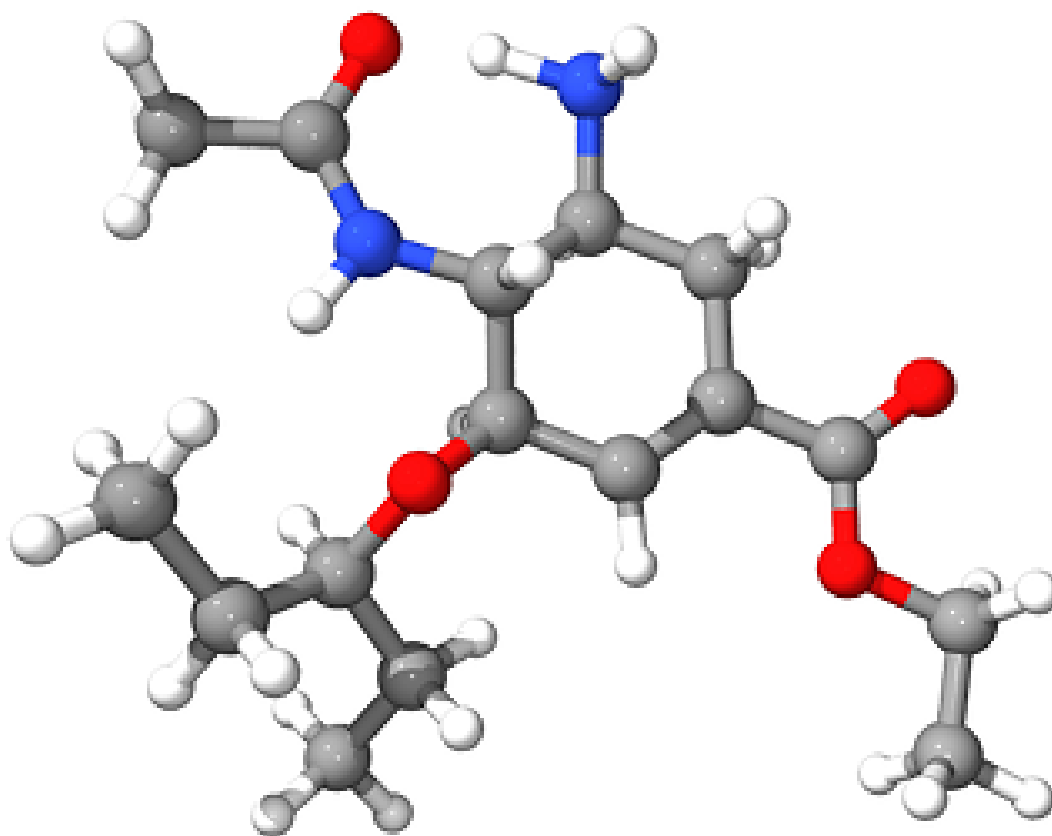


Figure S-1: Optimized structure of the protonated oseltamivir molecule from *ab initio* molecular modelling calculations.

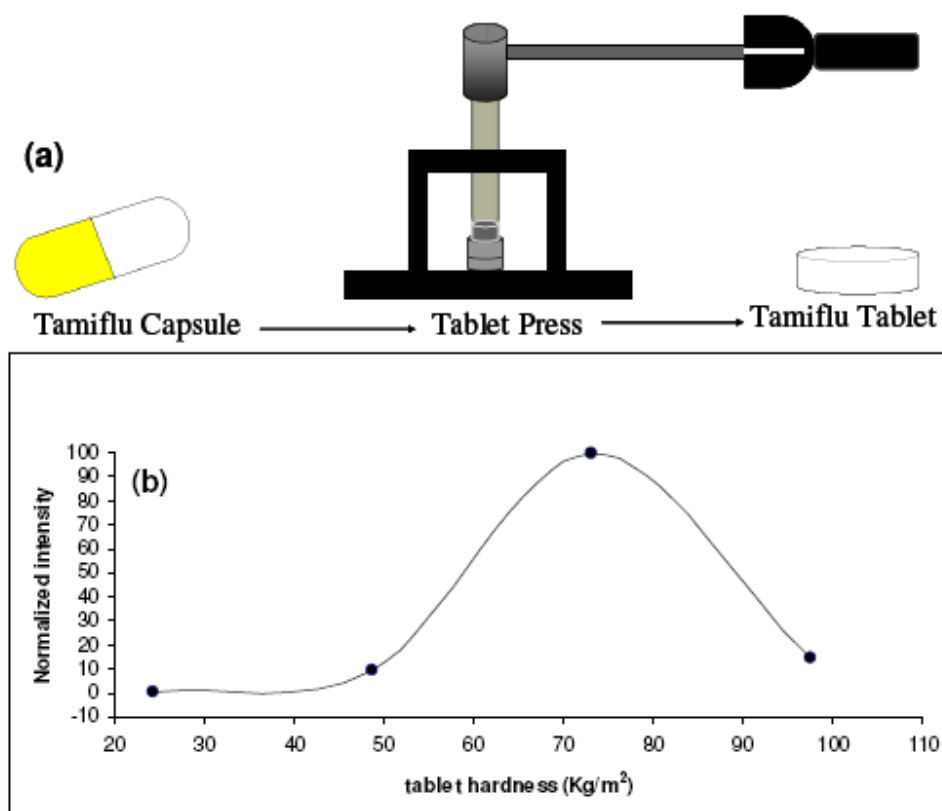


Figure S-2: (a) Samples were prepared by pressing the capsule content into a pellet at a hardness of $73 \pm 7 \text{ kg/m}^2$. (b) Dependence of the reserpine DESI signal intensity on pellet hardness. The DESI signal for the protonated reserpine molecule was normalized to that of the maximum signal.

Table S-1: Comparison of the robustness of the absolute DESI signal versus the signal intensity ratio of two different oseltamivir-crown ether complexes. Reactive DESI was performed by interrogating a genuine Tamiflu[®] capsule, pressed into a tablet, with an equimolar concentration (10 μ M) of 18-C-6 and 15-C-5 in neat acetonitrile.

DESI variable	RSD (%)	
	$I_{577} + I_{533}$	I_{577}/I_{533}
Solution flow rate (5-10 μ L min ⁻¹)	36.5	15.0
Nebulizer gas pressure (50-250 psi)	40.5	7.9
Tip-to-surface distance, d_1 (1-6 mm)	138.2	9.3
Spectrometer orifice-to-surface distance, d_2 (0.8–1.5 mm)	81.7	8.1
Sample-to-spectrometer orifice distance, x (2-7 mm)	30.1	10.3
Spray incident angle, α (50°-90°)	46.0	8.3