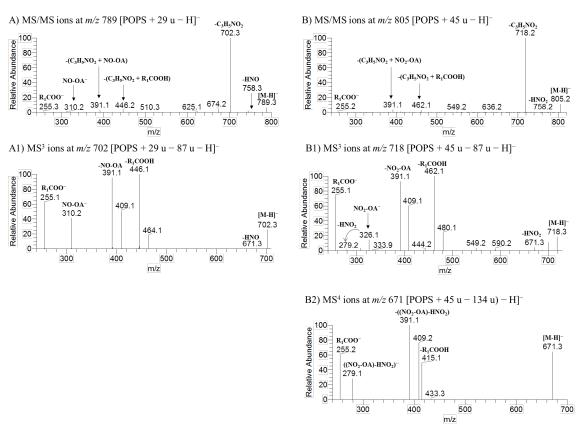
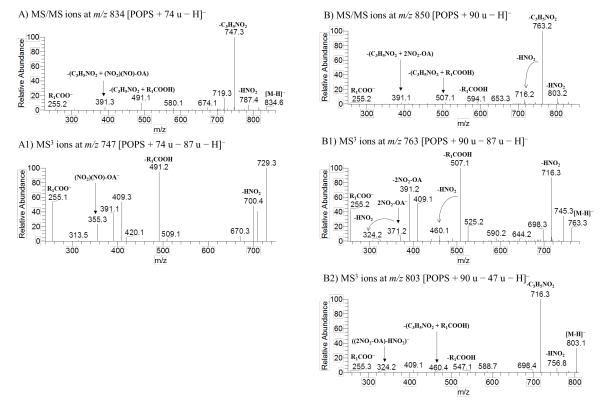
## Profile of Phosphatidylserine Modifications under Nitroxidative Stress Conditions Using a Liquid Chromatography-Mass Spectrometry Based Approach

Bruna Neves <sup>1</sup>, Pedro Domingues <sup>1</sup>, Maria Manuel Oliveira <sup>2</sup>, Maria do Rosário Domingues <sup>1,3</sup> and Tânia Melo <sup>1,\*</sup>

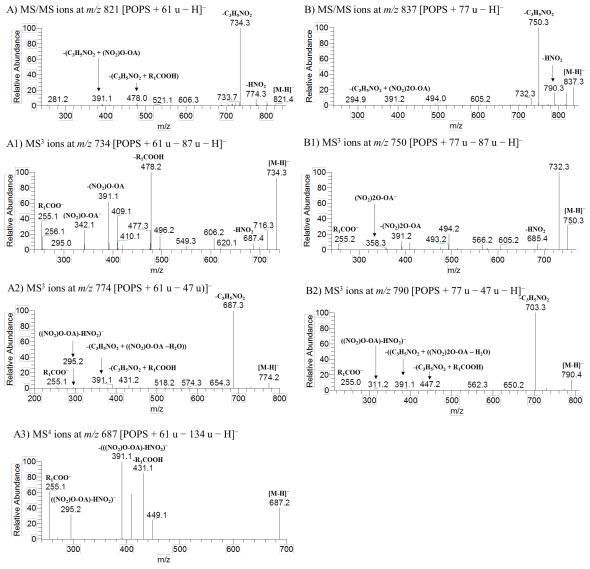
- <sup>1</sup> Mass Spectrometry Centre, UI QOPNA, Chemistry Department, University of Aveiro, 3810-193 Aveiro, Portugal; brunafbneves@gmail.com (B.N.); p.domingues@ua.pt (P.D.); mrd@ua.pt (M.R.D.)
- <sup>2</sup> Chemistry Department, University of Trás-os-Montes e Alto Douro, 5000-801 Vila Real, Portugal; mmso@utad.pt
- <sup>3</sup> Biology Department & CESAM & ECOMARE, University of Aveiro, 3810-193 Aveiro, Portugal
- \* Correspondence: <u>taniamelo@ua.pt</u>; Tel.: +351 23508



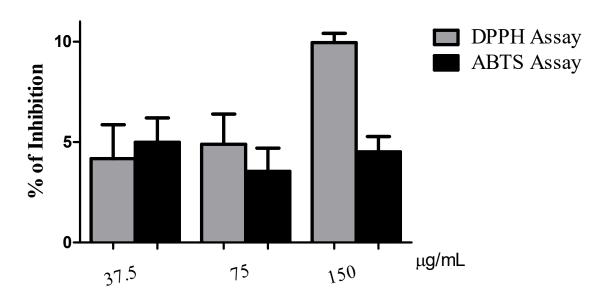
**Figure S1.** ESI-MS/MS spectra obtained in Linear Ion Trap of the  $[M - H]^-$  ions at m/z 789.3 corresponding to  $[POPS + 29 \text{ u} - H]^-$  (A), and at m/z 805.2 corresponding to  $[POPS + 45 \text{ u} - H]^-$  (B). MS<sup>3</sup> of ions at m/z 702.3 (A1) and m/z 718.3 (B1) that correspond, respectively, to  $[POPS + 29 \text{ u} - 87 \text{ u} - H]^-$  and  $[POPS + 45 \text{ u} - 87 \text{ u} - H]^-$  were also shown.



**Figure S2.** ESI-MS/MS spectra obtained in Linear Ion Trap of  $[M - H]^-$  ions at m/z 834.6 corresponding to  $[POPS + 74 \text{ u} - H]^-$  (A), and at m/z 850.3 corresponding to  $[POPS + 90 \text{ u} - H]^-$  (B). MS³ of ions at m/z 747.3 (A1) assigned as  $[POPS + 74 \text{ u} - 87 \text{ u} - H]^-$ , at m/z 763.3 (B1) that correspond to  $[POPS + 90 \text{ u} - 87 \text{ u} - H]^-$ , and at m/z 803.1 attributed to  $[POPS + 90 \text{ u} - HNO_2 - H]^-$  were also shown.



**Figure S3.** ESI-MS/MS spectra obtained in Linear Ion Trap of  $[M - H]^-$  ions at m/z 821.4 corresponding to  $[POPS + 61 \text{ u} - H]^-$  (A), and at m/z 837.3 corresponding to  $[POPS + 77 \text{ u} - H]^-$  (B). MS³ of ions at m/z 734.3 (A1) assigned as  $[POPS + 61 \text{ u} - 87 \text{ u} - H]^-$ , and at m/z 750.3 (B1) assigned as  $[POPS + 77 \text{ u} - 87 \text{ u} - H]^-$  were also shown.



**Figure S4.** Percentage of inhibition of DPPH• and ABTS•+ radicals obtained in the presence of non-modified POPS (37.5, 75 and 150  $\mu$ g/mL) after 120 min of reaction.