

Chemistry Department

## Physical Organic Chemistry

Physical Organic Chemistry  
Radical Chemistry  
Radiation Chemistry



Tecnologias de Radiação  
Processos e Produtos



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## Objectives

Development of new antioxidants

Identification and characterization of degradation products of biologically active compounds under oxidative stress

Generation of oxidizing radicals: radiomimetic methods (chemical, photochemical); gamma radiolysis

Mechanisms of radical oxidation reactions

Especies formadas	Captor	Reacção
$e_{aq}^-/H^+$	RH	$H_2O^+ + RH \rightarrow H^+ + H_2O$
$H^+$	RH ( $\omega H < 3$ )	$e_{aq}^- + H_2O^+ \rightarrow H_2O + H^+$ $H_2O^+ + R-H \rightarrow R^+ + H_2O$
$HO^•$	$N_2O$	$e_{aq}^- + N_2O \rightarrow N_2 + HO^• + OH^-$
$e_{ac}^-$	$HCOO^-$	$HO^• + HCOO^- \rightarrow H_2O + CO_2^{\bullet -}$ $H^+ + HCOO^- \rightarrow H_2 + CO_2^{\bullet -}$
$O_2^•-$	$H_2/H_2O_2$	$e_{aq}^- + O_2 \rightarrow O_2^•-$ $HO^• + HCOO^- \rightarrow H_2O + CO_2^{\bullet -}$ $H^+ + HCOO^- \rightarrow H_2 + CO_2^{\bullet -}$ $CO_2^{\bullet -} + O_2 \rightarrow CO_2 + O_2^•-$
$SO_4^{\bullet -}$	$S_2O_8^{2-}$ (Étalon)	$e_{aq}^- + S_2O_8^{2-} \rightarrow SO_4^{\bullet -} + SO_4^{2-}$ $HO^• + R-H \rightarrow R^+ + H_2O$

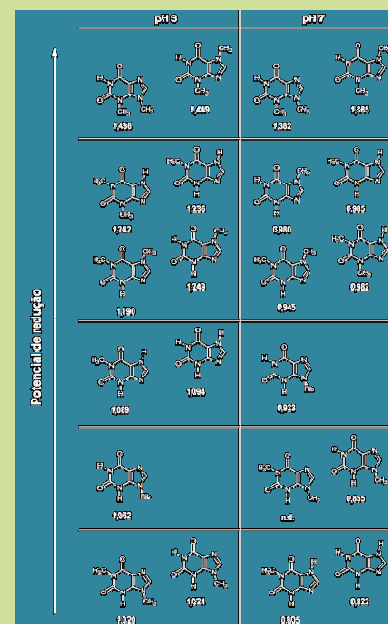
## Methodology

Chemical and photochemical generation of radicals

Gamma radiolysis; Pulse-radiolysis

HPLC/GC-MS techniques

ESR spectroscopy



## Expected Results

New protectors against oxidative stress

New types of antioxidant activity: scavenging, repairing and cascades

Kinetics of fast radical reactions

Structure of transient radicals by ESR

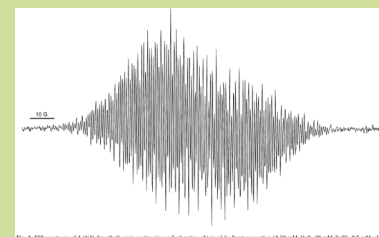


Fig. 5. ESR spectrum of 4-(N-dimethylamino)nitrobenzyl radical cation obtained by ferrous reaction (4.30 mM  $H_2O_2$ , 30 mM  $F_2SO_4$ , 0.5 mM, pH 1).

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