Supplementary Information

The Molecular Mechanism of the Photocatalytic Oxidation Reactions by Horseradish Peroxidase in the Presence of Histidine

Raheleh Ravanfar, Alireza Abbaspourrad*

Department of Food Science, Cornell University, Ithaca, NY, 14853, USA

*Corresponding Author: Alireza Abbaspourrad, email: alireza@cornell.edu

Supplementary Figures

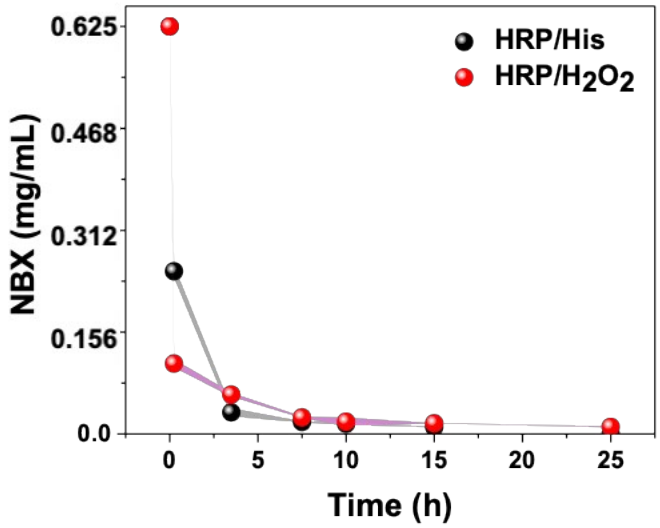
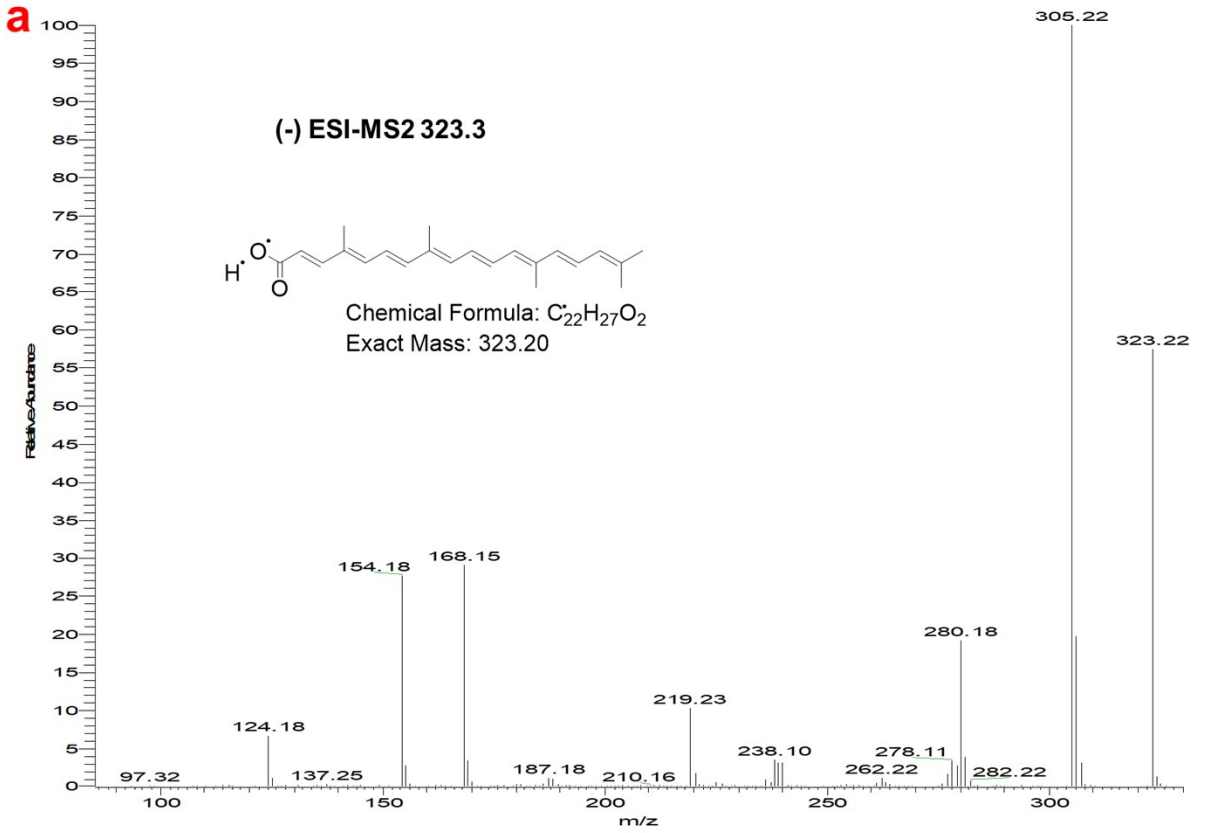


Figure S1. The concentration of NBX (mg/mL) at different time intervals up to 25 h in the HRP/His and HRP/H_2O_2 systems.


a
(-) ESI-MS2 323.3
Chemical Formula: C22H27O2
Exact Mass: 323.20
Relative Abundance
m/z
305.22
323.22
154.18
168.15
280.18
219.23
124.18
238.10
278.11
262.22
282.22
97.32
137.25
187.18
210.16

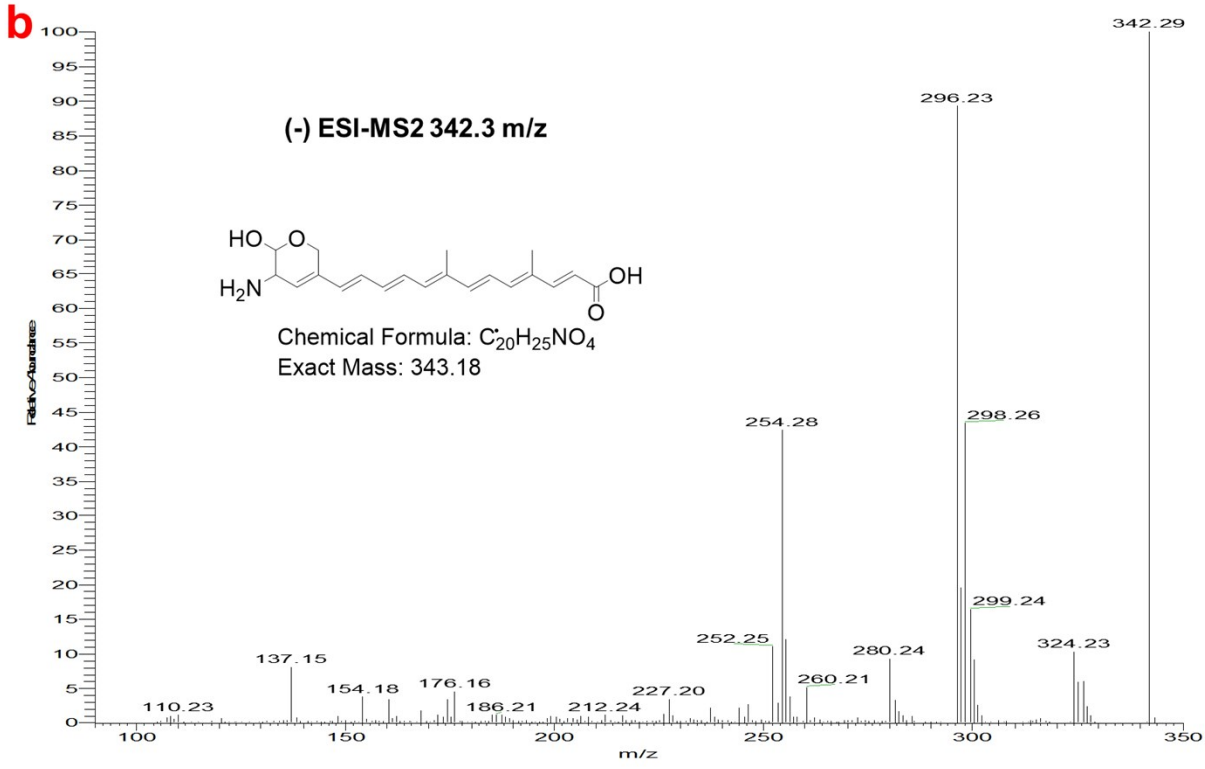

b
(-) ESI-MS2 342.3 m/z
Chemical Formula: C20H25NO4
Exact Mass: 343.18
Relative Abundance
m/z
342.29
296.23
298.26
254.28
299.24
252.25
280.24
324.23
260.21
137.15
154.18
176.16
227.20
186.21
212.24
110.23

Figure S2. a) The mass spectra from the LC-ESI-MS2 analysis of the oxidized product of NBX with a peak at 323 m/z, and its proposed structure formed upon the treatment by the HRP/His and HRP/H_2O_2 systems. b) The mass spectra from the LC-ESI-MS2 analysis of the oxidized product of NBX with a peak at 342 m/z, and its proposed structure formed only upon the treatment by the HRP/His system.

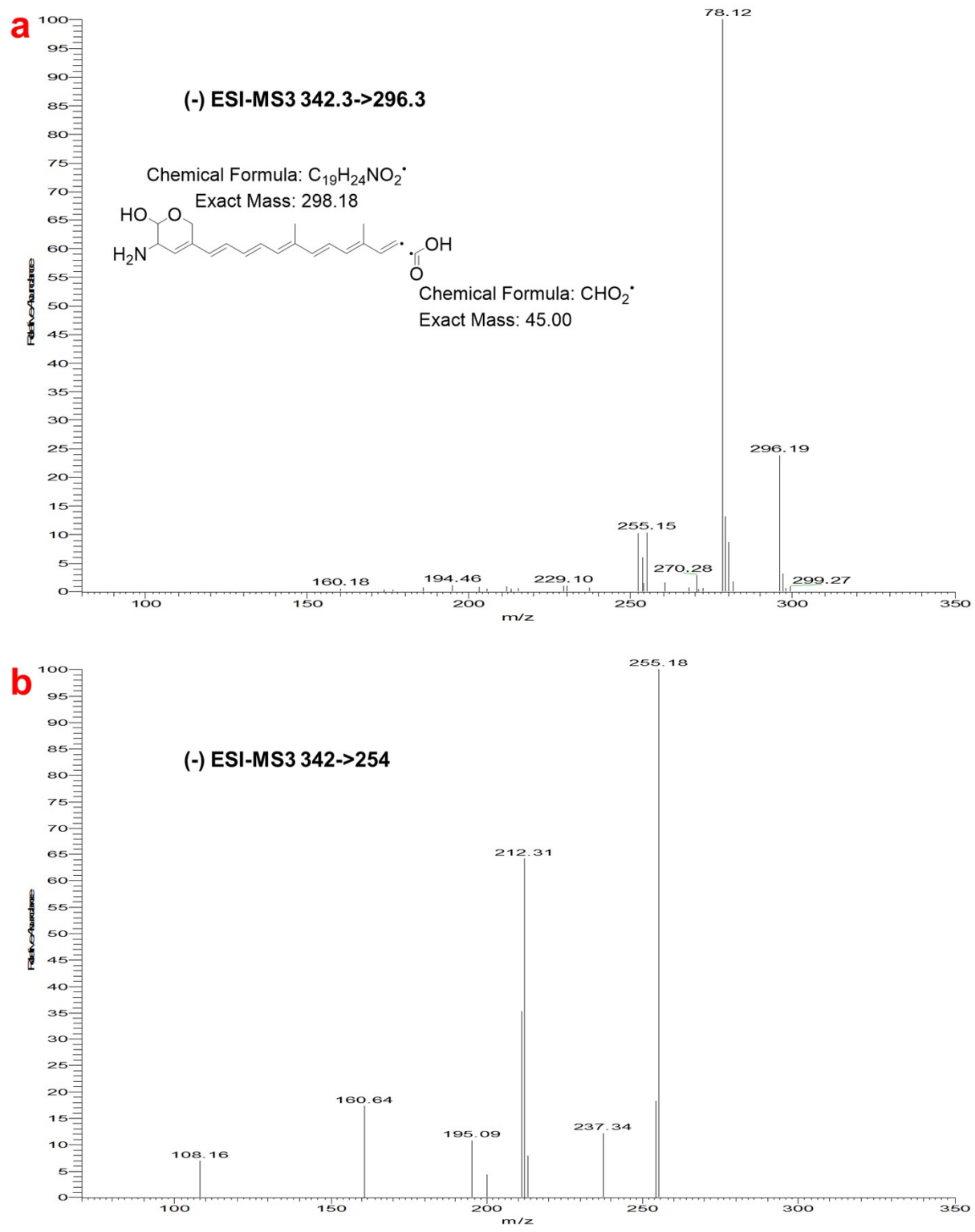


Figure S3. a) The mass spectra from the LC-ESI-MS3 analysis of the oxidized product of NBX at 296 m/z, and its proposed structure, originating from the peak at 342 m/z upon the treatment by

the HRP/His system. b) The mass spectra from the LC-ESI-MS3 analysis of the oxidized product of NBX at 254 m/z, originating from the peak at 342 m/z upon the treatment with the HRP/His system.