

Supporting Information:

Damage of Aromatic Amino Acids by the Nighttime Atmospheric Oxidant NO₃•

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Contents

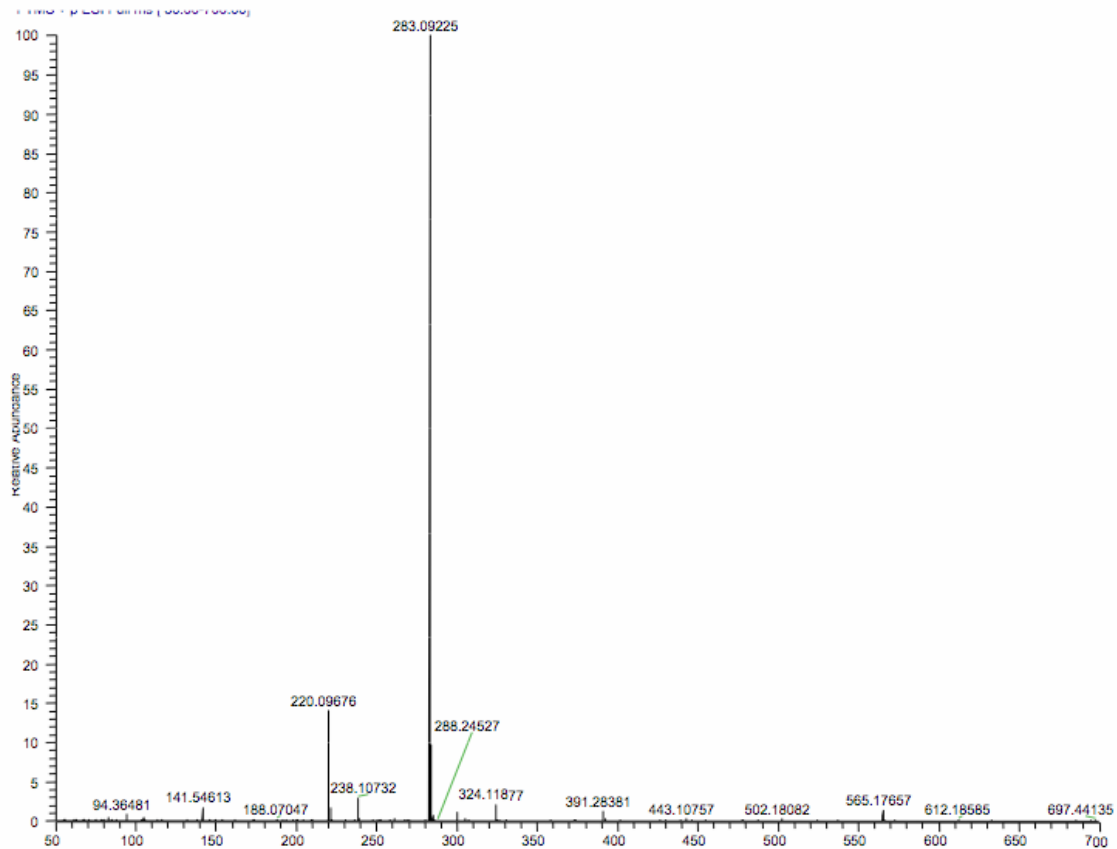
¹H NMR spectra for compounds **1b**, **5a**, **7b** and **14b**. LC/HR-MS(ESI) spectra the products of the reaction of **1**, **2** and **4** with NO₃•.

I	Reaction of NO₃• with phenylalanine 1	S2
II	Reaction of NO₃• with 4-methoxy phenylalanine 2	S8
III	Reaction of NO₃• with tyrosine 4	S12

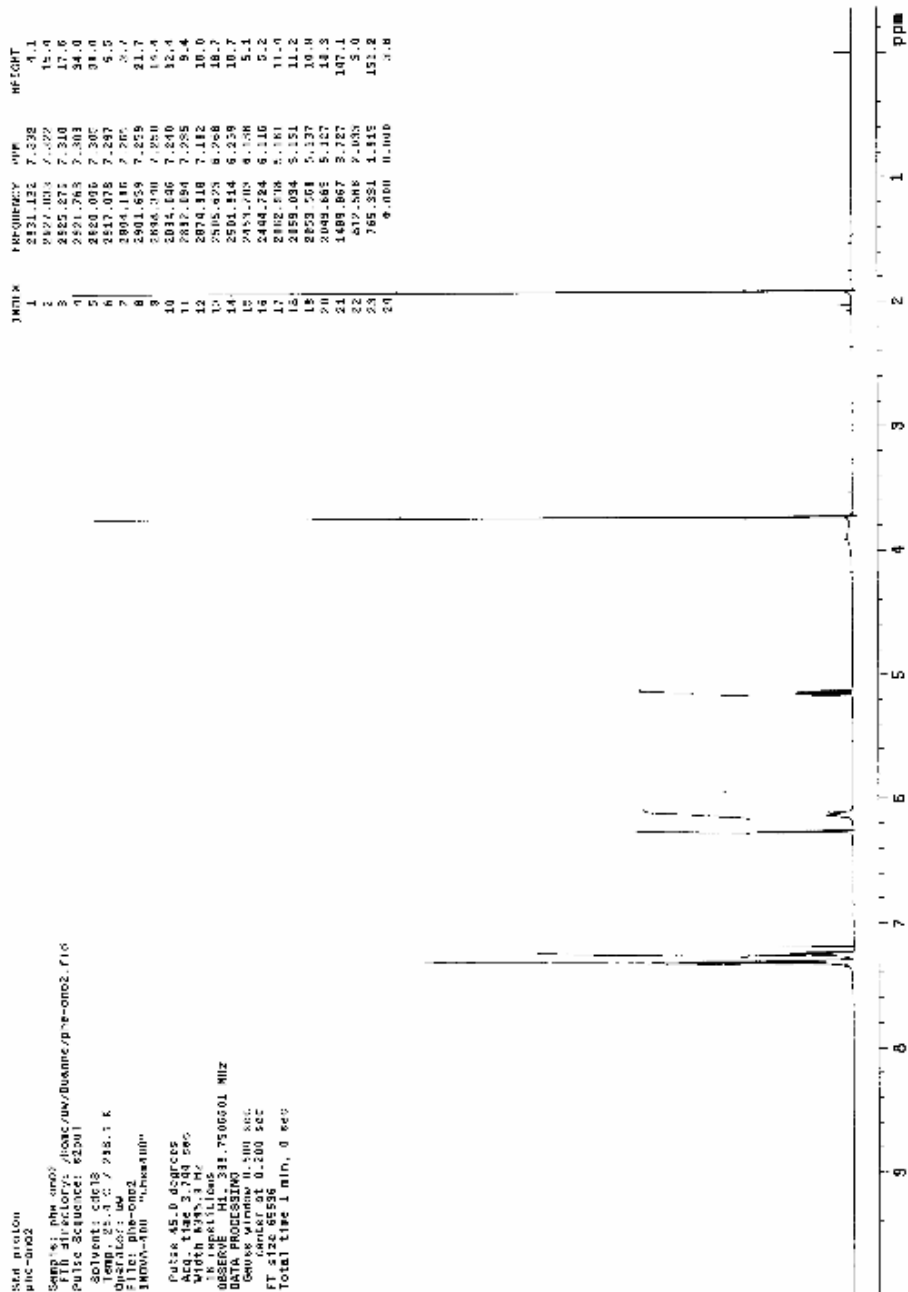
I Reaction of NO_3^\bullet with phenylalanine 1

1) Nitrate ester 5a

HR-MS(ESI)

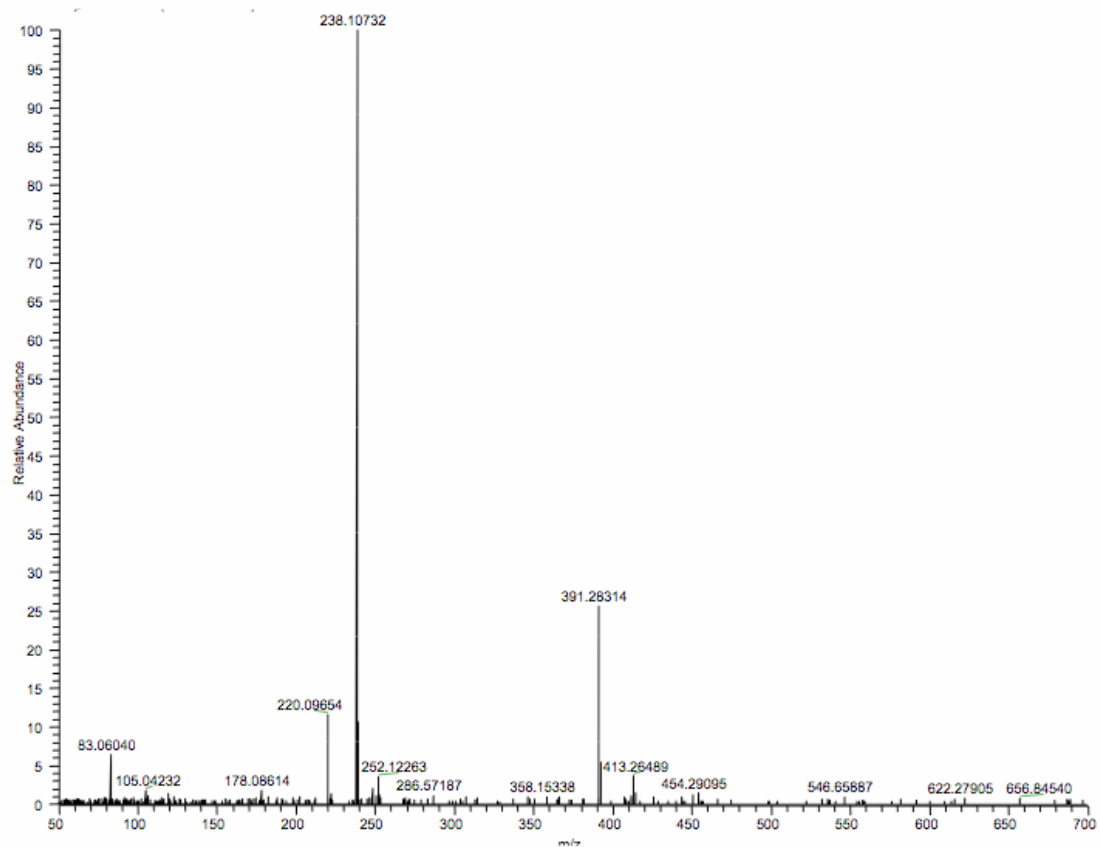


¹H NMR (CDCl₃, 400 MHz)



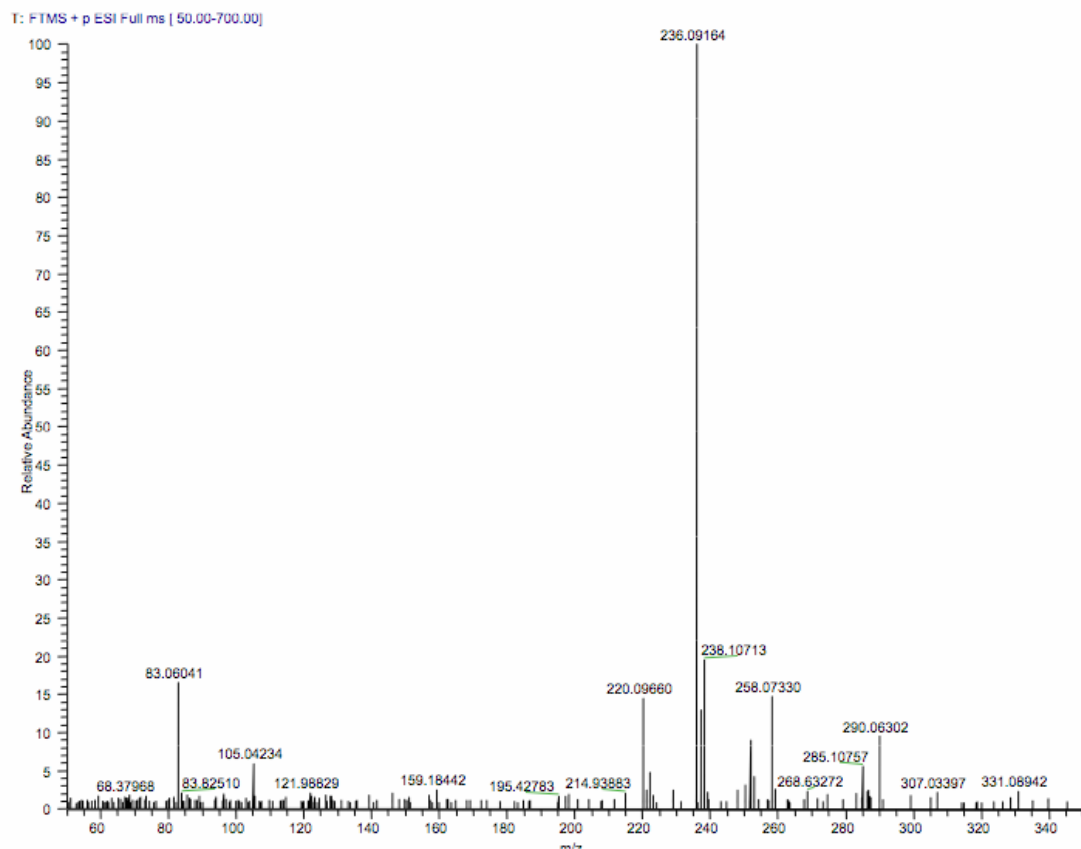
2) Alcohol 6a

HR-MS(ESI)



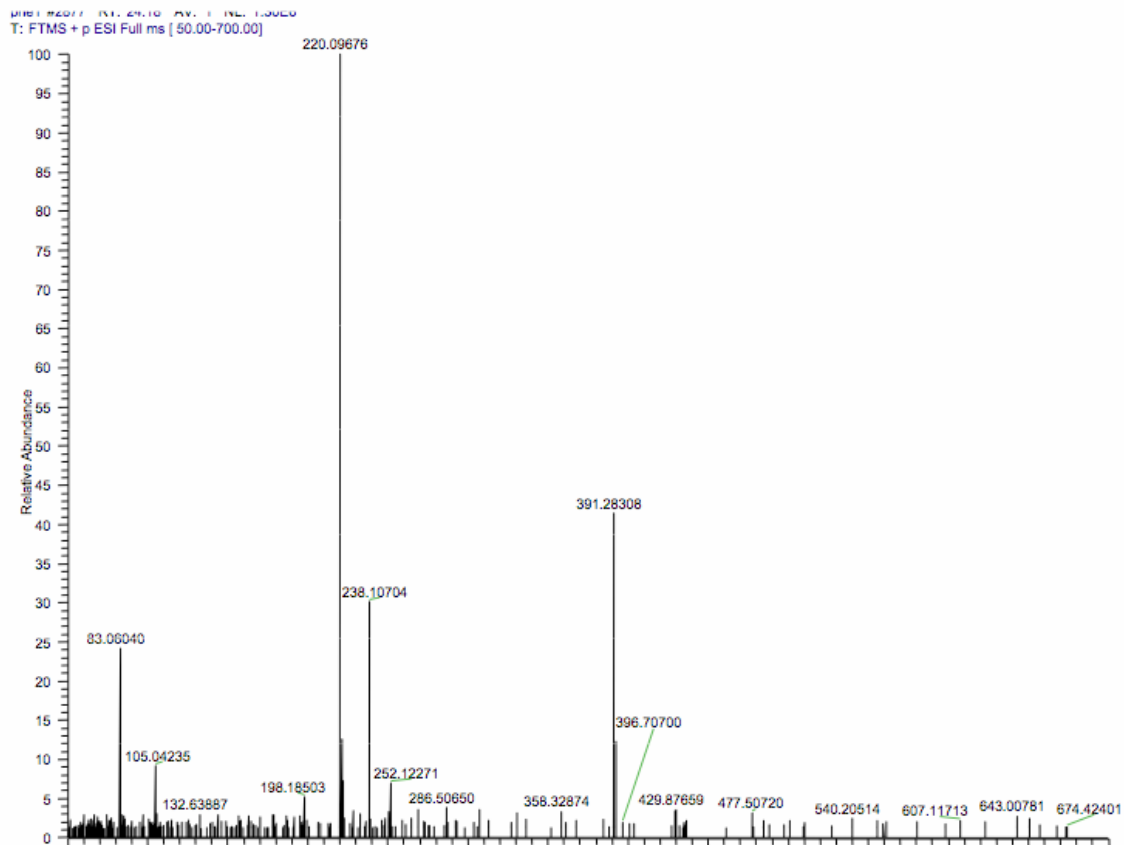
3) Carbonyl compound 7a

HR-MS(ESI)



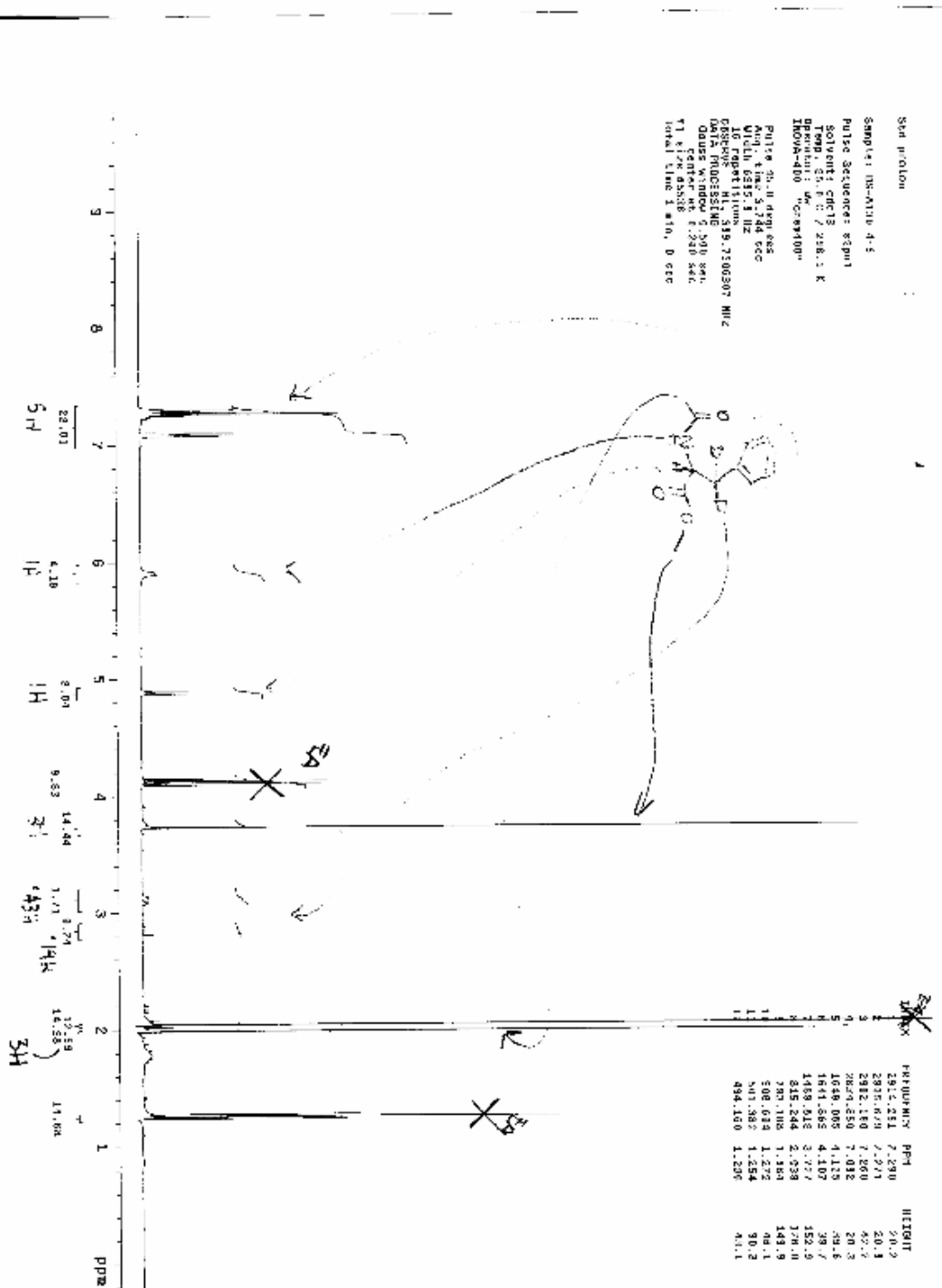
4) Alkene 8a

HR-MS(ESI)



5) Phenylalanine-D₂ 1b

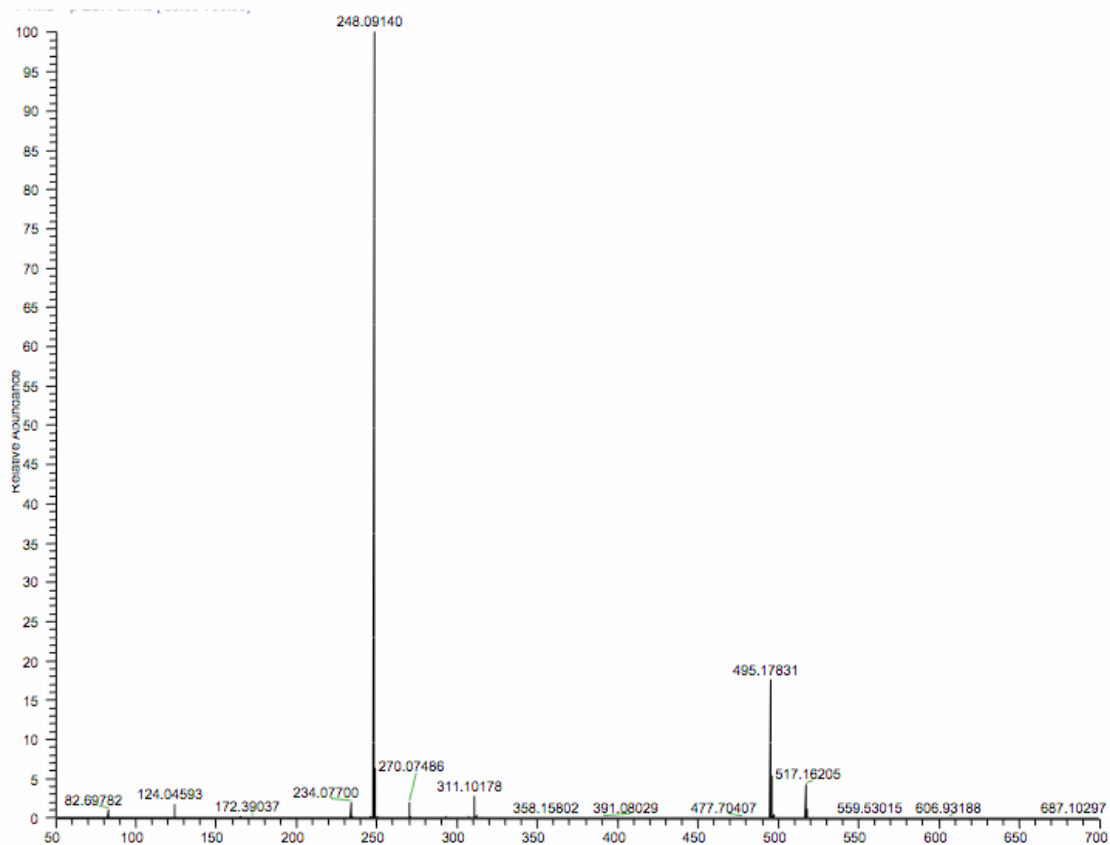
¹H NMR (CDCl₃, 400 MHz)



II Reaction of NO_3^\bullet with 4-methoxy phenylalanine 2

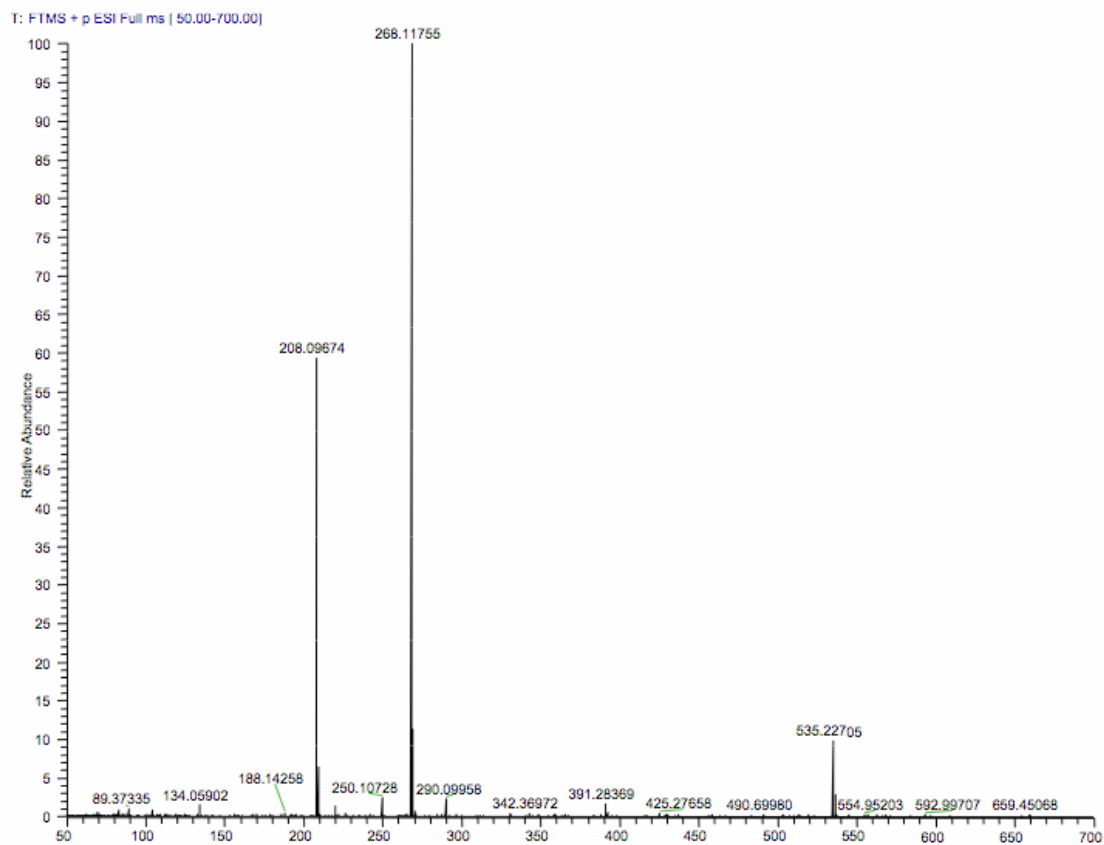
1) Carbonyl compound 7b

HR-MS(ESI)



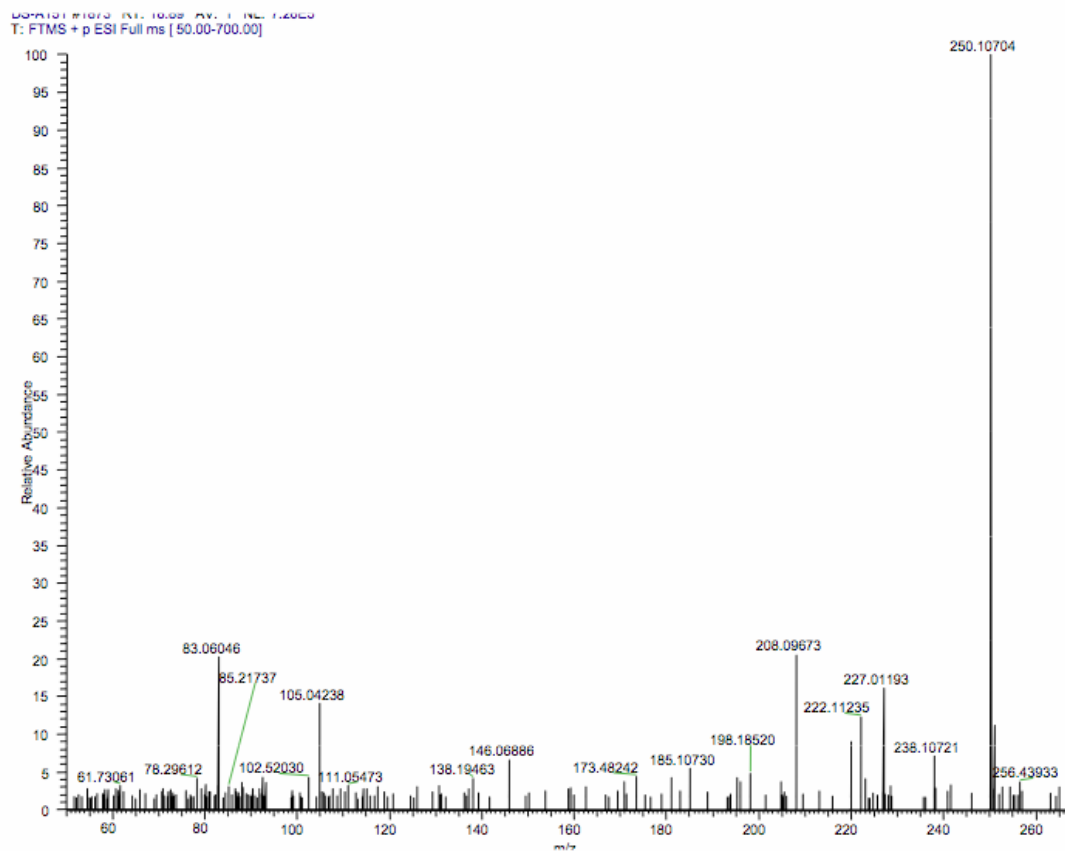
2) Alcohol 6c

HR-MS(ESI)



3) Alkene 8b

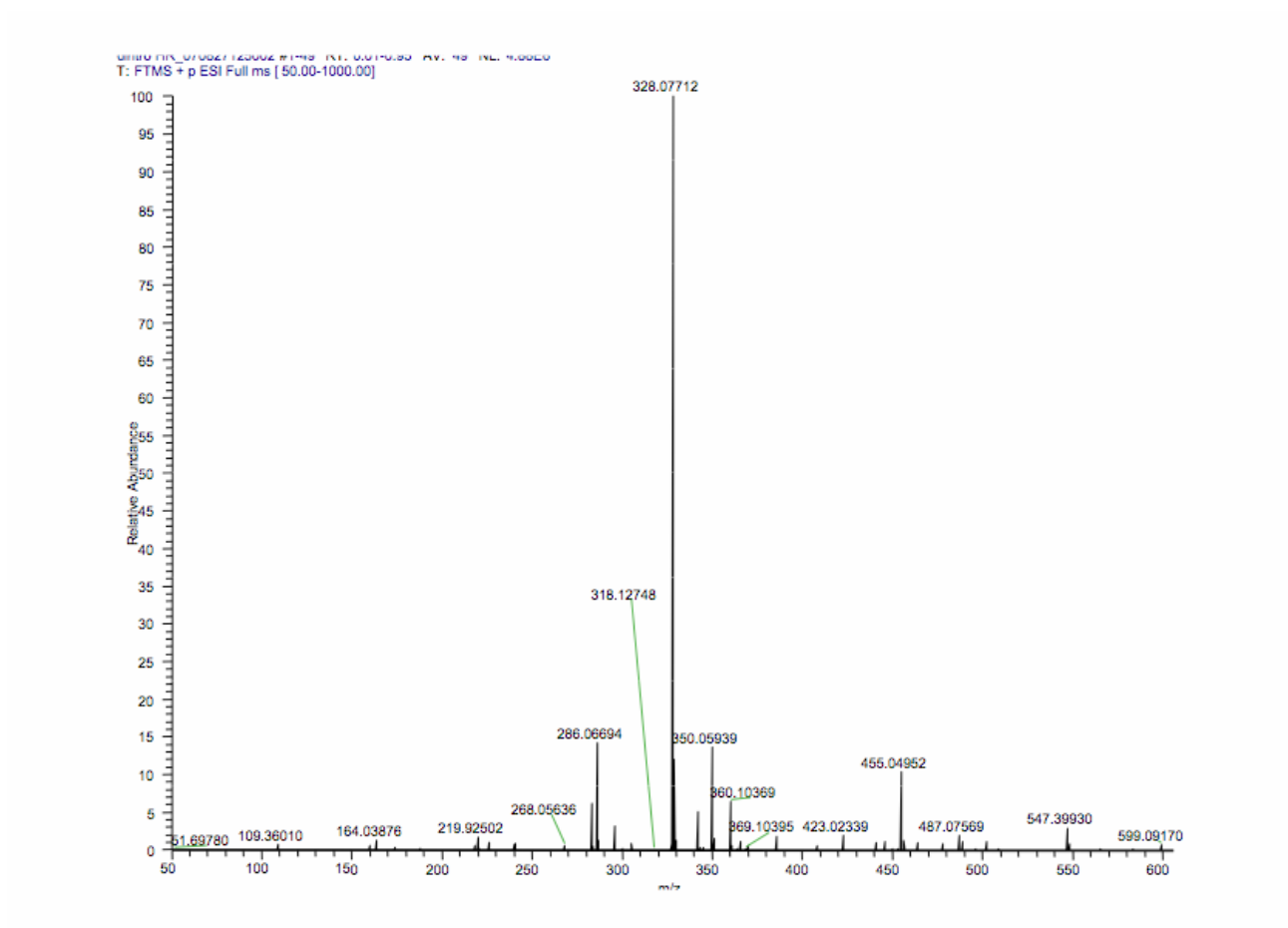
HR-MS(ESI)



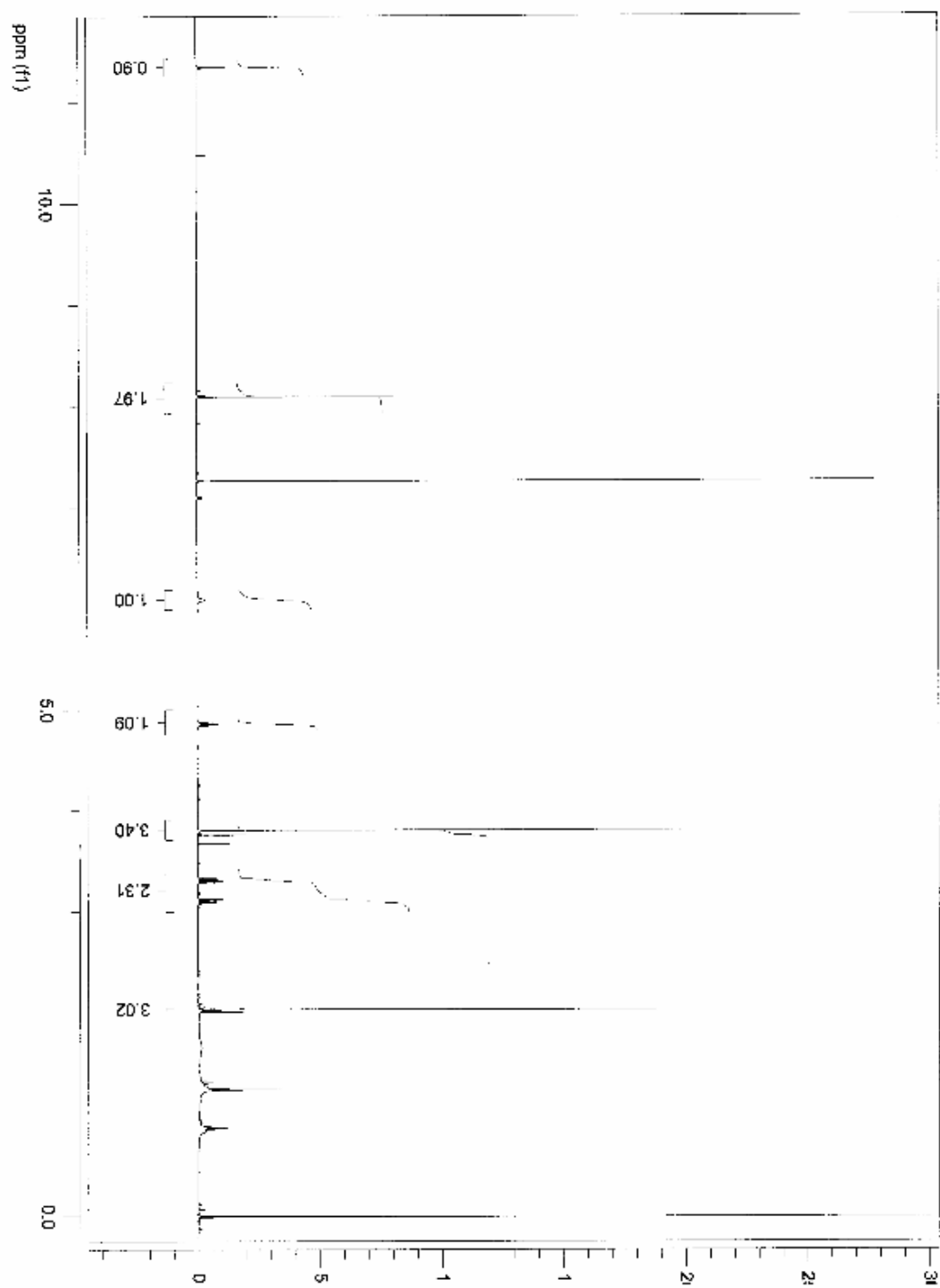
III Reaction of NO_3^\bullet with tyrosine 4

1) Dinitrotyrosine 14b

HR-MS(ESI)



^1H NMR (CDCl_3 , 400 MHz)



2) Nitrotyrosine 14a

HR-MS(ESI)

