

Electronic Supplementary Information

Molecular Characterization of Brown Carbon (BrC) Chromophores in Secondary Organic Aerosol Generated From Photo-Oxidation of Toluene

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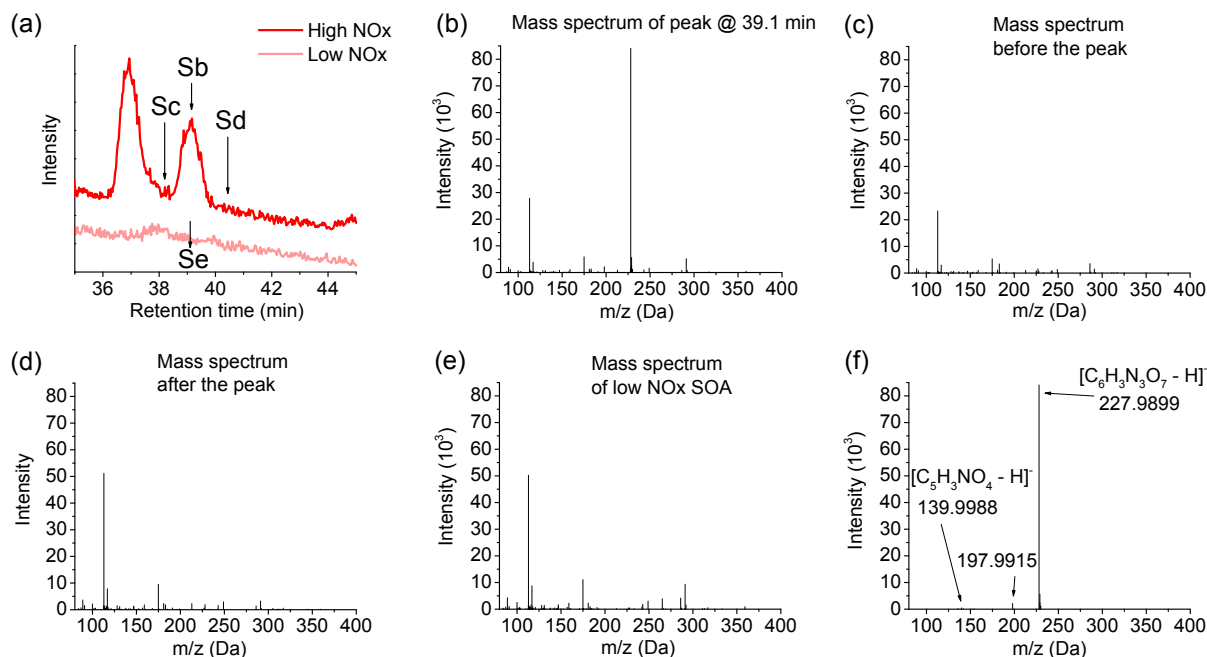
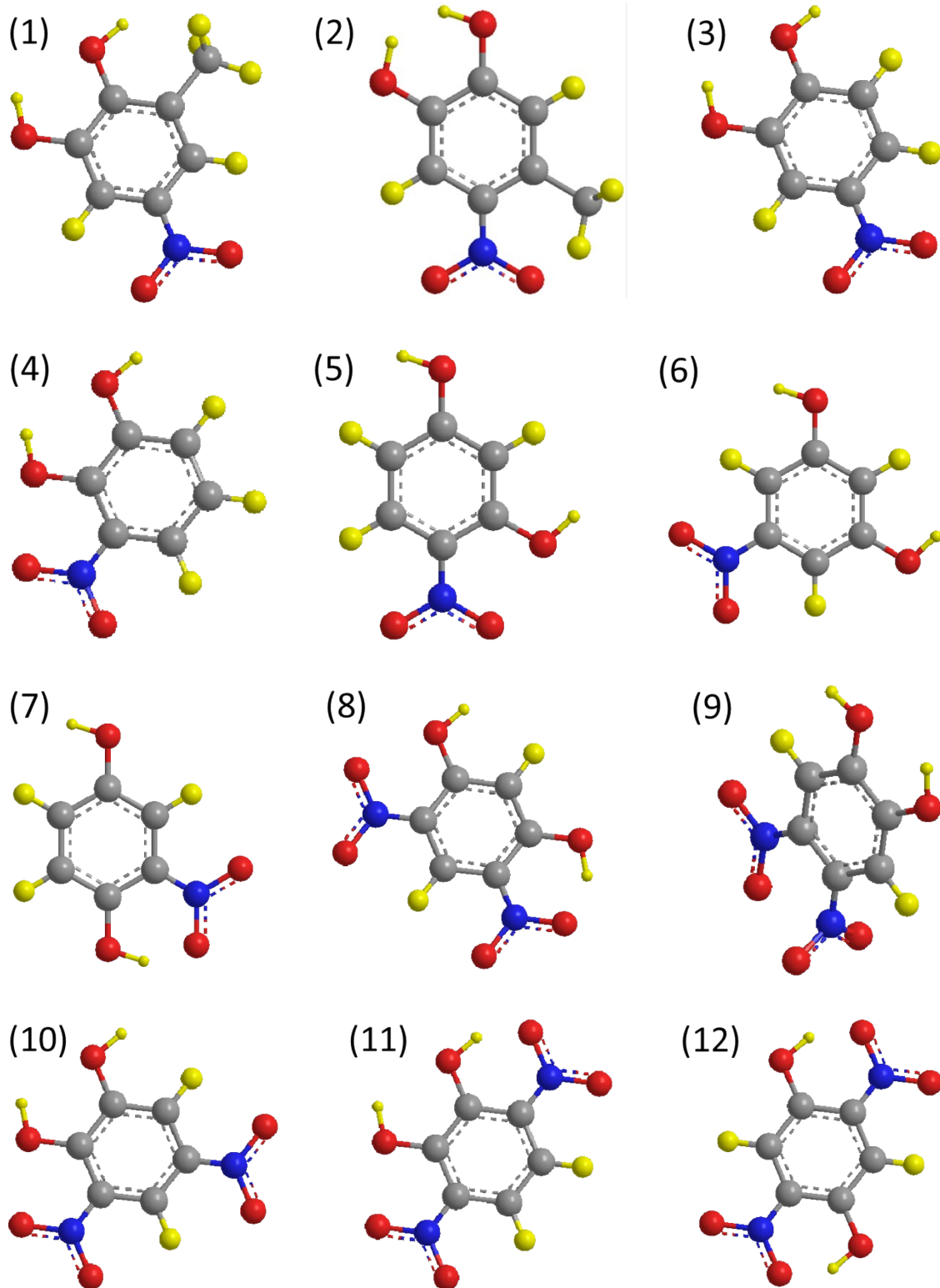


Figure S1: An example demonstrating the method used for identification of chromophoric compounds responsible for light absorption in high NO_x tol-SOA. (a) MS chromatogram around 39 min. (b) mass spectrum at the peak position (denoted as ‘Sb’). (c) mass spectrum before the peak (denoted as ‘Sc’). (d) mass spectrum after the peak (denoted as ‘Sd’). (e) mass spectrum around 39 min of low NO_x SOA. (f) mass spectrum of chromophoric compounds eluted at 39min obtained by removing peaks present in spectra(c, d and e) from spectrum(b).

Figure S1a shows the section of MS chromatogram around 39 min. Besides the mass spectrum at the peak position (denoted as ‘Sa’) of chromatogram from high NO_x sample (Figure S1b), the mass spectra before and after the peak (the positions are denoted as ‘Sc’ and ‘Sd’) were also extracted and defined as background spectra (Figure S1c and S1d). Ions present in both peak (Sa) and background (Sc or Sd) spectra, and with intensity ratio within a factor of 10 were considered as background signal, which were removed from the sample’s spectrum. The mass spectrum at RT= 39.1 min from chromatogram of low NO_x samples was also extracted (Figure S1e). As it is mentioned in the main text, SOA samples produced under low NO_x conditions is almost colorless. Thus ions detected in low NO_x samples are unlikely major light absorbing compounds. As a result, ions present commonly in these two spectra and with an intensity ratio < 100 were also removed. After these two steps, the resulted spectrum (e.g., Figure S1f) only contains several ions, with one or two abundant ones and others of low intensity. Finally, the extracted ion chromatogram (EIC) of these ions were exported and evaluated for their correspondence with the UV/Vis chromatogram (e.g., Figure 6a).

Figure S2.



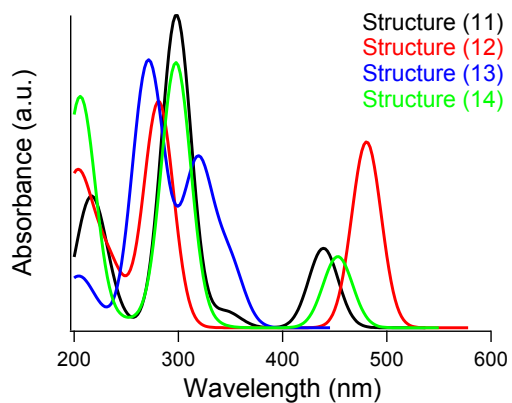
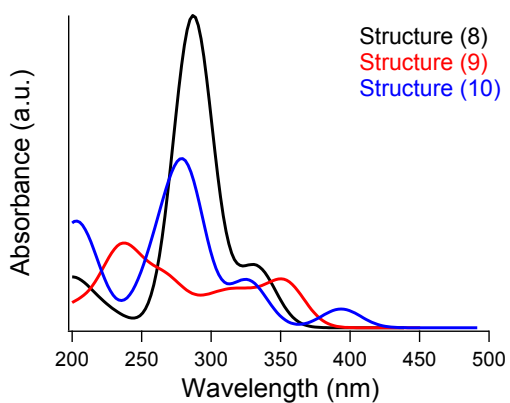
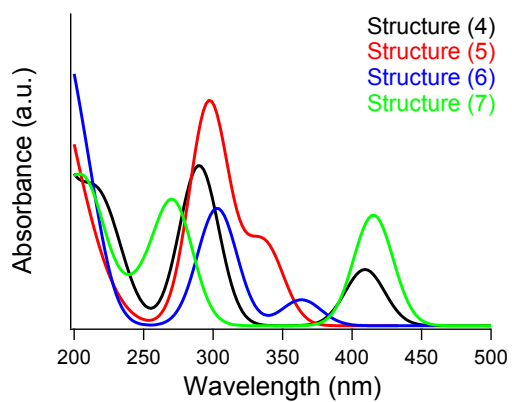
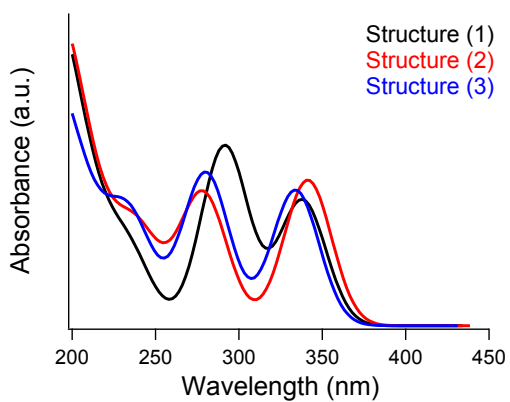
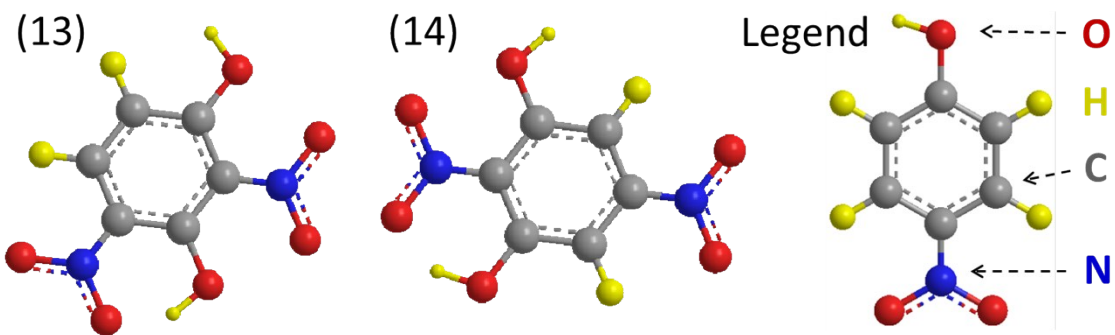


Figure S2: Molecular structures used for quantum chemistry calculations to understand the influence of functional groups location on the UV/Vis absorption spectrum. The calculated UV/Vis spectra of these 14 molecules are plotted in the four panels at the bottom.

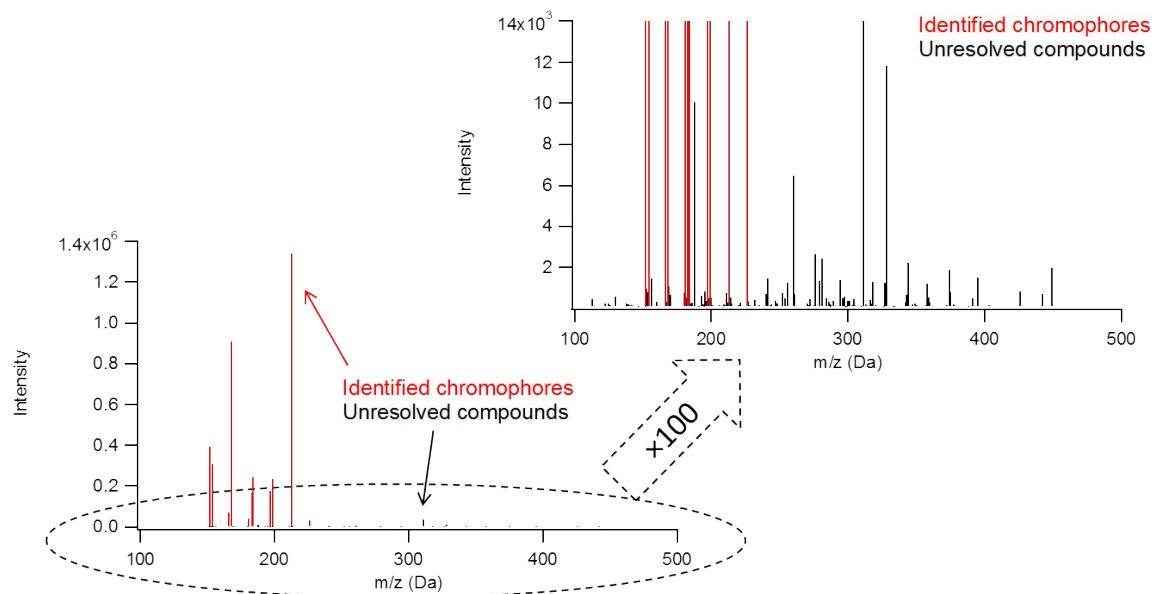


Figure S3: The averaged mass spectrum of LC fractions eluted at 15.0-30.0 min, which corresponds to the unresolved “hump” of UV/Vis chromatogram of high NO_x tol-SOA. Chromophores that have already been identified and listed in Table 1 are plotted in red. Other unresolved compounds are plotted in black.