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Supplement of

Chemical oxidative potential of secondary organic aerosol (SOA) generated from the photooxidation of biogenic and anthropogenic volatile organic compounds

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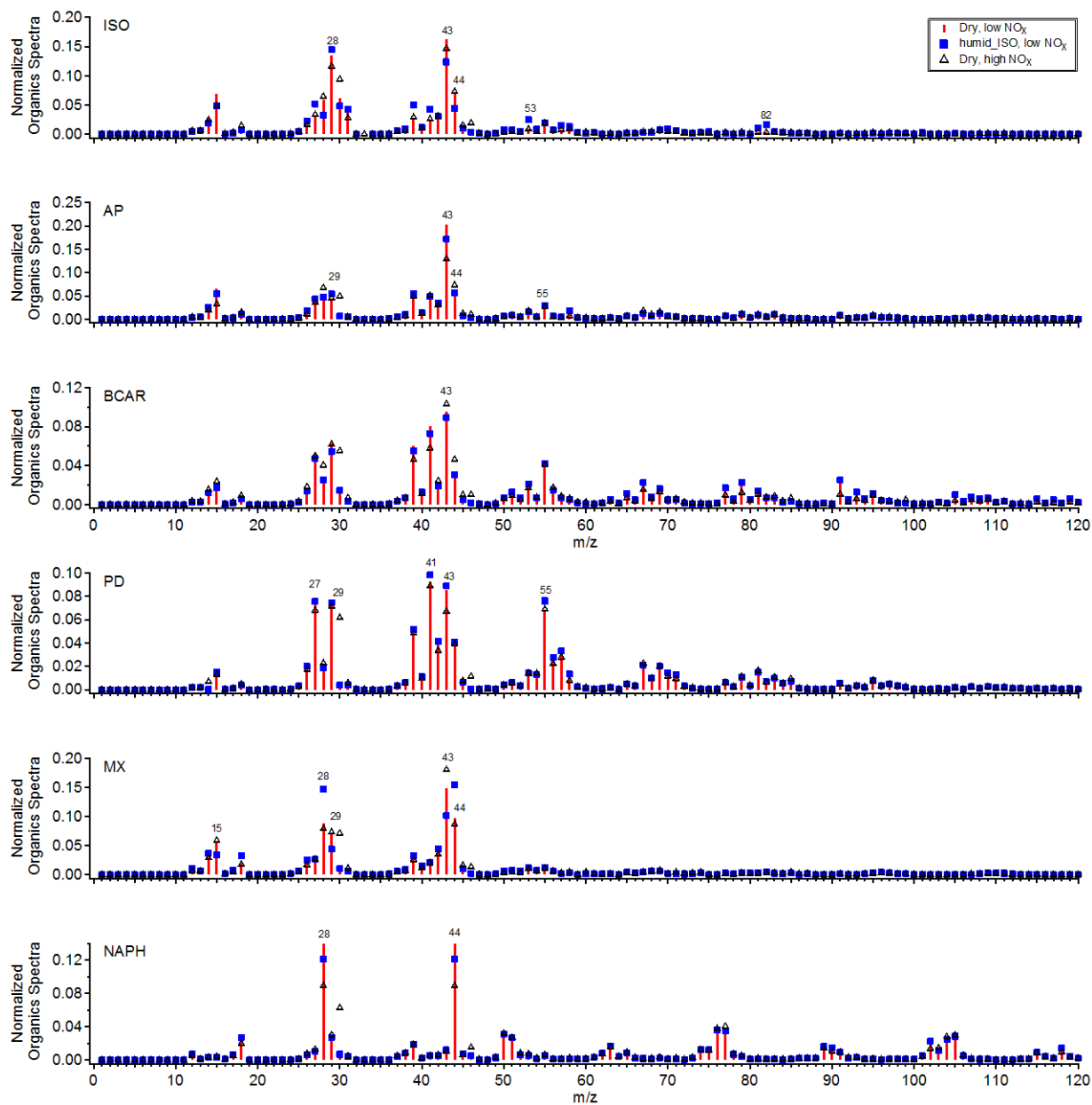


Figure S1. Aerosol mass spectra of SOA formed from the photooxidation of various hydrocarbon precursors (ISO: isoprene, AP: α -pinene, BCAR: β -caryophyllene, PD: pentadecane, MX: m-xylene, and NAPH: naphthalene) under various conditions (**red bars**: dry, RO₂ + HO₂; **blue squares**: humid, RO₂ + HO₂; and **black triangles**: dry, RO₂ + NO). Characteristic fragments for each system are labeled.

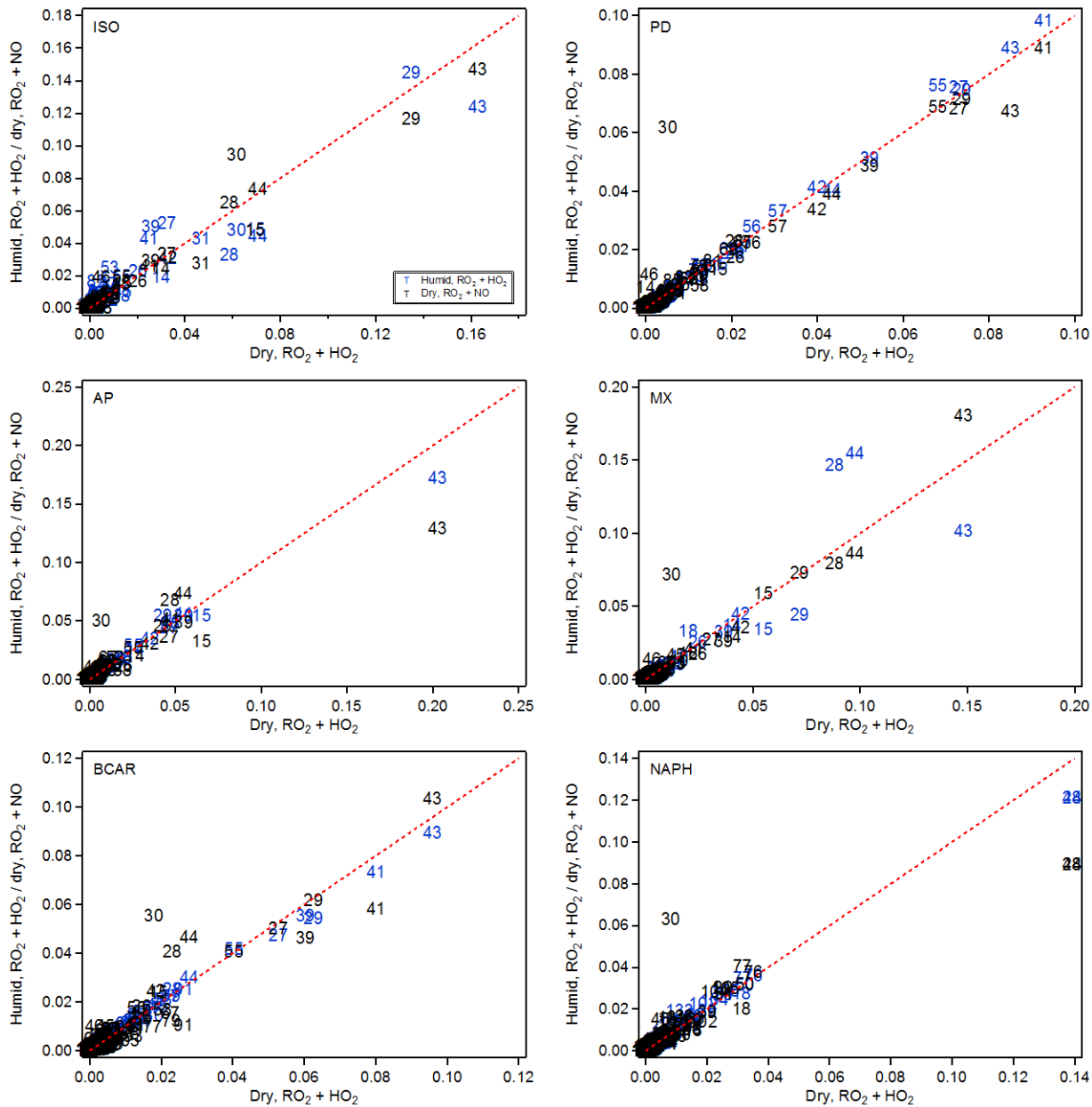


Figure S2. Comparison between mass spectra of SOA formed from the photooxidation of various hydrocarbon precursors (ISO: isoprene, AP: α -pinene, BCAR: β -caryophyllene, PD: pentadecane, MX: m-xylene, and NAPH: naphthalene) under various conditions (**blue**: humid, RO₂ + HO₂; and **black**: dry, RO₂ + NO). A 1:1 line is shown in red for reference.

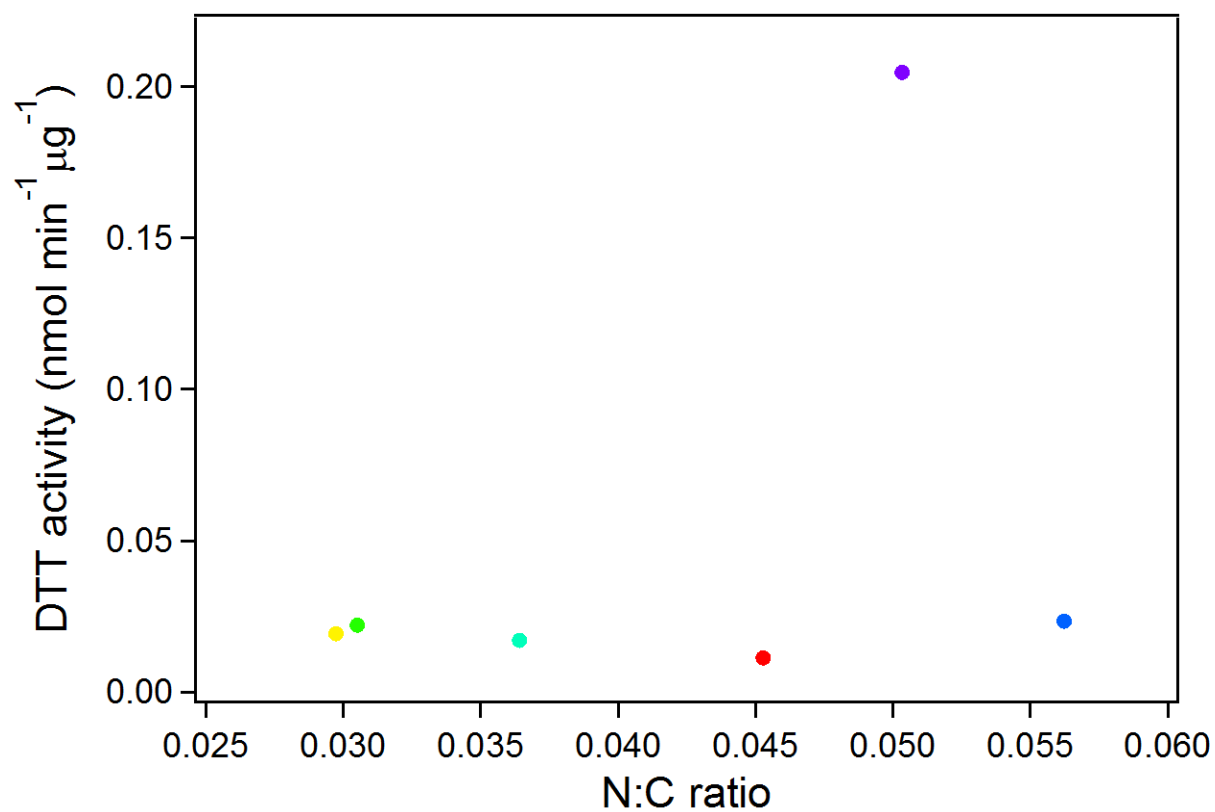
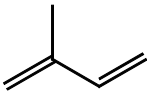
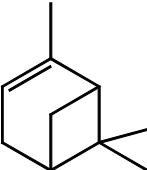
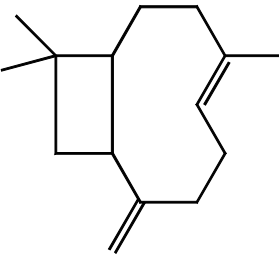

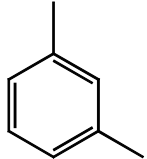
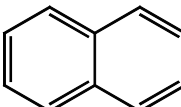


Figure S3. Intrinsic DTT activities (per μg) for various SOA systems spanning a wide range of N:C. Data points are colored by SOA system (red: isoprene, yellow: α -pinene, green: β -caryophyllene, light blue: pentadecane, blue: *m*-xylene, and purple: naphthalene).

Method for determining intrinsic OP^{WS-DTT} for various OA subtypes:

Verma et al. (2015) used multiple regression analysis to estimate the OP^{WS-DTT} of different OA subtypes (Verma et al., 2015; Xu et al., 2015a; Xu et al., 2015b). PMF analysis on AMS data collected in the southeastern U.S. resolved multiple OA factors, which represent different OA subtypes. The coefficients associated with each OA subtype from the multiple linear regression represented an estimation of the intrinsic DTT activity of that type of OA. These results are also included in Fig. 4 for comparison and discussed more below. The different aerosol subtypes with at least some contributions to DTT activity as determined by the multiple regression include isoprene-derived OA (Isoprene-OA), biomass burning OA (BBOA), more-oxidized oxygenated OA (MO-OOA), and cooking OA (COA) (Xu et al., 2015b; Verma et al., 2015).

Table S1. Hydrocarbon precursor structure and reaction rate constants.

Compound	Structure	k_{OH+HC} ($\text{cm}^3/\text{molec}^*\text{s}$)
Isoprene		1.01×10^{-10}
α -pinene		5.37×10^{-11}
β -caryophyllene		2.00×10^{-10}
Pentadecane		2.07×10^{-11}
m-xylene		2.31×10^{-11}
Naphthalene		2.44×10^{-11}

References:

Verma, V., Fang, T., Xu, L., Peltier, R. E., Russell, A. G., Ng, N. L., and Weber, R. J.: Organic Aerosols Associated with the Generation of Reactive Oxygen Species (ROS) by Water-Soluble PM_{2.5}, *Environmental Science & Technology*, 49, 4646-4656, 10.1021/es505577w, 2015.

Xu, L., Guo, H., Boyd, C. M., Klein, M., Bougiatioti, A., Cerully, K. M., Hite, J. R., Isaacman-VanWertz, G., Kreisberg, N. M., Knote, C., Olson, K., Koss, A., Goldstein, A. H., Hering, S. V., de Gouw, J., Baumann, K., Lee, S.-H., Nenes, A., Weber, R. J., and Ng, N. L.: Effects of anthropogenic emissions on aerosol formation from isoprene and monoterpenes in the southeastern United States, *Proceedings of the National Academy of Sciences*, 112, 37-42, 10.1073/pnas.1417609112, 2015a.

Xu, L., Suresh, S., Guo, H., Weber, R. J., and Ng, N. L.: Aerosol characterization over the southeastern United States using high-resolution aerosol mass spectrometry: spatial and seasonal variation of aerosol composition and sources with a focus on organic nitrates, *Atmos. Chem. Phys.*, 15, 7307-7336, 10.5194/acp-15-7307-2015, 2015b.