# Supplementary data for "Lower than expected volatility of secondary organic aerosols formed during α-pinene ozonolysis"

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Table S1. Molecules detected as sodium adduct ions during offline positive electrospray ionization analysis of α-pinene ozonolysis SOA samples.

| monomers | | | dimers | | |
|---|---|---|---|---|---|
| formula | m/z | carbon oxidation state | formula | m/z | carbon oxidation state |
| $C_8H_{12}O_4$ | 195.0628 | -0.50 | $C_{16}H_{24}O_6$ | 335.1465 | -0.75 |
| $C_8H_{12}O_5$ | 211.0577 | -0.25 | $C_{16}H_{24}O_7$ | 351.1414 | -0.63 |
| $C_8H_{12}O_6$ | 227.0526 | 0.00 | $C_{16}H_{24}O_8$ | 367.1363 | -0.50 |
| $C_8H_{12}O_7$ | 243.0475 | 0.25 | $C_{17}H_{26}O_6$ | 349.1622 | -0.82 |
| $C_8H_{14}O_5$ | 213.0733 | -0.50 | $C_{17}H_{26}O_7$ | 365.1571 | -0.71 |
| $C_8H_{14}O_6$ | 229.0683 | -0.25 | $C_{17}H_{26}O_8$ | 381.152 | -0.59 |
| $C_8H_{14}O_7$ | 245.0632 | 0.00 | $C_{17}H_{26}O_9$ | 397.1469 | -0.47 |
| $C_9H_{14}O_3$ | 193.0835 | -0.89 | $C_{17}H_{26}O_{10}$ | 413.1418 | -0.35 |
| $C_9H_{14}O_4$ | 209.0784 | -0.67 | $C_{17}H_{26}O_{11}$ | 429.1367 | -0.24 |
| $C_9H_{14}O_5$ | 225.0733 | -0.44 | $C_{17}H_{28}O_6$ | 351.1778 | -0.94 |
| $C_9H_{14}O_6$ | 241.0683 | -0.22 | $C_{17}H_{28}O_7$ | 367.1727 | -0.82 |
| $C_9H_{14}O_7$ | 257.0632 | 0.00 | $C_{17}H_{28}O_8$ | 383.1676 | -0.71 |
| $C_9H_{14}O_8$ | 273.0581 | 0.22 | $C_{17}H_{28}O_9$ | 399.1626 | -0.59 |
| $C_9H_{16}O_5$ | 227.089 | -0.67 | $C_{17}H_{28}O_{10}$ | 415.1575 | -0.47 |
| $C_9H_{16}O_6$ | 243.0839 | -0.44 | $C_{17}H_{30}O_5$ | 337.1985 | -1.18 |
| $C_9H_{16}O_7$ | 259.0788 | -0.22 | $C_{17}H_{30}O_6$ | 353.1935 | -1.06 |
| $C_9H_{16}O_8$ | 275.0737 | 0.00 | $C_{17}H_{30}O_7$ | 369.1884 | -0.94 |
| $C_{10}H_{14}O_5$ | 237.0733 | -0.40 | $C_{17}H_{30}O_8$ | 385.1833 | -0.82 |
| $C_{10}H_{14}O_6$ | 253.0683 | -0.20 | $C_{17}H_{32}O_5$ | 339.2142 | -1.29 |
| $C_{10}H_{14}O_7$ | 269.0632 | 0.00 | $C_{17}H_{32}O_6$ | 355.2091 | -1.18 |
| $C_{10}H_{16}O_3$ | 207.0992 | -1.00 | $C_{17}H_{32}O_7$ | 371.204 | -1.06 |
| $C_{10}H_{16}O_4$ | 223.0941 | -0.80 | $C_{17}H_{32}O_8$ | 387.1989 | -0.94 |
| $C_{10}H_{16}O_5$ | 239.089 | -0.60 | $C_{17}H_{32}O_9$ | 403.1939 | -0.82 |
| $C_{10}H_{16}O_6$ | 255.0839 | -0.40 | $C_{18}H_{28}O_5$ | 347.1829 | -1.00 |
| $C_{10}H_{16}O_7$ | 271.0788 | -0.20 | $C_{18}H_{28}O_6$ | 363.1778 | -0.89 |
| $C_{10}H_{16}O_8$ | 287.0737 | 0.00 | $C_{18}H_{28}O_7$ | 379.1727 | -0.78 |
| $C_{10}H_{16}O_9$ | 303.0687 | 0.20 | $C_{18}H_{28}O_8$ | 395.1676 | -0.67 |
| $C_{10}H_{18}O_5$ | 241.1046 | -0.80 | $C_{18}H_{28}O_9$ | 411.1626 | -0.56 |
| $C_{10}H_{18}O_6$ | 257.0996 | -0.60 | $C_{18}H_{28}O_{10}$ | 427.1575 | -0.44 |
| $C_{10}H_{18}O_7$ | 273.0945 | -0.40 | $C_{18}H_{28}O_{11}$ | 443.1524 | -0.33 |
| $C_{10}H_{18}O_8$ | 289.0894 | -0.20 | $C_{18}H_{30}O_8$ | 397.1833 | -0.78 |
| $C_{10}H_{18}O_9$ | 305.0843 | 0.00 | $C_{18}H_{30}O_9$ | 413.1782 | -0.67 |
| | | | $C_{18}H_{32}O_4$ | 335.2193 | -1.33 |
| | | | $C_{18}H_{32}O_5$ | 351.2142 | -1.22 |
| | | | $C_{18}H_{32}O_6$ | 367.2091 | -1.11 |
| | | | $C_{18}H_{34}O_5$ | 353.2298 | -1.33 |
| | | | $C_{18}H_{34}O_6$ | 369.2248 | -1.22 |
| | | | $C_{18}H_{34}O_8$ | 401.2146 | -1.00 |
| | | | $C_{19}H_{28}O_6$ | 359.1829 | -0.84 |
| | | | $C_{19}H_{28}O_7$ | 391.1727 | -0.74 |
| | | | $C_{19}H_{28}O_8$ | 407.1676 | -0.63 |
| | | | $C_{19}H_{28}O_9$ | 423.1626 | -0.53 |
| | | | $C_{19}H_{28}O_{10}$ | 439.1575 | -0.42 |
| | | | $C_{19}H_{28}O_{12}$ | 471.1473 | -0.21 |
| | | | $C_{19}H_{30}O_5$ | 361.1985 | -1.05 |
| | | | $C_{19}H_{30}O_6$ | 377.1935 | -0.95 |
| | | | $C_{19}H_{30}O_7$ | 393.1884 | -0.84 |
| | | | $C_{19}H_{30}O_8$ | 409.1833 | -0.74 |
| | | | $C_{19}H_{30}O_9$ | 425.1782 | -0.63 |
| | | | $C_{20}H_{30}O_6$ | 389.1935 | -0.90 |
| | | | $C_{20}H_{30}O_8$ | 421.1833 | -0.70 |
| | | | $C_{20}H_{30}O_9$ | 437.1782 | -0.60 |
| | | | $C_{20}H_{30}O_{10}$ | 453.1731 | -0.50 |
| | | | $C_{20}H_{32}O_5$ | 375.2142 | -1.10 |
| | | | $C_{20}H_{32}O_7$ | 407.204 | -0.90 |
| | | | $C_{20}H_{32}O_8$ | 423.1989 | -0.80 |
| | | | $C_{20}H_{32}O_9$ | 439.1939 | -0.70 |

Table S2. Saturation concentrations determined for α-pinene oxidation products by SPARC calculations and two previous parameterization methods.

| compound | $\log_{10}$ (saturation concentration / μg $m^{-3}$) | | |
|---|---|---|---|
| | SPARC (Sato et al., 2016) | 1D fit for α-pinene oxidation products (Shiraiwa et al., 2014) | 2D fit for oxygenated organic compounds (Li et al., 2016) |
| pinonic acid | 2.25 | 3.3 | 4.3 |
| pinic acid | -0.75 | 3.2 | 3.81 |
| 10-hydroxypinonic acid | -0.82 | 2.44 | 3.5 |
| MBTCA | -0.43 | 2.24 | 1.97 |
| $C_{10}H_{16}O_5$ | - | 1.59 | 2.59 |
| $C_{10}H_{16}O_6$ | - | 0.74 | 1.58 |
| $C_{10}H_{16}O_7$ | - | -0.11 | 0.50 |
| dimer of MW 348 (isomer 1) | -6.31 | -5.45 | -0.84 |
| dimer of MW 348 (isomer 2) | -7.4 | -5.45 | -0.84 |

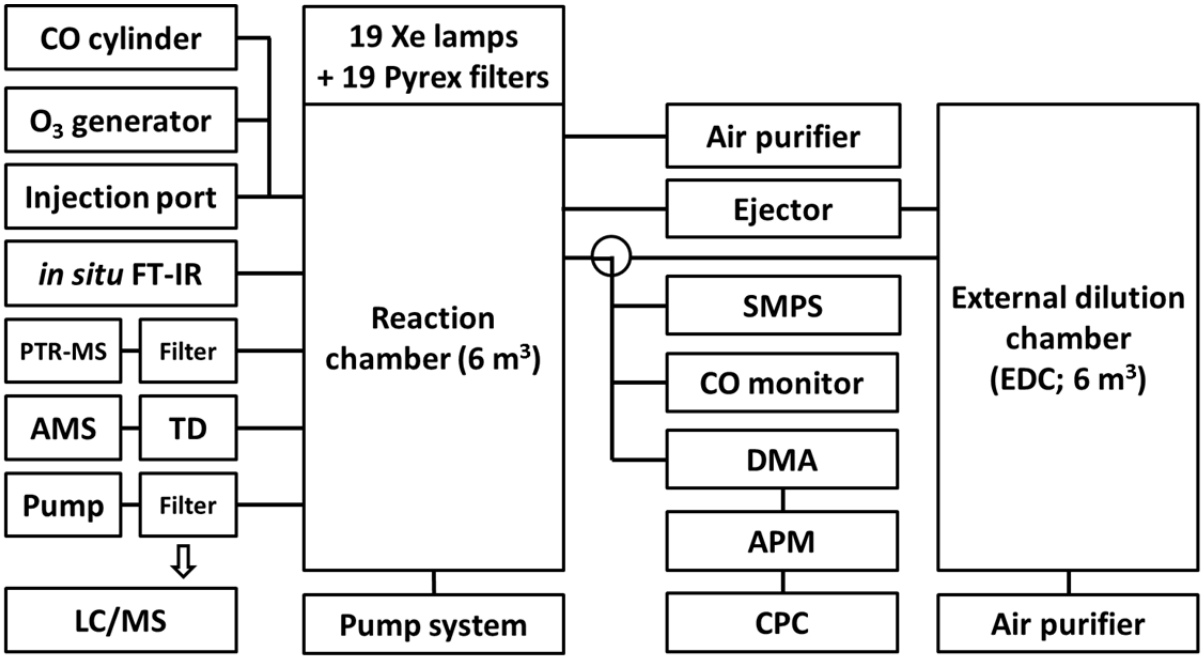


**Figure S1: Schematic diagram of the chamber system and analytical instruments used for the experiments at RH <1%; a Teflon bag was used instead of the reaction chamber with the pump system for the experiments at RH ~40%.**

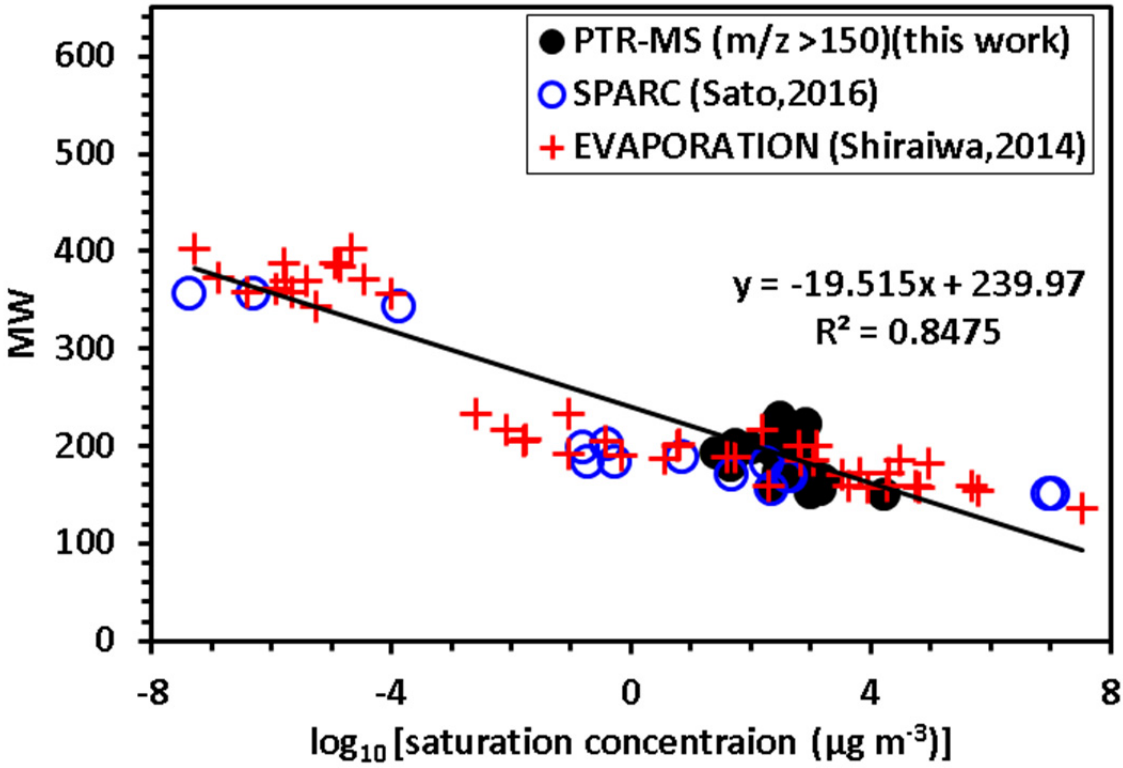


**Figure S2: MW plotted as a function of saturation concentration: Results of PTR-MS measurements, SPARC calculations, and EVAPORATION calculations.**

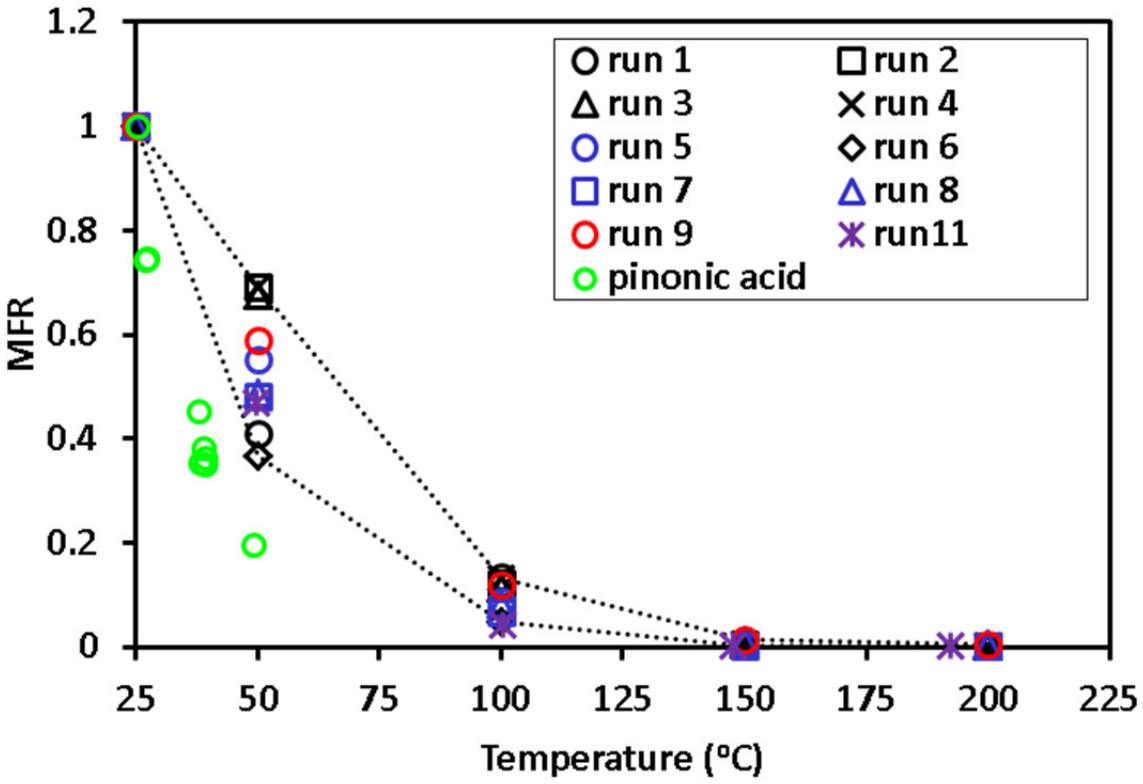


**Figure S3: Mass fraction remaining (MFR) measured for SOA and pinonic acid particles as a function of thermodenuder temperature.**

References

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