# Diagnostic Air Quality Model Evaluation of Source Specific Primary and Secondary Fine Particulate Carbon. 

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Table S1．Source speciation profiles for primary elemental and organic carbon emissions by category．All quantities are in（ug marker／ug carbon）．Boldfaced profiles were used in bias attribution analysis．

| Molecular Marker | Onroad Diesel | Nonroad Diesel | Onroad Gasoline | Nonroad Gasoline | Anthro． Biomass | Wildfire | Coal | Oil | Natural Gas | Food Cooking | Road Dust |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Data Source |  |  |  |  |  |  |  | 合宗 <br>  | －̈ <br> 둘 <br>  |  |  |
| Tetracosane | 3．37E－04 | 3．28E－04 | $1.31 \mathrm{E}-03$ | $1.64 \mathrm{E}-03$ | 8．36E－05 | $1.73 \mathrm{E}-05$ | 7．73E－04 | $1.01 \mathrm{E}-04$ | 2．68E－03 | $4.44 \mathrm{E}-04$ | $1.81 \mathrm{E}-04$ |
| Pentacosane | $2.51 \mathrm{E}-04$ | $2.48 \mathrm{E}-04$ | $1.38 \mathrm{E}-03$ | $1.78 \mathrm{E}-03$ | $1.29 \mathrm{E}-04$ | 3．60E－05 | $6.82 \mathrm{E}-04$ | $7.29 \mathrm{E}-05$ | $1.32 \mathrm{E}-03$ | $4.73 \mathrm{E}-04$ | 3．69E－04 |
| Hexacosane | $2.53 \mathrm{E}-04$ | $2.66 \mathrm{E}-04$ | $6.69 \mathrm{E}-04$ | $1.37 \mathrm{E}-03$ | $1.31 \mathrm{E}-04$ | $1.80 \mathrm{E}-05$ | 6．15E－04 | $3.70 \mathrm{E}-05$ | $5.67 \mathrm{E}-04$ | $1.09 \mathrm{E}-04$ | $2.35 \mathrm{E}-04$ |
| Heptacosane | $2.04 \mathrm{E}-04$ | $2.19 \mathrm{E}-04$ | $7.67 \mathrm{E}-04$ | $6.79 \mathrm{E}-04$ | 3．04E－04 | $9.01 \mathrm{E}-06$ | $5.07 \mathrm{E}-04$ | 2．93E－05 | 7．68E－04 | $1.72 \mathrm{E}-04$ | 4．34E－04 |
| Octacosane | $1.19 \mathrm{E}-04$ | $1.29 \mathrm{E}-04$ | $2.48 \mathrm{E}-04$ | $1.96 \mathrm{E}-04$ | $1.27 \mathrm{E}-04$ | $9.01 \mathrm{E}-06$ | 3．55E－04 | $1.50 \mathrm{E}-05$ | 3．03E－04 | $1.83 \mathrm{E}-04$ | 2．15E－04 |
| Nonacosane | $7.88 \mathrm{E}-05$ | 8．56E－05 | $2.41 \mathrm{E}-04$ | $1.81 \mathrm{E}-04$ | 7．47E－04 | $9.01 \mathrm{E}-06$ | 1．92E－04 | $2.49 \mathrm{E}-05$ | $1.20 \mathrm{E}-03$ | $2.01 \mathrm{E}-04$ | 8．87E－04 |
| Triacontane | $1.96 \mathrm{E}-04$ | $2.14 \mathrm{E}-04$ | $3.84 \mathrm{E}-04$ | $2.06 \mathrm{E}-04$ | 8．76E－05 | $0.00 \mathrm{E}+00$ | 8．49E－05 | $2.04 \mathrm{E}-05$ | $1.57 \mathrm{E}-04$ | $0.00 \mathrm{E}+00$ | $2.57 \mathrm{E}-04$ |
| Hentriacontane | $6.52 \mathrm{E}-05$ | $6.80 \mathrm{E}-05$ | $1.74 \mathrm{E}-04$ | $1.10 \mathrm{E}-04$ | 2．53E－04 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $1.05 \mathrm{E}-05$ | 3．96E－04 | $0.00 \mathrm{E}+00$ | 5．89E－04 |
| Dotriacontane | $1.45 \mathrm{E}-04$ | $1.43 \mathrm{E}-04$ | $1.61 \mathrm{E}-04$ | $1.05 \mathrm{E}-04$ | $6.30 \mathrm{E}-05$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | 3．64E－06 | $2.62 \mathrm{E}-05$ | $0.00 \mathrm{E}+00$ | 3．14E－04 |
| 22－29－30－trisnorhopane | $6.11 \mathrm{E}-05$ | $6.26 \mathrm{E}-05$ | $2.17 \mathrm{E}-04$ | $1.36 \mathrm{E}-04$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $6.94 \mathrm{E}-05$ |
| 17－a（H）－21b（H）－29－norhopane | $1.35 \mathrm{E}-04$ | $1.33 \mathrm{E}-04$ | 3．68E－04 | $4.01 \mathrm{E}-04$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | 6．60E－06 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ |
| 17－a（H）－21B（H）－hopane | $1.79 \mathrm{E}-04$ | $1.84 \mathrm{E}-04$ | $4.43 \mathrm{E}-04$ | $4.17 \mathrm{E}-04$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $1.05 \mathrm{E}-05$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | 2．63E－04 |
| 22R\＆S－17a（H）－21b（H）－30－homohopane | $1.64 \mathrm{E}-04$ | $1.75 \mathrm{E}-04$ | $5.24 \mathrm{E}-04$ | 3．16E－04 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | 4．94E－06 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $1.85 \mathrm{E}-04$ |
| 22R\＆S－17a（H）－21b（H）－30－31－bishomohopane | $9.40 \mathrm{E}-05$ | 9．93E－05 | $2.17 \mathrm{E}-04$ | $1.88 \mathrm{E}-04$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $1.47 \mathrm{E}-06$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $1.22 \mathrm{E}-04$ |
| 20R＋S－abb－cholestane | $2.99 \mathrm{E}-05$ | $2.59 \mathrm{E}-05$ | $4.51 \mathrm{E}-04$ | $1.92 \mathrm{E}-04$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | 8．31E－05 |
| 20R－aaa－cholestane | $1.42 \mathrm{E}-05$ | $1.24 \mathrm{E}-05$ | 3．53E－04 | 2．13E－04 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | 6．05E－06 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $9.48 \mathrm{E}-05$ |
| 20R＋S－abb－ergostane | $3.77 \mathrm{E}-05$ | $2.40 \mathrm{E}-05$ | 4．43E－04 | $1.81 \mathrm{E}-04$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $1.35 \mathrm{E}-05$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $1.19 \mathrm{E}-04$ |
| 20R＋S－abb－sitostane | $2.46 \mathrm{E}-05$ | $2.14 \mathrm{E}-05$ | 4．95E－04 | $2.61 \mathrm{E}-04$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | 5．81E－06 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | 8．59E－05 |


| Molecular Marker | Onroad <br> Diesel | Nonroad Diesel | Onroad Gasoline | Nonroad Gasoline | Anthro. <br> Biomass | Wildfire | Coal | Oil | Natural Gas | Food <br> Cooking | Road Dust |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Fluoranthene | $4.19 \mathrm{E}-05$ | $4.36 \mathrm{E}-05$ | 2.48E-04 | 6.45E-04 | 4.21E-04 | 7.40E-04 | $0.00 \mathrm{E}+00$ | $2.03 \mathrm{E}-05$ | $1.63 \mathrm{E}-02$ | 2.98E-05 | $3.15 \mathrm{E}-05$ |
| Acephenanthrylene | $5.97 \mathrm{E}-05$ | $6.54 \mathrm{E}-05$ | 2.96E-06 | 1.14E-04 | $1.91 \mathrm{E}-04$ | $3.40 \mathrm{E}-04$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | 0.00E+00 | 0.00E+00 | 0.00E+00 |
| Benzo(ghi)fluoranthene | $2.14 \mathrm{E}-05$ | $2.31 \mathrm{E}-05$ | 8.83E-05 | 3.29E-04 | 7.72E-05 | $1.15 \mathrm{E}-04$ | $0.00 \mathrm{E}+00$ | $1.48 \mathrm{E}-05$ | $9.48 \mathrm{E}-03$ | 8.62E-06 | 8.93E-06 |
| Cyclopenta(cd)pyrene | $1.43 \mathrm{E}-05$ | $1.57 \mathrm{E}-05$ | $1.09 \mathrm{E}-04$ | 6.20E-04 | 1.80E-04 | 1.98E-04 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | 0.00E+00 | 0.00E+00 |
| Benz(a)anthracene | $1.27 \mathrm{E}-05$ | $1.21 \mathrm{E}-05$ | 1.03E-04 | 1.03E-04 | $1.43 \mathrm{E}-04$ | $2.10 \mathrm{E}-04$ | $0.00 \mathrm{E}+00$ | $1.90 \mathrm{E}-05$ | $1.19 \mathrm{E}-02$ | 1.47E-05 | 5.98E-06 |
| Chrysene/Triphenylene | $3.25 \mathrm{E}-05$ | $3.32 \mathrm{E}-05$ | $1.07 \mathrm{E}-04$ | $1.03 \mathrm{E}-04$ | $1.43 \mathrm{E}-04$ | $2.12 \mathrm{E}-04$ | $0.00 \mathrm{E}+00$ | 6.74E-05 | $4.58 \mathrm{E}-02$ | 5.02E-05 | $5.29 \mathrm{E}-05$ |
| Retene | $1.03 \mathrm{E}-06$ | 0.00E+00 | 0.00E+00 | 0.00E+00 | 2.94E-03 | 5.23E-03 | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | 0.00E+00 | 0.00E+00 |
| Benzo(k)fluoranthene | 8.11E-06 | 5.91E-06 | $1.34 \mathrm{E}-04$ | 4.98E-04 | 6.58E-05 | $9.57 \mathrm{E}-05$ | 9.77E-03 | $1.67 \mathrm{E}-05$ | $9.39 \mathrm{E}-03$ | $1.06 \mathrm{E}-05$ | $3.78 \mathrm{E}-05$ |
| Benzo(b)fluoranthene | $7.93 \mathrm{E}-06$ | $6.01 \mathrm{E}-06$ | 3.59E-04 | 4.71E-04 | 7.20E-05 | $9.01 \mathrm{E}-05$ | $1.41 \mathrm{E}-02$ | $1.57 \mathrm{E}-05$ | $6.78 \mathrm{E}-03$ | 7.54E-06 | $3.02 \mathrm{E}-05$ |
| Benzo(j)fluoranthene | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | 3.46E-05 | 7.02E-05 | 3.31E-05 | $5.08 \mathrm{E}-05$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | 0.00E+00 | 0.00E+00 | $0.00 \mathrm{E}+00$ |
| Benzo(e)pyrene | $5.08 \mathrm{E}-06$ | 4.52E-06 | 8.00E-05 | 7.55E-05 | 5.10E-05 | 5.40E-05 | $1.04 \mathrm{E}-02$ | 7.57E-06 | $2.77 \mathrm{E}-03$ | 6.82E-06 | $1.85 \mathrm{E}-05$ |
| Benzo(a)pyrene | 6.40E-06 | 3.40E-06 | 7.92E-05 | 1.14E-04 | 8.49E-05 | $1.28 \mathrm{E}-04$ | $0.00 \mathrm{E}+00$ | 5.23E-07 | $0.00 \mathrm{E}+00$ | 6.82E-06 | $1.58 \mathrm{E}-05$ |
| Perylene | 3.05E-06 | $3.35 \mathrm{E}-06$ | 4.10E-05 | 3.21E-04 | $1.30 \mathrm{E}-05$ | $2.08 \mathrm{E}-05$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | 0.00E+00 | 1.08E-06 | 3.30E-06 |
| Indeno(cd)pyrene | $8.09 \mathrm{E}-09$ | $0.00 \mathrm{E}+00$ | 8.32E-05 | 1.47E-04 | 6.19E-05 | 8.11E-05 | $1.25 \mathrm{E}-02$ | $0.00 \mathrm{E}+00$ | 0.00E+00 | 0.00E+00 | 0.00E+00 |
| Benzo(ghi)perylene | 9.20E-06 | 3.98E-06 | 4.38E-04 | $1.81 \mathrm{E}-03$ | 4.02E-05 | 5.40E-05 | 9.45E-03 | $0.00 \mathrm{E}+00$ | 0.00E+00 | 0.00E+00 | $1.44 \mathrm{E}-05$ |
| Coronene | 7.76E-07 | $0.00 \mathrm{E}+00$ | $1.36 \mathrm{E}-04$ | 2.00E-04 | 6.54E-05 | $1.02 \mathrm{E}-04$ | 5.36E-03 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ |
| Tetradecanoic acid | $1.40 \mathrm{E}-04$ | $1.53 \mathrm{E}-04$ | $1.48 \mathrm{E}-03$ | $3.89 \mathrm{E}-05$ | $7.51 \mathrm{E}-04$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $1.84 \mathrm{E}-04$ | $1.42 \mathrm{E}-03$ | $3.62 \mathrm{E}-03$ | $1.17 \mathrm{E}-03$ |
| Pentadecanoic acid | $5.35 \mathrm{E}-05$ | $5.87 \mathrm{E}-05$ | $4.21 \mathrm{E}-04$ | $9.16 \mathrm{E}-06$ | $2.41 \mathrm{E}-04$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | 5.43E-05 | 3.41E-04 | $1.02 \mathrm{E}-03$ | $5.28 \mathrm{E}-04$ |
| Hexadecanoic acid | $4.68 \mathrm{E}-04$ | $5.13 \mathrm{E}-04$ | 7.92E-03 | $1.37 \mathrm{E}-04$ | $3.93 \mathrm{E}-03$ | $2.46 \mathrm{E}-03$ | $0.00 \mathrm{E}+00$ | $1.22 \mathrm{E}-03$ | $7.40 \mathrm{E}-03$ | $2.30 \mathrm{E}-02$ | $6.98 \mathrm{E}-03$ |
| Heptadecanoic acid | $1.35 \mathrm{E}-04$ | $1.49 \mathrm{E}-04$ | $1.81 \mathrm{E}-04$ | $9.47 \mathrm{E}-05$ | $1.69 \mathrm{E}-04$ | $1.29 \mathrm{E}-04$ | $0.00 \mathrm{E}+00$ | $3.52 \mathrm{E}-05$ | $2.98 \mathrm{E}-04$ | $1.95 \mathrm{E}-03$ | $3.27 \mathrm{E}-04$ |
| Octadecanoic acid | $1.37 \mathrm{E}-03$ | $1.50 \mathrm{E}-03$ | $1.65 \mathrm{E}-03$ | $1.80 \mathrm{E}-04$ | $1.31 \mathrm{E}-03$ | $1.11 \mathrm{E}-03$ | $0.00 \mathrm{E}+00$ | $4.47 \mathrm{E}-04$ | $1.95 \mathrm{E}-03$ | $1.30 \mathrm{E}-02$ | $3.57 \mathrm{E}-03$ |
| Eicosanoic acid | $9.87 \mathrm{E}-05$ | $1.08 \mathrm{E}-04$ | 3.95E-05 | $1.69 \mathrm{E}-05$ | $6.34 \mathrm{E}-04$ | $3.14 \mathrm{E}-04$ | $0.00 \mathrm{E}+00$ | $1.70 \mathrm{E}-05$ | $0.00 \mathrm{E}+00$ | $1.35 \mathrm{E}-04$ | $4.75 \mathrm{E}-04$ |
| Heneicosanoic acid | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $2.52 \mathrm{E}-06$ | $1.67 \mathrm{E}-04$ | $4.15 \mathrm{E}-05$ | $0.00 \mathrm{E}+00$ | $2.53 \mathrm{E}-06$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $9.03 \mathrm{E}-05$ |
| Docosanoic acid | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $1.01 \mathrm{E}-03$ | $4.23 \mathrm{E}-04$ | $0.00 \mathrm{E}+00$ | 7.68E-06 | $0.00 \mathrm{E}+00$ | $5.51 \mathrm{E}-05$ | 3.36E-04 |


| Molecular Marker | Onroad <br> Diesel | Nonroad Diesel | Onroad Gasoline | Nonroad Gasoline | Anthro. <br> Biomass | Wildfire | Coal | Oil | Natural Gas | Food Cooking | Road Dust |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Tricosanoic acid | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | 0.00E+00 | 4.11E-04 | $5.88 \mathrm{E}-05$ | 0.00E+00 | $1.43 \mathrm{E}-06$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | $1.20 \mathrm{E}-04$ |
| Tetracosanoic acid | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $2.26 \mathrm{E}-03$ | 8.69E-04 | $0.00 \mathrm{E}+00$ | $8.44 \mathrm{E}-06$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $4.54 \mathrm{E}-04$ |
| Pentacosanoic acid | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | 0.00E+00 | $2.14 \mathrm{E}-04$ | $1.38 \mathrm{E}-05$ | $0.00 \mathrm{E}+00$ | $1.08 \mathrm{E}-06$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | 8.31E-05 |
| Hexacosanoic acid | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $1.41 \mathrm{E}-03$ | 2.18E-04 | $0.00 \mathrm{E}+00$ | $1.71 \mathrm{E}-06$ | $1.26 \mathrm{E}-04$ | $0.00 \mathrm{E}+00$ | $3.67 \mathrm{E}-04$ |
| Heptacosanoic acid | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $1.14 \mathrm{E}-04$ | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | $7.81 \mathrm{E}-05$ |
| Octacosanoic acid | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | 7.45E-04 | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | $9.54 \mathrm{E}-05$ | $0.00 \mathrm{E}+00$ | $4.52 \mathrm{E}-04$ |
| Nonacosanoic acid | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | 0.00E+00 | $1.05 \mathrm{E}-04$ | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | $1.48 \mathrm{E}-04$ |
| Triacontanoic acid | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | 8.63E-04 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $3.34 \mathrm{E}-05$ | $0.00 \mathrm{E}+00$ | $4.30 \mathrm{E}-04$ |
| Butanedioic acid | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $2.68 \mathrm{E}-04$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | 0.00E+00 | $9.28 \mathrm{E}-04$ | $0.00 \mathrm{E}+00$ |
| Pentanedioic acid | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $6.81 \mathrm{E}-05$ | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | 0.00E+00 | $5.25 \mathrm{E}-04$ | $0.00 \mathrm{E}+00$ |
| Hexanedioic acid | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $1.76 \mathrm{E}-05$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | 6.38E-04 | $0.00 \mathrm{E}+00$ |
| Heptanedioic acid | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $1.29 \mathrm{E}-05$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ |
| Octanedioic acid | $9.58 \mathrm{E}-04$ | $1.05 \mathrm{E}-03$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $1.44 \mathrm{E}-04$ | $1.83 \mathrm{E}-04$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | 0.00E+00 | 6.14E-04 | $0.00 \mathrm{E}+00$ |
| Nonanedioic acid | $1.22 \mathrm{E}-03$ | $1.34 \mathrm{E}-03$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | 2.71E-04 | $1.60 \mathrm{E}-04$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ |
| 1-2-benzenedicarboxylic acid | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $5.40 \mathrm{E}-06$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ |
| 1-3-benzenedicarboxylic acid | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | 0.00E+00 | $7.30 \mathrm{E}-05$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ |
| 1-4-benzenedicarboxylic acid | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | 0.00E+00 | $3.31 \mathrm{E}-06$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | 5.13E-05 | 0.00E+00 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ |
| Nonadecanoic acid | $2.25 \mathrm{E}-05$ | $2.47 \mathrm{E}-05$ | 5.95E-05 | $1.60 \mathrm{E}-05$ | $1.58 \mathrm{E}-04$ | $5.31 \mathrm{E}-05$ | 0.00E+00 | 1.13E-05 | 0.00E+00 | $9.44 \mathrm{E}-05$ | $1.45 \mathrm{E}-04$ |
| 1-8-naphthalic anhydride | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | 0.00E+00 | $1.20 \mathrm{E}-05$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ |
| 1 H -phenalen-1-one | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $1.58 \mathrm{E}-04$ | $2.82 \mathrm{E}-04$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $1.47 \mathrm{E}-02$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ |
| Anthracen-9-10-dione | $7.18 \mathrm{E}-05$ | $7.88 \mathrm{E}-05$ | $5.45 \mathrm{E}-04$ | $5.57 \mathrm{E}-04$ | $5.06 \mathrm{E}-05$ | $9.11 \mathrm{E}-05$ | $0.00 \mathrm{E}+00$ | $5.49 \mathrm{E}-05$ | 4.71E-02 | $0.00 \mathrm{E}+00$ | 7.56E-06 |
| Benz(a)anthracene-7 12-dione | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | 2.95E-03 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ |
| Levoglucosan | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ | $9.31 \mathrm{E}-02$ | 1.13E-01 | 0.00E+00 | $0.00 \mathrm{E}+00$ | 0.00E+00 | $0.00 \mathrm{E}+00$ | $0.00 \mathrm{E}+00$ |



Figure S1. Monthly comparison of measured total carbon (OC + EC) to modeled carbon (primary organic, secondary organic, and elemental). There is a consistent underestimation during the warm months at all sites and the results are mixed at other times

Table S2. Paired model and observation quantities of each organic tracer at Bondville, IL in units of (ng/m ${ }^{\mathbf{3}}$ ) in the context of measurement detection limit (MDL ${ }^{\mathrm{a}}$ ) and measurement uncertainty ( $\mathrm{UNC}^{\mathrm{b}}$ ). Observations below the detection limit are denoted by ${ }^{\mathrm{c}}$.

| tracer | March04 |  | April04 |  | May04 |  | June04 |  | July04 |  | August04 |  | September04 |  | October04 |  | November04 |  | December04 |  | Janucry05 |  | February05 |  | $\mathrm{MDL}^{\text {a }} \quad \mathrm{UNC}^{\text {b }}$ |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | model | obs | model | obs | model | obs | model | obs | model | obs | model | obs | model | obs | mod | obs |  | obs |  | bs | model | obs | model | obs |  |  |
| Tetracosane | 1.87 |  | 2.11E-01 | 3.00E-02 | 1.90E-01 | $1.48 \mathrm{E}+00$ | 2.32E-01 | c | 01 | $9.40 \mathrm{E}-01$ | 01 | c | 3.15E-01 | c | 2.18E-01 | c | $3.44 \mathrm{E}-01$ | c | 01 | -01 | -01 | $1.55 \mathrm{E}+00$ | -01 |  | 7.78E-01 | 20\% |
| Penta | 185 E | 90E-01 | 2.04E-01 | 3.20E-01 | 1.70E-01 | 1.38E | 2.25E-01 | c | 2.60E-01 | 7.60E | 2.78E-01 | c | 3.11E-01 | c | 2.03E-01 |  | 3.34E-01 | c | 3.80E-01 | -01 | 2.63E-01 | $1.39 \mathrm{E}+00$ | 3.84E-0 | 90 E | $1.02 \mathrm{E}+00$ | 16\% |
| Hexacosane | 1.36E- | 9.00E-02 | 1.41 E | c | 1.11E-01 | $2.05 \mathrm{E}+00$ | 1.56E | c | 01 | 6.80E-01 | 1.73E-01 | c | 2.19E-01 | c | 1.35E-01 |  | 2.33E-01 | c | 2.77E-01 | 7.10E-01 | 1.82E-0) | $2.10 \mathrm{E}+00$ | 2.63E-01 | $1.40 \mathrm{E}+00$ | $1.30 \mathrm{E}+00$ | 16\% |
| Heptacosane | 1.97E-01 | c | 1.92E-01 | c | 1.31E-01 | $2.60 \mathrm{E}+00$ | 1.92E-01 | c | 45E-01 | 1.15E+00 | 1.51E-01 |  | 2.87E-01 |  | 1.49E-01 |  | 3.09E-01 |  | $4.30 \mathrm{E}-01$ | 2.20E-01 | 2.22E-01 | $2.48 \mathrm{E}+00$ | 3.24E-01 | $1.01 \mathrm{E}+00$ | $1.41 \mathrm{E}+00$ | 16\% |
| Octacosane | 9.14E-02 | c | 8.78E-02 | c | 6.16E-02 | $1.43 \mathrm{E}+00$ | 8.60E-02 | c | 6.90E-02 | 4.00E-01 | 7.28E-02 | c | 1.32E-01 | c | 7.27E-02 |  | 1.42E-01 | 1.90E-01 | 1.92E-01 | 5.40E-01 | 1.04E-01 | $1.55 \mathrm{E}+00$ | 1.52E-01 | 7.70E-01 | 7.88E-01 | 13\% |
| Nonacos | 3.56E- | c | 3.2 | 00E-01 | 1.91E-01 | $36 \mathrm{E}+0$ | 15E-01 | 9E+0 | $1.23 \mathrm{E}-01$ | 1.93E | 1.28E-01 |  | 4.76E-01 |  | $1.94 \mathrm{E}-$ |  | 5.15E-01 | DOE-01 | 8.28E | $1 \mathrm{E}+{ }^{\text {a }}$ | 3.46 E | OE+ | 5.01E-01 | 00 | 1.36E+00 | 27\% |
| Triacontane | 6.42E-02 | c | 6.58E-02 |  | 4.40E-02 | $2.14 \mathrm{E}+0$ | 6.23E-02 | OEE-0 | 5.36E-02 | $1.01 \mathrm{E}+0$ | 5.74E-02 | c | 9.42E-02 |  | 5.10E-02 |  | 1.06 E | 60E-01 | 1.37E-0 | 3.50E-0 | $7.16 \mathrm{E}-$ | 5.20E-0 | $1.08 \mathrm{E}-0$ | 7.40E-01 | 11E-2 | 40\% |
| Hentriacontane | $1.22 \mathrm{E}-01$ | c | 1.1 | 3.30E-01 | $6.63 \mathrm{E}-02$ | $1.87 \mathrm{E}+00$ | 1.09E-01 | 8.40E-01 | 4.59E-02 | 7.80E-01 | 4.75E-02 | c | 1.64E-01 | c | -02 | 6.20E-01 | 1.79E-01 | 9.50E-01 | 2.84E-01 | 4.50E-0 | 1.18E-01 | 5.80E-0 | 1.73E-01 | 6.20E-01 | 4.06E-01 | 40\% |
| Dotriacontane | 4.18E-02 | c | 4.27E-02 | c | 2.67E-02 | c | 3.95E-02 | $3.90 \mathrm{E}-01$ | 3.09E-02 | 4.50E-01 | 3.36E-02 | c | 5.99E-02 | c | 3.07E-02 | c | 6.85E-02 | 5.60E-01 | 9.03E-02 | 1.40E-01 | 4.43E-02 | 3.30E-01 | 6.70E-02 | 6.60E-01 | 3.40E-01 | 43\% |
| 22-29-30-trisnorhopane | 1.02E-02 | c | 1.33E-02 | c | 1.07E-02 | c | 1.36E-02 | c | 2.01E-02 | c | 2.21E-02 | c | 1.89E-02 | c | 1.36E-02 | c | 2.21E-02 | c | 1.95E-02 | c | 1.51E-02 | c | 2.31E-02 | c | 1.37E-02 | 28\% |
| 17-a(H)-21b(H)-29-norlopane | 2.17 | c | 2.8 |  | 2.32E-02 | c | 4E-0 | c | 4.59E-02 | c | -02 | c | 4.13E-02 |  | 2.94E-02 |  | 4.76E-02 | 4.00E-02 | 4.18E-12 | 6.00E-02 | 3.40E-02 |  | 5.09E-02 |  | 1.37E-02 | 14\% |
| 17-(H)-218(H)-hopane | 2.74E-02 | c | 3.58E-02 | c | 2.87E-02 | c | 3.74E-02 | 5.00E-02 | $5.52 \mathrm{E}-02$ | c | $6.03 \mathrm{E}-02$ | c | E-02 | 2.00E-02 | 3.67E-02 | 5.00E-02 | 5.93E-02 | 00E-02 | 5.22E-02 | .00E-02 | -02 | 5.00E-02 | -02 | 5.00E-02 | 1.37E | 14\% |
| 22R\&S-17a( | 2.5 | c | 3.32E-02 | c | 2.64E-02 | c | 3.34E-02 | c | 4.94E-02 | c | 5.46E-02 | c | 4.69E-02 | c | 3.39E-02 |  | 5.51E-02 | c | 4.85E-02 | c | 3.74E-02 | c | 5.76E-02 | c | 1.37E-02 | \% |
| 22R\&S-17a(H)-21b(H)-30-31bishomohopane |  |  | 1.76E-02 |  | 1.40E-02 | c | 1.3E-02 | c | 66E-02 | c | 2.92E-02 |  | E-02 |  | IE-02 |  | 2.91E-02 |  | $2.55 \mathrm{E}-02$ |  | 2.01E-02 |  | 3.09E-02 |  | 1.37E-02 | 14\% |
| $20 \mathrm{R}+\mathrm{S}$-ab--cholestane | 1.29E-02 | c | 1.71E-02 | c | 1.44E-02 | c | 1.86E-02 | c | 2.69E-02 | c | 2.98E-02 | c | 2.57E-02 | c | 1.84E-02 |  | 2.89E-02 | c | 2.59E-02 | c | 2.00E-02 | c | $2.96 \mathrm{E}-02$ |  | $1.37 \mathrm{E}-02$ | 32\% |
| 20R-aa-cholestane | 1.08E-02 | c | 1.4 | c | 1.25E-02 | c | 1.69E-02 | c | E-02 | c | E-02 | c | E-02 | c | 1.59E-02 |  | 2.45E-02 | c | 20E | c | 1.78E-02 | c | 78-210 | c | 37E | 28\% |
| 20R-S-abb-ergostane | 1.33E | c | 1.76E-02 | c | 1.47E-02 | c | 1.87E-02 | c | 2.71E-02 | c | 3.01E-02 |  | 2.61E-02 |  | 1.88E-02 |  | 2.96E-02 |  | 2.65E-02 |  | 2.04E-02 |  | 3.04E-02 |  | 37E-02 | 18\% |
| 20R+S-ab-sitostane | 1.4 | c | 1.94E-02 | c | 1.66E-02 | 00E-02 | 20E-21 | c | E-02 | c | 3.48E-02 | c | 2.96E-02 | c | 2.11E-02 | c | 3.28E-02 | c | 2.95E-02 | c | 2.33E-02 | c | 3.40E-02 | c | 1.37E-02 | 8\% |
| Fluoranthene | $4.16 \mathrm{E}-1$ | c | 4.61E-01 | $2.40 \mathrm{E}-01$ | 4.43E-01 | c | 01E-01 | c | $4.22 \mathrm{E}-01$ | 1.10E-01 | $4.61 \mathrm{E}-01$ | 1.00E-02 | 6.13E-01 | $2.00 \mathrm{E}-02$ | 3.76E-01 | 1.00E-02 | 7.10E-01 | 1.00E-02 | 1.03E+00 | 7.00E-02 | 5.86E-01 | 9.00E-02 | 9.51E-01 | 7.00E-02 | 2.73E-02 | 26\% |
| Acephenanthrylene | 8.46 | c | 7.65 | c | 4.04E-02 | c | 35E | c | 02 | c | $2.39 \mathrm{E}-02$ | c | 1.11 | c | 4.1 | c | 1.2 | c | 1.97 |  | 7.79 |  | 1.11E-01 |  | 2.73E-02 | 26 |
| Benzo(ghi) fluoranthene | 1.70 E | c | 2.04 | c | 2.2 | c | $2.30 \mathrm{E}-01$ | 3.00E-02 | 2.30E-01 | c | 2.52E-01 | c | 2.63E-01 | c | 1.85E-01 | c | 3.13E-01 | $8.00 \mathrm{E}-02$ | 4.32E-01 | $1.80 \mathrm{E}-01$ | 2.76E-01 | 2.2 | 4.61E-01 | $1.90 \mathrm{E}-01$ | 3.00E-02 | 25\% |
| Cyclopenta(cd)pyrene | 8.79E-02 | c | 8.40E-02 | c | 5.01E-02 | c | $9.06 \mathrm{E}-02$ | c | 5.15E-02 | c | 5.20E-02 | c | 1.26E-01 | c | -02 |  | -01 | c | $2.05 \mathrm{E}-01$ | 2.00E-02 | $9.34 \mathrm{E}-12$ | 9.00E-02 | 1.30E-01 |  | 2.73E-02 | 16\% |
| Benz(a)antracene | 2.26 | c | 2.64E-01 | c | 2.80E-01 | c | $2.90 \mathrm{E}-01$ | c | 2.71E-01 | $2.00 \mathrm{E}-02$ | 2.98E-01 | c | 3.39E-01 | 4.00E-02 | 2.30E-01 | 4.00E-02 | 4.02E-01 | 1.00E-02 | 5.72E-01 | 3.00E-02 | 3.48E-01 | 3.00E-02 | 5.83E-01 | 4.00E-02 | 2.73E-02 | 10\% |
| Chrysene/Triphenylene | $6.94 \mathrm{E}-01$ | c | 8.56E-20 | c | $9.97 \mathrm{E}-01$ | c | 9.61 E | c | $9.95 \mathrm{E}-01$ | $2.00 \mathrm{E}-02$ | 1.10E+00 |  | $1.07 \mathrm{E}+00$ |  | 8.01E-01 | c | 1.30E+00 | 4.00E-02 | 1.79E+00 | 8.00E-02 | $1.18 \mathrm{E}+00$ | 8.00E-02 | 2.02E+00 | 8.00E-02 | 2.73E-02 | 25\% |
| Retene | $1.21 \mathrm{E}+00$ | $5.90 \mathrm{E}-01$ | 1.06E | c | 5.29E-01 | c | 00 | c | 75E-01 | c | 1.64E-01 | 3.30E-01 | 1.55E+00 | c | 3E-01 | c | 1.66E+00 | c | $2.87 \mathrm{E}+00$ | 1.30 E | $1.06 \mathrm{E}+00$ | 1.00E | 1.49E+00 | 1.00E-02 |  | 29\% |
| Benzo(k)fluoranthene | $4.20 \mathrm{E}-01$ | c | 3.12E-01 | c | 3.91E-01 | c | 3.38E-01 | c | 4.93E-01 | c | 4.10E-01 | c | 6.16E-01 | c | 5.04E-01 | c | $5.68 \mathrm{E}-01$ | E-02 | 6.56E-01 | 4.00E-02 | 6.38E-01 | 4.0 | $9.34 \mathrm{E}-01$ | 5.00E-02 | 73E-02 | 38\% |
| Benzo(b)fluoranthene | 5.0 | 3.70E-01 | 3.21E-01 | c | 4.14E-01 | c | 9 E | 3.00E-02 | 56E-0 | 4.00E-02 | $4.20 \mathrm{E}-1$ | c | 25E | 6.00E-02 | 6.06E-01 | 5.00E-02 | 6.25E-01 | 9.00E-02 | 6.77E-01 | 1.00E-01 | 7.41 | 1.10E-0 | 1.04E+0 | 1.30E-0 | 2.73E-02 | 38\% |
| Benzo()ffluoranthene | 1.5 | c | 1.44 E | c | 25E-03 | c | 1.9E-02 | c | 7.04E-03 | c | $7.14 \mathrm{E}-03$ | c | 2.15E-02 | c | 8.62E-03 |  | $2.30 \mathrm{E}-02$ | c | 3.61E-02 | c | 1.55E-02 | 3.00E-02 | 2.16E-02 | c | 2.73E-02 | 38\% |
| Benzo(e)pyrene | 3.30E-01 | c | 1.86E-01 | c | $2.47 \mathrm{E}-01$ | c | 1.90E-01 | 2.00E-02 | 3.41E-01 | c | $2.35 \mathrm{E}-01$ | c | 4.67E-01 | $2.00 \mathrm{E}-02$ | 3.96E-01 | 5.00E-02 | 3.81E-01 | 5.00E-02 | 4.00E-01 | 7.00E-02 | 4.74E-01 | 1.00E-01 | 6.52E-01 | 7.00E-02 | 2.73E-02 | 25\% |
| Benzo(a)pyrene | 3.91E-02 | c | 3.61 | c | 2.02E-02 | c | 2E-02 | 2.00E-02 | 1.52E-02 | c | 1.56E-02 | c | 5.35E-02 | 1.00E-02 | 2.10E-02 | 2.00E-02 | 5.75E-02 | c | $9.13 \mathrm{E}-02$ | 7.00E-02 | 3.79E-02 | 4.00E-02 | 5.35E-02 | 6.00E-02 | 2.73E-02 | 25\% |
| Perylene | 1.19E-02 | c | 1.40E-02 | 20E-01 | 1.111--02 | c | 1.90E-02 | c | 2.11E-02 | 4.00E-02 | 2.16E-02 | c | 2.23E-02 | c | 1.30E-02 | c | 2.30E-02 | 1.00E-02 | $2.68 \mathrm{E}-02$ | 5.00E-02 | 1.89E-02 | 5.00E-02 | 2.53E-02 | 7.00E-02 | 2.73E-02 | 25\% |
| Indeno(cd) pyrene | 3.52E-01 | c | 1.67E-01 | c | 2.28E-01 | c | 1.65E-01 | c | 3.42E-01 | c | $2.06 \mathrm{E}-0$ | $4.00 \mathrm{E}-02$ | 4.92 | OOE-0 | 4.22E- | OE- | 3.73E | 6.00E-02 | 3.64 | 8.00E-02 | 4.92 | 1.00E-01 | 6.47E-0 | 1.00E-0 | 2.73E-02 | 29\% |
| Benzo(ghi) perylene | 3.00E | c | 1.75E-01 | c | 2.20E-01 | c | $2 \mathrm{E}-01$ | c | 3.69E-01 | c | $2.70 \mathrm{E}-01$ | 7.00E-02 | 4.54E-01 | 1.00E-01 | 3.77E-01 | 1.00E-01 | 3.66E-01 | 6.00E-02 | 3.48E-01 | 8.00E-02 | 4.47E-01 |  | 5.89E-01 | 1.00E-01 | 2.73E-02 | 12\% |
| Coronene | 1.71E-01 | c | 9.11E-02 | c | 1.10E-01 | c | 9.18E-02 | c | 1.60E-01 | c | 1.02E-01 | c | 2.41E-01 | c | 1.94E-01 | c | 1.92E-01 | $2.00 \mathrm{E}-02$ | 2.03E-01 | 4.00E-02 | $2.33 \mathrm{E}-01$ | 7.00E-02 | 3.08E-01 | 8.00E-02 | 3.41E-02 | 26\% |
| Tetradecanoic acid | 5.55E-01 | $3.45 \mathrm{E}+00$ | 5.80E-01 | $2.76 \mathrm{E}+00$ | 3.98E-01 | $1.03 \mathrm{E}+00$ | 5.64E-01 | c | 0E-01 | 9.90E-01 | 5.28E-01 | $2.85 \mathrm{E}+00$ | 8.29E-01 | c | 4.59E-01 | $1.66 \mathrm{E}+00$ | $9.03 \mathrm{E}-01$ | c | 1.21E+00 | c | 6.33 | $1.60 \mathrm{E}+01$ | 9.33E-01 | c | 2.17 E | 7\% |
| Pentadecanoic acid | 1.7 | 32E+00 | 1.75E | 27E+0 | 1.18E-01 | 5.30E-01 | 1.70E-0 | c | 1.24E-01 | 4.70E-01 | 1.52E-01 | $1.43 \mathrm{E}+0$ | 2.5 | c | 136E | .50E-01 | 2.73E-01 | c | 3.72 | c | 1.0E | $1.02 \mathrm{E}+01$ | 2.79E-01 | c | 1.33E+00 | 50\% |
| Hexadecanoic acid | 3.11E+ | $8.37 \mathrm{E}+00$ | 3.29E+00 | $3.80 \mathrm{E}+00$ | 2.29E+00 | $6.96 \mathrm{E}+00$ | 3.21E+00 | c | 2.56E+00 | 5.57E+00 | 3.17E+00 | $1.52 \mathrm{E}+01$ | 4.70E+00 | c | $2.67 \mathrm{E}+00$ | $9.17 \mathrm{E}+00$ | 5.11E+00 | c | 6.74E+00 | c | $3.61 \mathrm{E}+00$ | $6.82 \mathrm{E}+01$ | 5.32E+00 | c | 8.66E+00 | 53\% |
| Heptadecanoic acid | 1.89 | 7.30E- | 2.11E- | 5.40E-0 | 1.55E-01 | $2.40 \mathrm{E}-0$ | 2.07E-01 | c | $1.98 \mathrm{E}-01$ | 2.50E-01 | $2.48 \mathrm{E}-01$ | 4.50E-01 | 2.99E-01 | c | $1.88 \mathrm{E}-01$ | 2.00E-0 | 3.26E-01 | c | 01 | c | $2.36 \mathrm{E}-01$ | $1.76 \mathrm{E}+00$ | 3.50E-01 | c | 3.03E-01 | 76\% |
| Octadecanoic acid | $1.38 \mathrm{E}+00$ | $9.95 \mathrm{E}+00$ | 1.52E+00 | $2.83 \mathrm{E}+00$ | 1.10E+00 | 5.55E+00 | 1.47E+00 | c | 1.37E+00 | 3.63E+00 | 1.71E+00 | $1.22 \mathrm{E}+01$ | $2.14 \mathrm{E}+00$ | c | $1.33 \mathrm{E}+00$ | 6.80E-01 | $2.35 \mathrm{E}+00$ | c | 2.87E+00 | c | $1.68 \mathrm{E}+00$ | $1.28 \mathrm{E}+01$ | $2.50 \mathrm{E}+00$ | c | 4.56E+00 | 99\% |
| Eicosano | 2.78E-01 | $1.34 \mathrm{E}+00$ | 2.49E-01 | $1.07 \mathrm{E}+00$ | 1.30E-01 | 4.40E-01 | 2.35E-01 | c | E-02 | 7.70E-01 | 6.63E-02 | $2.47 \mathrm{E}+00$ | 3.63E-01 | c | $1.32 \mathrm{E}-01$ | c | 3.92E-01 | c | 6.49E-01 | c | 2.51E-01 | $1.35 \mathrm{E}+00$ | 3.59E-01 | c | 8.22E-01 | 8\% |
| Heneicosanoic acid | 6.911 | $4.30 \mathrm{E}-01$ | 6.05E-12 | c | 3.05E- | c | 5.75E-02 | c | 1.09E-02 | 1.80E-01 | 1.02E-12 | 1.40E-01 | 8.88E-02 | 1.00E-01 | 2.99E-02 | 6.90E-01 | 9.54E-02 | 8.00E-02 | 1.63E-0 | 5.90E-01 | 6.08E-02 | 3.20E-0 | 8.60E-02 | c | 8.22E-01 | 36\% |
| Docosanoic acid | $4.19 \mathrm{E}-1$ | $1.11 \mathrm{E}+00$ | 3.67E-01 | $9.60 \mathrm{E}-01$ | 1.86E-01 | 2.00E-01 | 3.49E-01 | c | 6.74E-02 | 7.40E-01 | 6.47E-02 | 1.12E+00 | 5.39E-01 | 1.10E-01 | $1.82 \mathrm{E}-01$ | 8.10E-01 | 5.79E-01 | c | $9.90 \mathrm{E}-01$ | 7.20E-01 | 3.69E-01 | $2.41 \mathrm{E}+00$ | 5.22E-01 | c | 2.23E-01 | 25\% |
| Tricosanoic acid | 1.70E-01 | $4.30 \mathrm{E}-01$ | 1.48E-01 | $4.40 \mathrm{E}-01$ | 7.46E-02 | c | 1.41E-01 | c | 2.56E-02 | 3.70E-01 | $2.39 \mathrm{E}-02$ | 2.80E-01 | 2.18E-01 | 1.60E-01 | 7.27E-02 | 2.60E-01 | 2.34E-01 | c | $4.02 \mathrm{E}-01$ | $2.00 \mathrm{E}-01$ | 1.49E-01 | 7.00E-01 | 2.10E-01 | c | 1.50E-01 | 24\% |
| Tetracosanoic acid | $9.34 \mathrm{E}-01$ | $1.61 \mathrm{E}+00$ | 8.17E-01 | $1.21 \mathrm{E}+00$ | 4.10E-01 | 6.70E-01 | 7.75E-01 | c | 1.39E-01 | 1.09E+00 | 1.30E-01 | 1.21E+00 | $1.20 \mathrm{E}+00$ | 4.10E-01 | 3.99E-01 | $1.32 \mathrm{E}+00$ | 1.29E+00 | c | 2.21E+00 | c | 8.18E-01 | $4.85 \mathrm{E}+00$ | 1.16E+00 | c | 6.29E-01 | 23\% |
| Pentacosanoic acid | 8.87E-02 | 6.40E-01 | 7.76E-02 |  | 3.90E-02 | c | 7.36E-02 | c | 1.35E-02 | 5.10E-01 | 1.26E-02 | 3.10E-01 | 1.14E-01 | 7.00E-02 | 3.81E-02 | $2.50 \mathrm{E}-01$ | 1.22E-01 | c | 2.10E-01 | c | 7.77E-02 | 6.00E-01 | 1.10E-01 | c | 3.72E-01 | 35\% |
| Hexacosanoic acid | 5.84E-01 | $1.00 \mathrm{E}+00$ | 5.12E-01 | $9.70 \mathrm{E}-01$ | 2.58E-01 | c | 4.86E-01 | c | 9.01E-02 | 8.10E-01 | 8.46E-02 | 5.80E-01 | 7.50E-01 | 3.60E-01 | 2.51E-01 | 8.00E-01 | 8.06E-01 | c | 1.38E+00 | 2.10E-01 | 5.13E-01 | $2.11 \mathrm{E}+00$ | 7.27E-01 | c | 4.60E-01 | 35\% |
| Heptacosanoic acid | 4.74E-02 | 6.40E-01 | 4.15E-02 |  | 2.10E-02 | c | 3.94E-02 | c | $7.51 \mathrm{E}-03$ | 4.70E-01 | 7.03E-03 |  | 6.09E-02 | 4.20E-01 | 2.06E-02 | 5.20E-01 | 6.55E-02 | c | 1.12E-01 | 5.00E-02 | 4.17E-02 | 1.90E-0 | 5.90E-02 | c | 3.05E-02 | 35\% |
| Octacosanoic acid | $3.11 \mathrm{E}-01$ | $1.54 \mathrm{E}+00$ | 2.72E-01 | $9.10 \mathrm{E}-01$ | 39E-1 | c | .59E-0 | c | 55E-02 | 8.00E-01 | 4.76E-02 | 8.30E-01 | 3.99E-01 | $1.04 \mathrm{E}+00$ | 1.35E-01 | $1.54 \mathrm{E}+00$ | 4.29E-01 | 2.70E-01 | 7.35E-01 | 5.30E-01 | 2.74E-01 | 6.90E-01 | 3.88E-01 | c | $2.34 \mathrm{E}-01$ | 47\% |
| Nonacosanoic acid | 4.39E-02 | c | 3.85E-02 | c | 1.96E-02 | c | 3.65E-02 | c | 7.56E-03 | 5.30E-01 | 7.10E-03 | 3.50E-01 | 5.66E-02 | 3.10E-01 | 1.94E-02 | 3.80E-01 | 6.08E-02 | 6.00E-02 | 1.04E-01 | 5.00E-02 | 3.88E-02 | 1.40E-01 | 5.50E-02 | 1.00E-02 | 2.34E-01 | 32\% |
| Triacontanoic acid | $3.58 \mathrm{E}-01$ | $1.01 \mathrm{E}+00$ | 3.13E-01 | 7.40E-01 | 1.58E-01 | c | 2.98E-01 | $3.80 \mathrm{E}-01$ | 5.60E-02 | 7.60E-01 | 5.25E-02 | c | 4.60E-01 | $1.53 \mathrm{E}+00$ | 1.55E-01 | $2.32 \mathrm{E}+00$ | 4.94E-01 | 6.30E-01 | 8.47E-01 | 6.00E-01 | 3.15E-01 | 4.10E-01 | 4.45E-01 | 1.00E-02 | 2.34E-01 | 17\% |
| Butanedioic acid | 1.58E-01 | $4.41 \mathrm{E}+00$ | 1.57E-01 | $3.40 \mathrm{E}-01$ | 9.77E-02 | $3.08 \mathrm{E}+00$ | 1.52E-01 | 4.10E-01 | 9.00E-02 | 5.04E+00 | 1.12E-01 | $1.32 \mathrm{E}+00$ | 2.26E-01 | $4.79 \mathrm{E}+00$ | 1.11E-01 | 8.70E-01 | $2.43 \mathrm{E}-01$ | 3.50E-01 | 3.53E-01 | $9.30 \mathrm{E}-01$ | 1.67E-01 | 4.10E-01 | 2.41E-01 | $2.92 \mathrm{E}+00$ | 1.28E+00 | 42\% |
| Pentanedioic acid | 5.51E-02 | $1.83 \mathrm{E}+00$ | 5.85E-02 |  | 4.02E-02 | 5.90E-01 | 5.74E-02 | c | 4.59E-02 | 7.90E-01 | 5.85E-02 | 6.00E-02 | 8.38E-02 | 1.03E+00 | 4.82E-02 | c | $9.01 \mathrm{E}-02$ | c | 1.18E-01 | 6.00E-02 | 6.43E-02 | 7.00E-02 | 9.35E-02 | $9.50 \mathrm{E}-01$ | 1.52E+00 | 42\% |
| Hexanedioic acid | 4.02E-02 | 6.20E-01 | 4.77E-02 | 1.90E-01 | 3.71E-02 | c | 4.76E-02 | c | 5.20E-02 | 1.00E-01 | 6.75E-02 | c | 6.75E-02 | 1.00E-01 | 4.72E-02 | c | 7.26E-02 | c | 7.97E-02 | c | 5.47E-02 | 8.00E-02 | 8.06E-02 | c | $1.31 \mathrm{E}+00$ | 42\% |
| Heptanedioic acid | 5.29E-03 | 90e-01 | 4.62E-03 | c | 31E-03 | c | -39E-0 | c | 7.67E-0 | c | 15E-04 | c | 8E-0 | 1.80E-01 | 2.24E-0 | c | $28 \mathrm{E}-0$ | c | .25E-02 | c | 4.62E-03 | c | 6.53E-03 | 2.10E-0 | 1.32E+0 | 42\% |
| Octanedioic acid | 1.53E-01 |  | 1.69E-01 |  | 1.10E-01 | c | 1.44E-01 | c | 1.46E-01 | 9.00E-02 | 1.73E-01 | 6.00E-02 | 2.22E-01 | $2.90 \mathrm{E}-01$ | 1.34E-01 |  | 2.65E-01 | c | 3.03E-01 | 3.10E-01 | 1.70E-01 | 7.00E-02 | 2.69E-01 | 1.20E-01 | $1.32 \mathrm{E}+00$ | 42\% |
| Nonanedioic acid | 1.90E-01 | 7.60E-01 | 1.96E-01 | $2.80 \mathrm{E}-01$ | 1.14E-01 | 7.00E-02 | 1.62E-01 | $2.50 \mathrm{E}-01$ | 1.29E-01 | 1.00E-01 | 1.44E-01 | $6.30 \mathrm{E}-01$ | 2.58E-01 | 4.70E-01 | $1.32 \mathrm{E}-01$ | 3.60E-01 | 3.10E-01 | $4.50 \mathrm{E}-01$ | 3.95E-01 | $4.60 \mathrm{E}-01$ | 1.89E-01 | 4.00E-01 | 3.00E-01 | $3.50 \mathrm{E}-01$ | $1.18 \mathrm{E}+00$ | $42 \%$ |


| tracer | March04 |  | April04 |  | May04 |  | June04 |  | July04 |  | August04 |  | September04 |  | October04 |  | November04 |  | December04 |  | Janucry05 |  | February05 |  | MDL ${ }^{\text {a }}$ | UNC ${ }^{\text {b }}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1-2-ben | $2.22 \mathrm{E}-03$ | $1.14 \mathrm{E}+00$ | 1.94E-03 | LOE-M | 9.72E-04 | $1.07 \mathrm{E}+00$ | 1.84E-03 | c | 3.22E-04 | $1.70 \mathrm{E}+00$ | 3.01E-04 | $2.90 \mathrm{E}-01$ | 2.85E-03 | 00 | $9.43 \mathrm{E}-04$ | 1.00E-01 | 3.06E-03 |  | 5.27E-03 | 1.70E-01 | $1.94 \mathrm{E}-03$ |  | 2.75E-03 | $9.60 \mathrm{E}-01$ | 1.29E+00 | 38\% |
| 1-3-b | 2.00E-04 | 1.90E-01 | 3.19E-04 |  | 1.70E-04 |  | 1.52E-04 | c | 2.21E-04 |  | 1.79E-04 |  | 5.07E-04 |  | 2.38E-04 |  | 3.30E-04 |  | 5.10E-04 |  | 7.76E-04 |  | 6.15E-04 | .60E-01 | $1.34 \mathrm{E}+00$ | 38\% |
| 1-4-benzenedicarboxylic acid | 1.50E-03 | OE- | 1.41E-03 | 1.00E-0 | 7.14E-04 | 3.70E-01 | 1.24E-03 | c | 3.52E-04 | 30E-0 | 3.10E-04 | 3.50E-0 | 2.10E-03 | 7.70E-01 | 7.45E-04 | $2.60 \mathrm{E}-01$ | 2.11E-03 | 9.00E-02 | 3.58E-03 | 2E+00 | 1.74 | $2.20 \mathrm{E}-01$ | 2.111 | 5.70E-01 | 1.27 E | 38\% |
| Nonadecanoic acid | 7.34E-02 | 0e-01 | 6.73E-02 | 1.30E-0 | 3.69E-02 | c | 6.40E-02 | c | 2.29E-02 | 1.60E-01 | 2.52E-02 | 1.30E-01 | 9.80E-02 | c | 3.87E-02 | 1.50E- | 1.06E-01 | c | 1.70E-01 | c | $6.88 \mathrm{E}-02$ | $2.20 \mathrm{E}-01$ | 9.8 | c | 1.45E-01 | 73\% |
| 1-8-naphthalic anhydride | 4.95E-03 | c | 4.32E-03 | c | 2.16E-03 | c | 4.10E-03 | c | 7.17E-04 | c | 6.69E-04 | c | $6.34 \mathrm{E}-03$ |  | 2.10E-03 | c | 6.81E-03 |  | 1.17E-02 |  | $4.32 \mathrm{E}-03$ | c | $6.11 \mathrm{E}-03$ |  | 2.78E+00 | 16\% |
| 1 H -phenalen-1-one | $2.66 \mathrm{E}-01$ | c | 3.12E-01 | c | 3.38E-01 | c | 3.43E-01 | c | 3.21E-01 | c | 3.54E-01 |  | 3.98E-01 |  | $2.73 \mathrm{E}-01$ |  | 4.75E-01 | c | 6.79E-01 |  | $4.15 \mathrm{E}-01$ |  | $6.99 \mathrm{E}-01$ |  | 1.74E+00 | 16\% |
| Anthracen-9-10-dione | $6.88 \mathrm{E}-01$ |  | $8.65 \mathrm{E}-01$ | c | 1.02E+00 |  | $9.80 \mathrm{E}-01$ | c | 1.05E+00 | c | 1.17E+00 |  | 1.08E+00 |  | 8.28E-01 |  | 1.31E+00 | .00E-2 | 1.77E+00 | 10E | $1.20 \mathrm{E}+00$ | 00E | 2.06E+ | 1.10E- | 7.41E-1 | 16\% |
| Benz(a)antracen | $4.03 \mathrm{E}-02$ | c | 5.11 E | c | 6.19E-02 | c | 5.79E-02 | c | 6.24E-02 | c | $6.92 \mathrm{E}-02$ | c | 6.30E-02 | c | 4.92E-02 | c | .11E | c | 1.05 E | 10 E | 7.17 E | c | 1.24E-0 | c | 7.06E-01 | 16\% |
| Levoglucosan | 3.83E+01 | $4.23 \mathrm{E}+01$ | 3.35E | c | 1.77E | 28+01 | 18E+01 | $3.04 \mathrm{E}+01$ | 5.55E+00 | $2.53 \mathrm{E}+01$ | 5.18E+00 | $1.60 \mathrm{E}+01$ | 4.91E+01 | 1.64E+01 | 1.63E+01 | $3.77 \mathrm{E}+01$ | 5.27E+01 | 7.76E+0 | 9.08 E | $7.30 \mathrm{E}+01$ | 3.35E+01 | $1.32 \mathrm{E}+01$ | 4.73E+01 | $5.50 \mathrm{E}+01$ | 2.70E+00 | 37\% |
| 3-Acetylpentanedioic acid | 3.31E-02 | c | 1.77 E | OE-0 | 1.32E-01 | OE+00 | 1.42 | OE+ | 4.49E-01 | $1.33 \mathrm{E}+01$ | 3.36E-01 | $6.60 \mathrm{E}+00$ | 4.2 | c | 8.0 | 1.70E+00 | 1.40E-01 | $1.60 \mathrm{E}+00$ | 6.79 | $1.10 \mathrm{E}+00$ | 1.0 | c | 3.39E-02 | c | 1.00 |  |
| 2-Hydroxy-4-isopropyladipic a | 6.04E-02 | E+ | 3.23E-01 | E+00 | 2.40E-01 | $2.33 \mathrm{E}+01$ | 2.59E-01 | $2.49 \mathrm{E}+01$ | 8.19E-01 | 4.91E+01 | 6.13E-01 | $3.14 \mathrm{E}+01$ | 7.78E-01 | $1.30 \mathrm{E}+00$ | 1.47E-01 | $1.25 \mathrm{E}+01$ | 2.55E-01 | 2.79E+01 | 1.24E-01 | $2.42 \mathrm{E}+01$ | 1.86E-01 |  | 6.17E-02 | 3.00E+00 | 1.00E-01 |  |
| 3 -Acetyl hexanedioic acid | $4.16 \mathrm{E}-01$ | OE-0 | 23E | OE-0 | 1.65E | 50E+0 | 1.79E+ | $2.20 \mathrm{E}+0$ | 5.65E | $7.50 \mathrm{E}+0$ | 4.23E+ | $4.10 \mathrm{E}+0$ | 5.37E | 4.00E-01 | 1.02 E | 8.00E- | 1.7 | 7.00E-0 | 8.53 | Oe- | $1.28 \mathrm{E}+00$ | c | 4.26E-01 | 1.00E-01 | 1.00E- |  |
| 3-Hydroxyglutaric acid | 4.67E-02 | 7.20E+00 | $2.50 \mathrm{E}-0$ | $1.31 \mathrm{E}+01$ | 1.86E-10 | $2.83 \mathrm{E}+01$ | 2.00E-0 | 3.11E+01 | 6.34E-1 | 2 + + | 4.74E | $3.67 \mathrm{E}+01$ | 6.02E | 3.60E+ | 1.14E-01 | E+0 | 1.97E-01 | $1.41 \mathrm{E}+01$ | 9.57E-02 | 1.70E+01 | 1.44E-01 | c | 4.78E-02 | 20 E | 1.00E |  |
| ${ }_{\text {acid }}{ }^{2-H y}$ | 3.44E-02 | 4.00E-01 | E-0 | E-0 | 1.37E-01 | E+0 | $1.48 \mathrm{E}-01$ | 1.80E+0 | 4.67E-01 | OE+0 | 3.49E-01 | OE+0 | 4.44E-01 |  | 8.41E-02 | .00E-01 | 1.45E-01 | $1.30 \mathrm{E}+00$ | 7.05E-02 | $1.40 \mathrm{E}+00$ | 1.06E-01 |  | $3.52 \mathrm{E}-02$ | 1.00E-01 | 1.00E-01 |  |
| 3-(2-Hydroxy-ethyl)-2-2-dimethyl-cyclobutane-carboxylic acid | $2.29 \mathrm{E}-01$ |  | 1.23E+00 |  | 9.11E-01 | E-01 | E-01 | $2.00 \mathrm{E}-01$ | 3.11E+ | 1.00E-01 | 2.33E+0 | $6.00 \mathrm{E}-01$ | $2.96 \mathrm{E}+00$ | 1.00E-01 | $5.60 \mathrm{E}-01$ | $2.00 \mathrm{E}-01$ | 9.67E-01 | 1.00E-01 | 4.70E-01 | 3.00E-01 | 7.05E-01 |  | 2.35E- |  | 1.00E-01 |  |
| Pinic acid | 1.69E-01 | c | $9.01 \mathrm{E}-01$ | 8.00E-01 | 6.70E-01 | 7.00E-01 | 7.23E-01 | 5.00E-01 | 2.29E+00 | 2.00E-01 | $1.71 \mathrm{E}+00$ | 9.00E-01 | 2.17E+00 | 5.00E-01 | 4.12E-01 | 4.00E-01 | 7.11E-01 | 5.00E-01 | 3.46E-01 | $1.70 \mathrm{E}+00$ | 5.18E-01 | c | 1.72E-01 | c | 1.00E-01 |  |
| Pinonic ac | 8.13E-02 | c | 4.3 | DE-2 | 3.23E-01 | 00E-01 | 88E-01 | OE-0 | 1.10E+00 | OOE-0 | 8.25E- | OOE-01 | 1.05E+ | . $00 \mathrm{E}-01$ | 1.98E-01 | 3.00E-0 | 3.43E-01 | 3.00E- | $1.66 \mathrm{E}-01$ | 1.20 E | 2.50 E | c | 8.31 | c | 1.00E |  |
| 2-3-Dihydroxy-4-oxopentanoic acid | 1.64E-01 | 8.00E-01 | 2.41E-01 | 4.00E-01 | 2.08E-01 | $1.60 \mathrm{E}+00$ | 1.95E-01 | $1.70 \mathrm{E}+00$ | 3.98E-01 | $2.40 \mathrm{E}+00$ | 3.25E-01 | $1.80 \mathrm{E}+00$ | 4.39E-01 | 3.00E-01 | 1.77E-01 | $9.00 \mathrm{E}-01$ | 1.90E-01 | $1.00 \mathrm{E}+00$ | 2.35E-01 | $1.00 \mathrm{E}+00$ | 1.02E-01 |  | 3.58E-01 | 8.00E-01 | 1.00E-01 |  |
| 2-Methylglyceric acic | 5.96E-01 | 1.80E+00 | 8.10E-01 | $2.00 \mathrm{E}+00$ | 1.55E+00 | $1.31 \mathrm{E}+01$ | 1.49E+00 | $2.09 \mathrm{E}+01$ | $4.10 \mathrm{E}+00$ | $3.44 \mathrm{E}+01$ | $2.66 \mathrm{E}+00$ | $1.85 \mathrm{E}+01$ | 3.13E+00 | 1.20E+00 | 4.35E-01 | $3.60 \mathrm{E}+00$ | 6.60E-01 | $2.60 \mathrm{E}+0$ | 1.09E+ | $2.00 \mathrm{E}+0$ | 7.24E-0 | c | 1.02E+0 | E+00 | 1.00E-01 |  |
| 2-Methylthreitol | 1.1E+00 | 0E-01 | 137E+00 | 00E-01 | $2.61 \mathrm{E}+00$ | 3.21E+01 | 2.51E+00 | 4.07E+01 | 92E+00 | 5.55E+0 | 49E+0 | 61E+0 | 5.28E+00 | c | .33E-0 | .20E+0 | 11E+0 | $4.00 \mathrm{E}-0$ | 1.84E+00 | 1.00E-01 | $122 \mathrm{E}+0$ | c | 1.72E+0 |  | 1.00E-01 |  |
| 2 -Methylerythritol | 1.65E+00 | OE-01 | 2.25E+00 | 1.00E+00 | 4.29E+00 | 6.41E+01 | 4.12E+00 | $7.92 \mathrm{E}+01$ | 1.14E+01 | $1.13 \mathrm{E}+02$ | 7.39E+00 | $3.61 \mathrm{E}+01$ | 8.69E+00 | c | 1.21E+00 | $2.60 \mathrm{E}+00$ | 1.83E+00 | 9.00E-01 | 3.02E+00 | 1.00E-01 | $2.01 \mathrm{E}+00$ | c | $2.82 \mathrm{E}+00$ | 2.00E-01 | 1.00E-01 |  |
| Caryophyllinic aci | $1.08 \mathrm{E}-02$ | $2.80 \mathrm{E}+00$ | 7.12E-01 | 1.6 | $1.16 \mathrm{E}+00$ | 1.50 | $1.28 \mathrm{E}+00$ | $1.00 \mathrm{E}+00$ | $4.51 \mathrm{E}+00$ | $5.40 \mathrm{E}+00$ | 3.61 | 3.30 E | 2.72 | $2.50 \mathrm{E}+0$ | 4.14E-01 | 2.60 E | 3.55E | 3.10E | 2.67 | 2.90 E | 2.49E-02 |  | 1.09 E | 3.00 E | 1.00 |  |

Table S3. Paired model and observation quantities of each organic tracer at Northbrook, IL in units of ( $\mathbf{n g} / \mathrm{m}^{\mathbf{3}}$ ) in the context of measurement detection limit (MDL ${ }^{\text {a }}$ ) and measurement uncertainty ( $\mathrm{UNC}^{\mathrm{b}}$ ). Observations below the detection limit are denoted by ${ }^{\mathrm{c}}$.

| tracer | March04 |  | April04 |  | May04 |  | June04 |  | July04 |  | August04 |  | September04 |  | October04 |  | November04 |  | December04 |  | nucry05 |  | February05 |  | MDL ${ }^{\text {a }}$ | UNC ${ }^{\text {b }}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | m | bs | model | obs | model | obs | model | obs | model | obs | model | obs | model | bs | mo | bs |  | obs | mo | obs | mod | bs | mod | obs |  |  |
| Tetracosane | $3.97 \mathrm{E}-01$ | 1.37E+00 | 3.94E-01 | 2.70E-01 | 3.36E-01 |  | 7.12E-01 | 1.2 | 4.14E-01 | c | $6.85 \mathrm{E}-01$ |  | 8.95E-01 | 5.10E-01 | 4.72E-01 | $2.45 \mathrm{E}+00$ | 6.15E-01 | $3.40 \mathrm{E}-01$ | 01 | $1.31 \mathrm{E}+00$ | $2.98 \mathrm{E}-01$ | 01 | 5.52E-01 | 0 | 7.78E-01 | 20\% |
| Pentac | 3.69E-01 | 1.36 | 3.79E | 8.10 E | 3.18E-01 |  | 7.15E-01 | 2.42E | 4.00E-01 |  | 6.71E-01 | c | 8.42E-01 |  | $4.47 \mathrm{E}-01$ | $2.86 \mathrm{E}+00$ | 5.83E-01 | 2.70 E | $4.25 \mathrm{E}-01$ |  | $2.88 \mathrm{E}-01$ | 9.70E-01 | .24E-01 | 00 | -02E+00 | 16\% |
| Hexacosan | 2.32 | 1.39 E | 2.43E | 9.20E-01 | 2.01 |  | 4.80E-01 | $1.73 \mathrm{E}+00$ | 2.63E-01 | 1.00E-02 | 4.31 | c | 5.37E-01 |  | 2.86E-01 | $3.99 \mathrm{E}+00$ | 3.75E-01 | +00 | 3.00E-01 | $9.00 \mathrm{E}-02$ | 2.07E-01 | EE+00 | 01 | 6E+00 | 1.30E+00 | \% |
| Heptacosane | 2.63E-01 | 1.79E+00 | 2.64E-01 | $9.60 \mathrm{E}-01$ | 1.77E-01 |  | 3.51E-01 | $3.16 \mathrm{E}+00$ | 1.95E-01 |  | 3.03E-01 |  | 4.65E-01 | $4.30 \mathrm{E}-01$ | $2.60 \mathrm{E}-01$ | $3.87 \mathrm{E}+00$ | 4.01E-01 | $2.43 \mathrm{E}+00$ | 3.88E-01 | c | 2.53E-01 | $1.78 \mathrm{E}+00$ | 3.87E-01 | $2.33 \mathrm{E}+00$ | $1.41 \mathrm{E}+00$ | \% |
| Octacosane | 1.28E-01 | 6.30E-01 | 1.26E-01 | 2.20E-01 | 8.43E-02 | c | 1.50E-01 | $1.37 \mathrm{E}+00$ | 8.89E-02 | 6.30E-01 | 1.38E-01 | c | 2.19E-01 | c | 1.23E-01 | $2.45 \mathrm{E}+00$ | 1.91E-01 | $2.27 \mathrm{E}+00$ | 1.75E-01 |  | $1.13 \mathrm{E}-01$ | 6.60E-01 | 1.82E-01 | $1.06 \mathrm{E}+00$ | 7.88E-01 | 13\% |
| Nona | 3.49E-01 | $2.06 \mathrm{E}+00$ | 3.53E | $2.63 \mathrm{E}+00$ | 1.75E-01 |  | 2.67E-01 | 5.43E+00 | 1.25E-01 | 3.31E+00 | 1.77E-01 |  | 4.52E-01 | 10E-01 | 2.56E-01 | 6.36E+00 | 5.06E-01 | $1.20 \mathrm{E}+01$ | 6.49E-1 | 1.03E+00 | 4.17E-01 | $2.78 \mathrm{E}+00$ | 5.43E-01 | $3.11 \mathrm{E}+00$ | 1.36E+00 | 27\% |
| Triaconta | $9.35 \mathrm{E}-02$ | 4.60E-01 | 9.20E |  | 5.94 E |  | 1.21E-01 | 3E+ | 7.44E-02 | 4.20E-01 | 1.05E |  | 1.55E-01 |  | 9.76 E | $1.33 \mathrm{E}+00$ | 1.4 | 9E+ | 1.29 E | 190E-I | 8.06E | 8.60E-0 | 1.31E-2 | 0 | 11 | 40\% |
| Hentriacontane | 1.19 | 70 | 1.21 | $2.90 \mathrm{E}-01$ | 5.95 | 7.00E-02 | 1.00E-01 | $1.55 \mathrm{E}+00$ | 4.87E-02 | -01 | 6.50E-02 | 3.90E-01 | 1.55E-01 | $1.19 \mathrm{E}+00$ | 9.26E-02 | $1.30 \mathrm{E}+00$ | 1.77E-01 | 2.26 | 2.24E-01 | 4.50E-01 | 1.44E-01 | 1.6 | 1.87E-01 | 6.10E-01 | 4.06E-01 | 40\% |
| Dotriacontane | $5.73 \mathrm{E}-02$ | 6.70E-01 | 5.68E-02 | c | 3.39E-02 | c | 6.94E-02 | c | $4.28 \mathrm{E}-02$ | $2.10 \mathrm{E}-01$ | 5.78E-02 | c | 8.76E-02 | $2.60 \mathrm{E}-01$ | 5.80E-02 | 4.00E-01 | 9.07E-02 | $1.15 \mathrm{E}+00$ | 8.21E-02 | 2.20E-01 | 5.05E-02 | $1.72 \mathrm{E}+00$ | 8.07E-02 | 6.00E-01 | 3.40E-01 | 43\% |
| 22-29-30-trisnorhopane | 2.62E-02 |  | 2.67E-02 |  | 2.20E-02 | 6.00E-02 | 5.48E-02 | c | 3.29E-02 | 6.00E-02 | 5.06E-02 |  | 5.75E-02 | c | 3.57E-02 | 5.00E-02 | 4.47E-02 | c | $2.68 \mathrm{E}-02$ | 4.00E-02 | 1.64E-02 | c | 3.47E-02 |  | 1.37E-02 | 28\% |
| 17-a(H)-21b(H)-29-nortopane | 5.76E-02 | $2.40 \mathrm{E}-0$ | 6.09E-02 | 1.40E-01 | 5.29E-02 | 20e-01 | 1.40E-01 | 1.90E-01 | 8E-02 | - | 1.27E-01 | $1.20 \mathrm{E}-01$ | 1.40E-01 | $2.30 \mathrm{E}-01$ | 8.21E-02 | 1.60E-01 | 9.99E-02 | 6.00E-02 | 6.05E-02 | 1.30E-01 | 3.86E-02 |  | 7.99E-02 | 1.50E-01 | 1.37E-02 | 14\% |
| 17-a(H)-218(H)-hopane | 7.00E-02 | 2.40E-01 | $7.24 \mathrm{E}-02$ | 1.40E-01 | 6.08E-02 | 1.20E-01 | 56E | c | 9.19E-02 | -02 | $1.43 \mathrm{E}-01$ | 1.00E-01 | 1.60E-01 | $2.10 \mathrm{E}-01$ | 9.71E-02 | 1.50E-01 | 1.20 | 8.00E-02 | 7.25E-02 | 9.0 | $4.58 \mathrm{E}-12$ | 1.50E- | $9.51 \mathrm{E}-02$ | 1.60E-01 | 1.37E-02 | 14\% |
| 22R\&S-17a(H) homohopane | 6.5 | c | 6.60E-02 | 1.42E-01 | 5.35E-02 | $1.30 \mathrm{E}-01$ | $1.32 \mathrm{E}-01$ | c | $8.03 \mathrm{E}-02$ | $1.20 \mathrm{E}-01$ | $1.22 \mathrm{E}-01$ | c | 1.40E-01 | c | 8.78E-02 | 1.80E-01 | 1.11E-01 | c | $6.62 \mathrm{E}-02$ | 9.00E-02 | 4.01E-02 | c | $8.58 \mathrm{E}-02$ | 3.20E-01 | 1.37E-02 |  |
| 22R\&S-17a(H)-21b(H)-30-3 bishomohopane |  |  |  |  |  |  |  |  | 4.39E-02 |  | 6.73E-02 |  | 7.62E-02 |  | $4.69 \mathrm{E}-02$ |  | 5.87E-02 |  | 3.52E-02 |  | $2.19 \mathrm{E}-12$ |  | 4.61E-02 |  | 1.37E-02 | 14\% |
| 20R + S-ab--cholestane | 3.45E-02 | c | 3.56E-02 | c | 3.02E-02 | 6.00E-02 | 7.58E-02 | c | 4.40E-02 | c | $6.99 \mathrm{E}-02$ | c | 7.87E-02 | c | 4.79E-02 | 5.00E-02 | 5.92E-02 |  | 3.61E-02 | 6.00E-02 | 2.20E-02 |  | 4.58E-02 |  | 1.37E-02 | 32\% |
| 20R-aaa-cholestane | $2.91 \mathrm{E}-02$ | c | 3.12E-02 | c | 2.79E-02 | 4.00E-02 | 7.37E-02 | c | 4.09E-02 | c | $6.72 \mathrm{E}-02$ | c | 7.34E-02 |  | 4.25E-02 | 5.00E-02 | 5.07E-02 |  | 3.16E-02 | 3.00E-02 | 2.03E-02 |  | 4.06E-02 |  | 1.37E-02 | \% |
| 20R+S-ab-ergostane | 3.51E-02 |  | 3.58E-02 |  | 2.99E-02 | 5.00E-02 | 7.40E-02 | 00E-02 | 02 | c | $6.86 \mathrm{E}-02$ | c | 7.79E-02 |  | $4.80 \mathrm{E}-02$ | OE-02 | -02 |  | 3.65E-02 | 2.00E-02 | 2.21E-02 |  | 4.62E-02 |  | 37E-02 | 18\% |
| 20R + S-ab-sitostane | 3.93E-02 |  | 4.15E-02 |  | 3.64E-02 | 00E-02 | 44E-6 | c | 5.31E-02 | c | 8.64E-02 | c | $9.54 \mathrm{E}-12$ | c | 5.62E-02 | 9.00E-02 | 6.80E-02 | c | 4.20E-02 | 6.00E-02 | 2.63E-02 | c | 5.36E-02 | c | 1.37E-02 | 28\% |
| Fluoranthene | 7.02E | 2.80E-01 | 6.25E-01 | $1.20 \mathrm{E}-01$ | 4.91 E | 8.00E-02 | 6.75E-01 | $2.90 \mathrm{E}-01$ | 4.22E-01 | 8.00E-02 | 6.86E-01 | 1.70E-01 | 1.36E+00 | 3.00E-01 | 6.4 | 1.60E-0 | 9.67E-01 | 3.50E-01 | 8.59E-01 | $1.63 \mathrm{E}+00$ | 6.58E-01 | $3.19 \mathrm{E}+00$ | 9.93E-01 | 1.27E+0 | 2.73E-02 | 26\% |
| Acephenanthrylene | 7.5 | c | 7.99E-02 | c | 3.65E-02 | c | 6.79E-02 | c | 2.88E-02 | c | -02 | c | 9.36E-02 | c | 5.60E-02 | c | 1.14E-10 | c | 1.55E | c | $9.77 \mathrm{E}-02$ | 4.00 | 1.23E-01 | c | 2.73E-02 | 26\% |
| Benzo(ghi)fluoranthene | 3.48E-01 | $2.20 \mathrm{E}-0$ | 3.00E-01 | c | 2.59E-01 | 1.30E-01 | 3.49E-01 | c | $2.30 \mathrm{E}-01$ | c | 3.79E-01 | 1.90E-01 | 7.24E-01 | $4.20 \mathrm{E}-01$ | 3.35E-01 | 2.30E-01 | 4.73E-01 | $1.01 \mathrm{E}+00$ | 3.70E-01 | $2.86 \mathrm{E}+00$ | 3.0 | +00 | 4.79E-01 | 4.20E+00 | 3.00E-02 | 25\% |
| Cyclopenta(cd)pyrene | $9.66 \mathrm{E}-02$ |  | 1.10E |  | 7.42E-02 |  | 1.91E-01 | c | 02 | c | 1.48E-01 | c | 1.97 E | c | 1.03E-01 | 8.00E-02 | 1.57E-01 | 5.00E-02 | 1.80E | 1.50E-0 | 1.20E-0 | 4.20E-01 | 1.63E-0 | 2.80E-01 | 2.73E-02 | 16\% |
| Benz(a)antrracene | $4.32 \mathrm{E}-2$ | 7.00E-02 | 3.68E-01 | 5.00E-02 | 3.04E-01 | 3.00E-02 | 3.65E-01 | 4.00E-02 | 2.51E-01 | 1.00E-02 | 4.06E-01 | 5.00E-02 | 8.51E-01 | 1.00E-01 | 3.94E-0 | 5.00E-12 | 5.79E-01 | 7.00E-02 | 4.74E-1 | 1.30E-01 | 3.80E-01 | 3.20E-01 | 5.92E-01 | $2.30 \mathrm{E}-01$ | 2.73E-02 | 10\% |
| Chrysene/Triphenylene | 1.51 E | 1.80E-01 | 1.25E+00 | 1.30E-01 | 1.09E+00 | 8.00E-02 | 1.25E+00 | 6.00E-02 | 9.06E-01 | 5.00E-02 | 1.48E+00 | 7.00E-02 | 3.08E+00 | $2.50 \mathrm{E}-01$ | 1.40E+00 | $1.30 \mathrm{E}-01$ | $1.99 \mathrm{E}+00$ | 1.90E-01 | 1.50E | 4.30E-01 | $1.26 \mathrm{E}+0$ | 5.90E-01 | 2.02E+00 | 6.40E-01 | 2.73E-02 | 25\% |
| Retene | 9.29 | 3.80E-01 | 9.79E-01 | c | 3.45E-01 | c | $4.61 \mathrm{E}-01$ | c | 1.06E-01 | c | 7.10E-02 | c | 8.63E-01 | c | 5.25E-01 | 1.30E-01 | $1.35 \mathrm{E}+00$ | c | $2.14 \mathrm{E}+00$ | 1.50E-01 | $1.34 \mathrm{E}+0$ | 3.10E-01 | 1.56E+00 | c |  | 29\% |
| Benzo(k)fluoranthen | 5.76E-01 | E-01 | 4.4 | E-01 | 4.39E-01 | D0E-02 | 4.87E-01 | c | 4.18E-01 | 00E-02 | 5.78E-01 | 00E-02 | 1.25 | OE-01 | $5.33 \mathrm{E}-01$ | 1.10E-01 | E-01 | c-01 | 6.52E-01 | 2.60E-01 | 5.85E-0 | c | 8.67 | c | $2.73 \mathrm{E}-12$ | 38\% |
| Benzo(b)fluoranthene | $6.03 \mathrm{E}-01$ | 3.00E-01 | 4.49E-01 | 8.00E-02 | 4.58E-01 | 1.00E-01 | 4.68E-01 | 1.30E-01 | 4.48E-01 | c | 5.74E-01 | 1.00E-01 | $1.32 \mathrm{E}+00$ | 2.70E-01 | 5.48E-01 | 1.40E-01 | 7.57E-01 | $2.90 \mathrm{E}-01$ | 7.10E- | 5.90E-01 | 6.48E-01 | 6.10E-0 | 9.38E-0 | 6.60E-01 | 2.73E-02 | 38\% |
| Benzo(i)fluoranthene | 1.56E |  | 1.73E-02 |  | 1.04E-02 |  | 2.45E-02 |  | 1.09E-02 |  | 1.79E-02 |  | 2.72E-02 |  | 1.47E-02 |  | 2.47E-02 |  | 3.03E-02 |  | 1.97E-02 |  | 2.60E-02 |  | 2.73E-02 | 38\% |
| Benzo()pyrene | $3.51 \mathrm{E}-01$ | 1.70E-01 | 2.46E-01 | ce-0 | 2.59E-01 | 1.00E-01 | $2.10 \mathrm{E}-01$ | 3.00E-02 | -01 | 3.00E-02 | 2.84E-01 | 8.00E-02 | 7.52E-01 | $2.50 \mathrm{E}-01$ | 3.00E-01 | $1.10 \mathrm{E}-01$ | $4.23 \mathrm{E}-01$ | 3.10E-01 | 4.27E-01 | 8.50E-01 | 3.99E-01 | $2.09 \mathrm{E}+00$ | 5.60 | $4.13 \mathrm{E}+00$ | 2.73E-02 | 5\% |
| Benzo(a)pyre | 3.84E-02 | 5.00E-02 | 4.14E-02 | 6.00E-02 | 2.26E-02 | OoE-22 | 4.82E-02 | c | 2.14E-02 | .00E-02 | 3.37 | 3.00E-02 | 5.8 | $2.10 \mathrm{E}-01$ | 3.30 | 1.50E-4 | 5.93E | 9.00E-21 | 7.46 | 3.00E-11 | 4.76E | $1.38 \mathrm{E}+00$ | 6.2 | 7E | 2.73 E | 25\% |
| Perylene | 2.35E-02 | E--12 | 2.90E-02 | OOE-22 | 2.84E-02 | OOE-0 | 49E | 8.00E-02 | 4.10E-02 | 3.00E-02 | 7.33E-02 | .OOE-02 | 7.67E-02 | $2.50 \mathrm{E}-01$ | 3.75E-02 | 1.00E-01 | 4.23E-02 | 6.50E-21 | 3.38E-02 | $2.52 \mathrm{E}+$ | $2.48 \mathrm{E}-02$ | $4.34 \mathrm{E}+00$ | 4.06E-02 | $2.03 \mathrm{E}+00$ | $3 \mathrm{E}-12$ | 25\% |
| Indeno(cd) pryene | 3.18 E | 5.00E-02 | 2.13E--1 | 5.00E-02 | 2.37E-01 | 1.00E-0 | 1.77E-01 | c | 39E-01 | c | $2.48 \mathrm{E}-01$ | 8.00E-02 | 6.97E-01 | 1.50E-01 | 2.67 E | 1.30E-01 | 74E-01 | 3.40E-2 | $4.17 \mathrm{E}-01$ | 9.70E-01 | 3.97E-01 | 6.70E-01 | 5.38E--1 | $1.13 \mathrm{E}+00$ | 2.73E-02 | 29\% |
| Benzo(ghi)perylene | $3.46 \mathrm{E}-01$ | 3.90E-01 | 2.94E-01 | c | 3.24E-01 | $1.30 \mathrm{E}-01$ | 5.78E-01 | c | 3.99E-01 | 3.00E-02 | 5.79E-01 | 1.30E-01 | 9.19E-01 | $2.70 \mathrm{E}-01$ | 3.93E-01 | 2.00E-01 | 4.81E-01 | 7.40E-01 | 4.45E-01 | $2.25 \mathrm{E}+00$ | 4.00E-01 | $1.38 \mathrm{E}+00$ | 5.88E-01 | $2.85 \mathrm{E}+00$ | 2.73E-02 | 12\% |
| Coronene | 1.61E-01 | c | 1.18E-01 | c | 1.20E-01 | 3.00E-02 | 1.21E-01 | c | 1.24E-01 | c | 1.42E-01 | c | 3.47E-01 | c | 1.40E-01 | 1.10E-01 | 1.99E-01 | 5.00E-01 | 2.21E-01 | $1.25 \mathrm{E}+00$ | 1.98E-01 | $9.90 \mathrm{E}-01$ | 2.70E-01 | $2.36 \mathrm{E}+00$ | 3.41E-02 | 26\% |
| Tetradecanoi | $9.71 \mathrm{E}-01$ | 12E+00 | $9.63 \mathrm{E}-01$ | $1.26 \mathrm{E}+00$ | 6.43E-01 | c | 1.2E+ | 55E+0 | 5.85E-01 | c | 1.05E+00 | 4.23E+0 | 1.61E+00 | c | 8.80E-01 | E- | 1.39E+00 | c | 0 | c | 6.5 | c | 1.24E+ | $1.97 \mathrm{E}+00$ | 2.17E+00 | 47\% |
| Pentadecanoic acid | 2.84E-01 | c | 2.82E-01 | c | 1.85E-01 | c | 3E-2 | 6.60E-0 | 1.68E-01 | c | 98E | $1.27 \mathrm{E}+0$ | 4.62E-01 | c | 5E-1 | $3.90 \mathrm{E}+$ | 4.07E | c | 3.37E | c | 1.99 E | c | 3.68E--1 | 6.40E-0 | 1.33E+6 | 50\% |
| Hexadecanoic acid | $5.71 \mathrm{E}+00$ | $4.73 \mathrm{E}+00$ | 5.67E+00 | $7.23 \mathrm{E}+00$ | 3.86E+00 | c | 12E+00 | 22E+00 | 3.53E+00 | c | $6.45 \mathrm{E}+00$ | $4.21 \mathrm{E}+01$ | 9.65E+00 | c | $23 \mathrm{E}+00$ | $7.71 \mathrm{E}+01$ | 8.15 | c | 6.31 | c | $3.67 \mathrm{E}+00$ | 3.50E-01 | $7.24 \mathrm{E}+00$ | $1.64 \mathrm{E}+01$ | 8.66E+00 | 53\% |
| Heptadecanoic acid | $4.18 \mathrm{E}-01$ | c | 4.15E-01 | c | 3.00E-01 | c | $4.93 \mathrm{E}-01$ | 3.60E-01 | 2.90E-01 | c | 5.38E-01 | $9.50 \mathrm{E}-01$ | 7.99E-01 | c | $4.02 \mathrm{E}-01$ | $1.20 \mathrm{E}+00$ | 5.96E-01 | c | $4.01 \mathrm{E}-01$ | c | $2.27 \mathrm{E}-01$ | c | 5.10E-01 | 1.10E-01 | 3.03E-01 | 76\% |
| Octadecanoic acid | $2.92 \mathrm{E}+00$ | $3.09 \mathrm{E}+00$ | 2.89E+00 | $5.26 \mathrm{E}+00$ | 2.04E+00 | c | 3.31E+00 | $5.04 \mathrm{E}+00$ | 1.97E+00 | c | $3.60 \mathrm{E}+00$ | $1.39 \mathrm{E}+01$ | 5.10E+00 | c | 2.78E+00 | $2.30 \mathrm{E}+01$ | $4.18 \mathrm{E}+00$ | c | $2.87 \mathrm{E}+00$ | c | $1.62 \mathrm{E}+0$ | 1.10E-01 | 3.58E+00 | 8.15E+00 | 4.56E+00 | 99\% |
| Eicosanoic acid | 2.43 E | 70E-01 | 2.52E-0 | 10E-01 | 1.04 E | c | 52E-1 | 40E-01 | 5.94E | c | 7.21 E | 6.00E-02 | 2.61E-01 | c | 1.60 E | $2.20 \mathrm{E}-01$ | 3.55E-01 | c | 4.97E-1) | c | 3.10E-0 | 30E-01 | 3.87E--1 | 1.27E+00 | 8.22E-01 | 48\% |
| Heneicosanoic acid | 5.33 |  | 5.62E-02 |  | 2.01E-02 | c | 2.73E-02 | c | 6.89E-0 | c | 5.15E-03 | 2.60E-01 | 5.04E-02 | $3.50 \mathrm{E}-01$ | 3.07E-02 | 5.40E-01 | 7.75E-02 | c | 1.22E-01 | 2.50E-01 | 7.69E-0 | c | 8.94E-02 | 1.40E-01 | 8.22E-01 | $36 \%$ |
| Docosanoic acid | 3.29E-01 | 6.10E-01 | 3.46E-01 | 6.80E-01 | 1.26E-01 | c | 1.71E-01 | 3.60E-01 | 4.52E-02 | c | $3.98 \mathrm{E}-02$ | $1.06 \mathrm{E}+00$ | 3.16E-01 |  | 1.91E-01 | $1.41 \mathrm{E}+00$ | 4.77E-01 | c | 7.40E-01 | 1.90E-01 | $4.65 \mathrm{E}-01$ | 7.90E-01 | 5.47E-01 | $1.62 \mathrm{E}+00$ | 2.23E-01 | 25\% |
| Tricosanoic acid | 1.31E-01 | 2.50E-01 | 1.37E-01 | 2.80E-01 | 4.86E-02 | c | 6.52E-02 | 2.50E-01 | 1.56E-02 | c | 1.07E-02 | 3.60E-01 | 1.22E-01 | 8.00E-02 | 7.43E-02 | 3.50E-01 | 1.89E-01 | c | 3.00E-01 | c | 1.88E-01 | 2.60E-01 | 2.19E-01 | 4.50E-01 | 1.50E-01 | 24\% |
| Tetracosanoic acid | 7.18E-01 | $1.33 \mathrm{E}+00$ | 7.56E-01 | 1.59E+00 | 2.67E-01 | c | 3.58E-01 | $1.01 \mathrm{E}+00$ | 8.46E-02 | c | 5.75E-02 | 1.59E+00 | 6.69E-01 | c | $4.08 \mathrm{E}-01$ | 8.90E-01 | 1.04E+00 | c | 1.65E+00 | c | 1.04E+00 | 7.70E-01 | $1.20 \mathrm{E}+00$ | 2.10E+00 | 6.29E-01 | 23\% |
| Pentacosanoic acid | 6.82 E | 4.50E-01 | 7.18E-12 | 5.00E-0 | 2.55E-02 | c | 3.41E-02 | 5.50E-01 | 8.26E-03 | c | 5.69E-03 | 3.10E-01 | 6.38E-02 | c | 3.89E-02 | 4.50E-01 | 9.90E-02 | c | 1.56E-0 | c | $9.84 \mathrm{E}-12$ | 6.00E-02 | 1.14E-01 | $2.60 \mathrm{E}-01$ | 3.72E-01 | 35\% |
| Hexacosanoic acid | 4.52 E | $9.60 \mathrm{E}-01$ | 4.75E-01 | 1.15E+00 | 1.70E-01 | c | 2.27E-01 | 8.00E-01 | 5.56E-02 | c | 4.02E-02 | $1.25 \mathrm{E}+00$ | 4.26E-01 |  | $2.58 \mathrm{E}-01$ | $7.90 \mathrm{E}-0$ | 6.55E-01 | c | 1.03E+00 |  | $6.50 \mathrm{E}-01$ | OE-0 | 7.56E-01 | 9.10E-01 | 4.60E-01 | 35\% |
| Heptacosanoic acid | $3.65 \mathrm{E}-12$ | 4.00E-01 | 3.84E-0 | , $60 \mathrm{E}-0$ | 1.37E-02 | c | 84E-02 | c | 461-0 | c | 3.24E-03 | 5.50E-01 | 3.43E-02 | 8.80E-01 | 2.10E-02 | 1.00E-01 | 5.31E-02 | c | 8.36E-02 | c | 5.27E-02 | c | 6.13E-02 | $1.10 \mathrm{E}+00$ | 3.05E-02 | 35\% |
| Octacosanoic acid | $2.41 \mathrm{E}-01$ | c | 2.53E-01 | 9.00E-01 | 9.13E-02 | c | $1.22 \mathrm{E}-01$ | c | 3.16E-02 | 6.00E-02 | 2.38E-02 | $1.35 \mathrm{E}+00$ | 2.30E-01 | 3.80E-01 | 1.39E-01 | 8.90E-01 | 3.50E-01 | $2.32 \mathrm{E}+00$ | 5.48E-01 | c | $3.46 \mathrm{E}-01$ | 1.71E+0 | 4.03E-01 | $1.65 \mathrm{E}+0$ | 2.34E-01 | 4\% |
| Nonacosanoic acid | 3.40E-02 | 6.30E-01 | 3.57E-02 | 6.30E-01 | 1.28E-02 | 2.00E-02 | 1.74E-02 | c | 4.70E-03 | 5.00E-02 | $3.45 \mathrm{E}-03$ | c | 3.23E-02 | $9.50 \mathrm{E}-01$ | 1.99E-02 | 1.20E-01 | 4.93E-02 | 4.40E-01 | 7.72E-02 | c | 4.88E-02 | c | 5.69E-02 | c | 2.34E-01 | 32\% |
| Triacontanoic acid | 2.76E-01 | $9.40 \mathrm{E}-01$ | 2.91E-01 | $1.03 \mathrm{E}+00$ | 1.04E-01 | 2.40E-01 | 1.39E-01 | c | 3.45E-02 | $4.40 \mathrm{E}-01$ | $2.45 \mathrm{E}-02$ | 7.80E-01 | 2.60E-01 | $1.47 \mathrm{E}+00$ | 1.58E-01 | $1.02 \mathrm{E}+00$ | 4.01E-01 | $4.54 \mathrm{E}+00$ | 6.31E-01 | 2.30E-01 | 3.98E-01 | $2.11 \mathrm{E}+00$ | 4.63E-01 | $1.95 \mathrm{E}+00$ | 2.34E-01 | 17\% |
| Butanedioic acid | 2.37E-01 | $6.63 \mathrm{E}+00$ | 2.40E-01 | $1.00 \mathrm{E}+00$ | 1.50E-01 | 3.00E-01 | 2.34E-01 | 4.60E-01 | 1.24E-01 | $1.81 \mathrm{E}+00$ | $2.31 \mathrm{E}-01$ | $1.01 \mathrm{E}+00$ | 3.72E-01 | $3.63 \mathrm{E}+00$ | 2.00E-01 | $7.90 \mathrm{E}-01$ | 3.36E-01 | $1.20 \mathrm{E}-01$ | 3.07E-01 | $1.40 \mathrm{E}+00$ | 1.80E-01 | 8.30E-01 | 3.16E-01 | $6.26 \mathrm{E}+00$ | $1.28 \mathrm{E}+00$ | 42\% |
| Pentanedioic acid | 1.08E-01 | $1.80 \mathrm{E}+00$ | 1.08E-01 | 3.00E-02 | 7.49E-02 | c | 1.19E-01 | c | 6.70E-02 | $2.10 \mathrm{E}-01$ | 1.29E-01 | 1.10E-01 | 1.86E-01 | $1.02 \mathrm{E}+00$ | 9.79E-02 | 1.90E-01 | 1.52E-01 | c | 1.13E-0 | $1.90 \mathrm{E}-0$ | 6.38E-02 | c | 1.34E-0 | $1.06 \mathrm{E}+00$ | 1.52E+6 | 42\% |
| Hexanedioic acid | OE-01 | 7.60E-01 | 10E-01 | c | 34E-02 | c | 35E-01 | c | 7.91E-02 | c | 1.55E- | c | 2.07E-01 |  | . 07 E -0 | 6.00E-02 | 1.55E-0 | c | 8.96E-02 | c | 4.78E-02 | c | 1.29E-0 | 2.00E-01 | E+ | 42\% |
| Heptanedioic acid | 4.06E-03 | 3.00E-01 | 4.28E-03 |  | 1.51E-03 |  | $2.02 \mathrm{E}-03$ | c | 4.64E-04 | 9.00E-02 | 3.10E-04 | c | 3.77E-03 | 1.80E-01 | 2.29E-03 | 1.50E-01 | 5.89E-03 | c | $9.34 \mathrm{E}-03$ | c | 5.87E-03 | c | 6.81E-03 | c | $1.32 \mathrm{E}+00$ | 42\% |
| Octanedioic acid | 2.93 | 4.70E-01 | 2.78E-01 | 1.60E-01 | 1.75E-01 | 3.70E-01 | 2.98E-01 |  | 2.10E-01 |  | 3.00E-01 | 5.20E-01 | $4.40 \mathrm{E}-01$ | $2.30 \mathrm{E}-01$ | 2.90E-01 | 5.10E-01 | 4.45E-01 |  | 3.05E-01 | 1.60E-01 | 1.69E-0 |  | 3.59E-0 |  | $1.32 \mathrm{E}+00$ | 42\% |
| Nonanedioic acid | $2.73 \mathrm{E}-01$ | 6.90 | 2.57E-01 | 1.70 | $1.34 \mathrm{E}-01$ | 8.20E-01 | $2.32 \mathrm{E}-01$ | 1.90E-01 | 1.75E-01 | $1.35 \mathrm{E}+00$ | 1.95E-01 | 1.42 | 3.39E-01 | $1.23 \mathrm{E}+00$ | $2.57 \mathrm{E}-01$ | $1.37 \mathrm{E}+00$ | E-1 | $4.30 \mathrm{E}-01$ | 3.58E-01 | $6.80 \mathrm{E}-01$ | 2.07E-01 | 2.60E-01 | 3.58E-01 | $1.03 \mathrm{E}+0$ | $1.18 \mathrm{E}+00$ | 42\% |


| trace | March04 |  | April04 |  | May04 |  | June04 |  | July04 |  | August04 |  | September04 |  | October04 |  | November04 |  | December04 |  | Janucry05 |  | February05 |  | $\mathrm{MDL}^{\text {a }}$ UNC ${ }^{\text {b }}$ |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1-2-benzened | 1.71E-03 | $2.13 \mathrm{E}+00$ | 1.8 | -02 | 6.33E-04 | 7.00E-02 | 8.47E-04 | 1.90E-01 | 1.95E-04 | c | $1.30 \mathrm{E}-04$ | $2.10 \mathrm{E}-01$ | 1.59E-03 | $2.15 \mathrm{E}+00$ | $9.64 \mathrm{E}-04$ | 6.40E-01 | $2.48 \mathrm{E}-03$ | 01 | 3.93E-03 | -01 | 2.47E-03 | 01 | 2.86E-03 | $1.99 \mathrm{E}+00$ | 0 | 38\% |
| $1-3$-benzenedicarboxylic ac | 3.72E-04 |  | 4.82E-04 |  | 2.91E-04 |  | 3.43E-04 | c | 2.33E-04 | c | 4.19E-04 |  | 8.73 | OE-M | 3.63E-04 |  | 32 E |  | 6.85 E |  | 5.24 E |  | 7.74E-04 | OE | 34 | 38\% |
| 1-4-benzenedicarboxylic acid | 1.31E-03 | 6.80E-01 | 1.44 | 1.70E-01 | 5.92E-04 | c | 7.59E-04 | c | 2.83E-04 | c | 3.74E-04 | 3.30E-01 | 1.58E-03 | 60E-01 | 8.46E-04 | 2.40E-0 | 1.96E-03 | 7.00E-02 | 2.89E-03 | 1.20E-01 | 1.88E-03 | 1.90E-01 | 2.30E-03 | 5.10E-01 | 1.27E+00 | 38\% |
| Nonadecanoic acid | 7.32E-02 | c | 7.5 | c | 3.59E-02 | c | 02 | c | 2.54E-02 | c | E-02 | 2.30E-01 | 9.01E-02 | c | 5.33E-02 | 1.10E-01 | 1.07E-01 | c | 1.34E-01 | c | 8.27 | c | 1.11 | c | 1.45 E | 73\% |
| 1-8-naphthalic anhydride | 3.80E-03 | c | 4.00 | c | 1.41 E | c | 1.88E-3 | c | 4.34E-04 | c | $2.90 \mathrm{E}-04$ | c | 3.53E-03 | c | 2.15E-03 | c | 5.51E-03 | c | 8.73 |  | 5.49E-31 |  | 6.37E-03 |  | 2.78E+00 | 16\% |
| 1 H -phenalen-1-one | 5.12E-01 |  | 4.31E-01 |  | 3.58E-01 | c | 4.06E-01 | c | 77-01 | c | 4.62 | c | 1.01E+00 |  | 4.61E-01 |  | 01 | $2.30 \mathrm{E}-0$ | 5.56E-01 | 1.22E+00 | 4.51E-01 |  | 7.00E-01 |  | E+00 | 16\% |
| Anthracen-9-10-dione | 1.56E+00 | 6.40E-01 | $1.30 \mathrm{E}+00$ | 7.30E-01 | 1.16E+00 | $2.90 \mathrm{E}-01$ | 1.40E+00 | 5.20E-01 | $9.96 \mathrm{E}-01$ | $2.70 \mathrm{E}-01$ | $1.63 \mathrm{E}+00$ | c | 3.26E+00 | 7.50E-01 | 1.49E+00 | 3.70E-0 | $2.08 \mathrm{E}+00$ | 2.20E-01 | $1.52 \mathrm{E}+0$ | 5.30E-01 | $1.28 \mathrm{E}+00$ | 4.00E-0 | $2.09 \mathrm{E}+00$ | 6.10E-0 | 7.41E-01 | 16\% |
| Benz()antriracene-7 12-dione | 9.26 |  | 7.57E-02 |  | $6.80 \mathrm{E}-02$ |  | 7.62E-02 |  | 5.62E-02 |  | 9.18E-02 |  | 1.92E-01 |  | 8.65E-02 | 2.40 E | 1.22E-01 |  | $8.83 \mathrm{E}-12$ | 4.10 | 7.59E-02 |  | 1.23 |  | 7.06E-01 | 16\% |
| Levoglucosan | $2.94 \mathrm{E}+01$ | 3.73E | 3.10E+01 | 5.71E | 1.09E+01 | $3.91 \mathrm{E}+01$ | 1.46E+01 | 30E+01 | E +00 | $2.13 \mathrm{E}+01$ | 2.24E+00 | $3.57 \mathrm{E}+01$ | $2.73 \mathrm{E}+01$ | 6.18E+01 | 1.66E+01 | 5.14E | 4.27E+01 | $6.48 \mathrm{E}+01$ | $6.77 \mathrm{E}+01$ | 8.73E+01 | $4.25 \mathrm{E}+01$ | $7.48 \mathrm{E}+01$ | $4.94 \mathrm{E}+01$ | 1.10E+02 | 0E+00 | 37\% |
| 3-Acetylpentanedioic acid | 7.49E-02 | 8.00E-01 | 1.90E-01 | $4.00 \mathrm{E}-01$ | 1.02E-01 | c | 1.85E-01 | $2.30 \mathrm{E}+00$ | 5.62E-01 | 1.35E+01 | 5.14E-01 | $4.10 \mathrm{E}+00$ | 3.59E-01 | $4.10 \mathrm{E}+00$ | $1.32 \mathrm{E}-01$ | $1.00 \mathrm{E}+00$ | 1.68E-01 | $1.10 \mathrm{E}+00$ | 3.99E-02 | c | 1.79E-01 | c | 3.86E-02 | c | 1.00E-01 |  |
| 2-Hydroxy-4-isopropyladipic acid | 1.37 E | +00 | 3.47E | $4.60 \mathrm{E}+00$ | 1.87E-01 | $1.51 \mathrm{E}+01$ | 3.36E-01 | $1.18 \mathrm{E}+01$ | E+00 | $2.39 \mathrm{E}+01$ | $9.37 \mathrm{E}-01$ | $1.14 \mathrm{E}+01$ | 6.54E | $1.22 \mathrm{E}+01$ | 2.40E-01 | $6.10 \mathrm{E}+00$ | 3.07E-01 | $1.02 \mathrm{E}+01$ | 7.27E-12 | $2.10 \mathrm{E}+00$ | 3.27E-01 | E-01 | 7.04E-02 | 00 | 1.00E-uI |  |
| 3-Acetyl hexanedioic acid | 9.42E-0 | 7.00E-01 | $2.39 \mathrm{E}+0$ | $1.10 \mathrm{E}+0$ | 1.29E+00 | 1.10E+00 | $2.32 \mathrm{E}+00$ | $2.20 \mathrm{E}+00$ | 7.07E+00 | $7.80 \mathrm{E}+00$ | 6.46E+00 | $3.20 \mathrm{E}+00$ | $4.51 \mathrm{E}+00$ | $3.00 \mathrm{E}+00$ | 1.66E+00 | 6.00E-01 | 2.12E+00 |  | 5.01E-01 | 7.00E-01 | $2.25 \mathrm{E}+00$ | 7.00E-01 | 4.86E-01 | $1.60 \mathrm{E}+00$ | 1.00E-01 |  |
| 3-Hydroxylutaric acid | 1.06E-01 | $1.39 \mathrm{E}+01$ | $2.68 \mathrm{E}-01$ | $1.21 \mathrm{E}+01$ | $1.44 \mathrm{E}-01$ | $4.55 \mathrm{E}+01$ | 2.60E-01 | $2.71 \mathrm{E}+01$ | 7.93E-01 | 4.53E+01 | 7.25E-01 | $3.31 \mathrm{E}+01$ | $5.06 \mathrm{E}-01$ | $3.08 \mathrm{E}+01$ | 1.86E-01 | $1.48 \mathrm{E}+01$ | $2.38 \mathrm{E}-01$ | $1.34 \mathrm{E}+0$ | 5.62E-02 | 8.50E+ | 2.53E-01 | $2.60 \mathrm{E}+00$ | 5.44E-02 | 9.00E | 1.00E- |  |
| acid | 7.78E-02 | 3.00E-01 | 1.98E-01 | -01 | -01 | $1.50 \mathrm{E}+0$ | 1.92E-01 | +00 | 5.84E-01 | 5.30 | 5.34E-0 | $1.60 \mathrm{E}+0$ | 3.73 | $1.70 \mathrm{E}+0$ | 1.37E-01 | E-0 | 1.75E-01 | $1.20 \mathrm{E}+00$ | 4.14E-02 | 1.00E-01 | 1.86E-01 |  | 4.01E-02 | $2.00 \mathrm{E}-01$ | 1.00E-01 |  |
| cyclobutane-carboxylic acid | 5.19E-01 | $1.50 \mathrm{E}+00$ | $1.32 \mathrm{E}+00$ | 1.10E+00 | 7.09E-01 | c | 1.28E+00 | $2.60 \mathrm{E}+00$ | 3.89E+00 | 1.18E+01 | 3.56E+00 | $2.90 \mathrm{E}+00$ | $2.48 \mathrm{E}+00$ | 3.10E+00 | 9.12E-01 | $1.80 \mathrm{E}+00$ | 1.17E+00 | $1.80 \mathrm{E}+00$ | 2.76E-01 | 7.00E-01 | 1.24E+00 | c | 2.67E-01 | 1.20E+00 | 1.00E-01 |  |
| Pinic acid | $3.81 \mathrm{E}-01$ | 5.00E-01 | 9.68E-01 | $1.00 \mathrm{E}+00$ | 5.21E-01 | 5.00E-01 | 9.40E-01 | $1.50 \mathrm{E}+00$ | $2.86 \mathrm{E}+00$ | $2.60 \mathrm{E}+00$ | $2.62 \mathrm{E}+00$ | 1.60E+00 | $1.83 \mathrm{E}+00$ | 6.00E-01 | 6.71E-01 | 5.00E-01 | 8.58E-01 | $1.00 \mathrm{E}+00$ | 2.03E-01 | $1.70 \mathrm{E}+00$ | 9.13E-01 | 5.00E-0 | 1.97E-01 | 5.00E-01 | 1.00E-01 |  |
| Pinonic ac | 1.84E-01 | 0E-01 | 66E-01 | . 50 E +00 | 51E-01 | .00E-01 | 53E-01 | 80E+00 | . $38 \mathrm{E}+00$ | 60E+00 | 1.26E+00 | 1.00E-01 | 8.80E-01 | 1.00E+00 | $23 \mathrm{E}-0$ | 7.00E-01 | 4.13E-01 | . $00 \mathrm{E}+0$ | 9.78E-02 | OE- | $4.40 \mathrm{E}-0$ | c | 9.47E- | OOE | 00E |  |
| ${ }^{2 \text { acid }}$ | $2.39 \mathrm{E}-01$ | 8.00E-01 | 2.05E-01 | $7.00 \mathrm{E}-01$ | 2.00E-01 | 1.40E+00 | 2.75E-01 | $1.20 \mathrm{E}+00$ | 4.16E-01 | $2.50 \mathrm{E}+00$ | 3.60E-01 | $1.30 \mathrm{E}+00$ | 5.24E-01 | $1.70 \mathrm{E}+00$ | 2.31E-01 | 7.00E-01 | 1.788-01 | 8.00E-01 | 1.75E-01 | 6.00E-0 | 1.25E-0 | 3.00E-01 | 3.188-01 | 6.00E-0 | 1.00E-01 |  |
| 2-Methylglyceric acid | 1.02E+0 | 1.60E+00 | 9.10E-01 | $1.40 \mathrm{E}+00$ | 1.40E+00 | 9.70E+00 | 1.65E+00 | $1.45 \mathrm{E}+01$ | 4.12E+00 | $2.15 \mathrm{E}+01$ | 2.87E+00 | $1.41 \mathrm{E}+01$ | $2.95 \mathrm{E}+00$ | $1.64 \mathrm{E}+01$ | 7.90E-01 | $2.90 \mathrm{E}+00$ | 7.68E-01 | $2.10 \mathrm{E}+00$ | 1.04E+00 | $1.40 \mathrm{E}+00$ | $1.13 \mathrm{E}+0$ | 7.00E-01 | 1.20E+00 | 1.30E+00 | 1.00E-01 |  |
| 2-Methyltrreitol | $1.72 \mathrm{E}+00$ | 3.00E-01 | $1.54 \mathrm{E}+00$ | 7.00E-01 | $2.36 \mathrm{E}+00$ | 1.14E+01 | 2.78E+00 | $1.39 \mathrm{E}+01$ | 6.95E+00 | $2.51 \mathrm{E}+01$ | 4.84E+00 | $1.46 \mathrm{E}+01$ | 4.97E+00 | $3.06 \mathrm{E}+01$ | 1.33E+00 | 1.00E+00 | $1.30 \mathrm{E}+00$ | 3.00E-01 | $1.76 \mathrm{E}+00$ | 1.00E-01 | $1.90 \mathrm{E}+00$ | 2.00E-01 | $2.03 \mathrm{E}+00$ | c | 1.00E-01 |  |
| 2-Methylerythritol | $2.83 \mathrm{E}+00$ | 9.00E-01 | $2.52 \mathrm{E}+00$ | $1.50 \mathrm{E}+00$ | 3.88E+00 | $2.81 \mathrm{E}+01$ | 4.56E+00 | $3.00 \mathrm{E}+01$ | $1.14 \mathrm{E}+01$ | $6.19 \mathrm{E}+01$ | 7.96E+00 | $3.58 \mathrm{E}+01$ | 8.18E+00 | $5.60 \mathrm{E}+01$ | 2.19E+00 | $2.50 \mathrm{E}+00$ | 2.13E+00 | 7.00E-01 | 2.89E+00 | 5.00E-01 | 3.13E+00 | 1.00E-01 | 3.34E+00 |  | 1.00E-01 |  |
| b-Caryophyllinic acid | -02 | $20 \mathrm{E}+0$ | 3.20E-01 | 3.20 E | 4.55E-01 | 3.70 | 7.99E-01 | 2.30 | $2.28 \mathrm{E}+00$ | $3.50 \mathrm{E}+00$ | $1.48 \mathrm{E}+00$ | $3.60 \mathrm{E}+0$ | 1.89E+00 | E+0 | $2.93 \mathrm{E}-01$ | +00 | $2.20 \mathrm{E}-01$ | OE+ | 1.16E-02 | 5.40E | 5.79E-02 | 2.8 |  | 6.30E+00 | 1.00E-01 |  |

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Table S4. Paired model and observation quantities of each organic tracer at Cincinnati, OH in units of ( $\mathrm{ng} / \mathrm{m}^{\mathbf{3}}$ ) in the context of measurement detection limit (MDL ${ }^{\text {a }}$ ) and measurement uncertainty ( $\mathrm{UNC}^{\mathrm{b}}$ ). Observations below the detection limit are denoted by ${ }^{\mathrm{c}}$.

| tracer | March04 |  | April04 |  | May04 |  | June04 |  | July04 |  | August04 |  | September04 |  | October04 |  | November04 |  | December04 |  | nucry05 |  | February05 |  | MDL ${ }^{\text {a }}$ | UNC ${ }^{\text {b }}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | m | bs | model | obs | model | obs | mode | obs | model | obs | model | obs | model | obs | mo | bs |  | obs | mo | obs | mod | obs | model | obs |  |  |
| Tetracosane | $5.68 \mathrm{E}-01$ | 7.30E-01 | 5.7 | 4.90E-01 | 5.07E-01 | $2.43 \mathrm{E}+00$ | 5.05E-01 | $3.06 \mathrm{E}+00$ | 8.48E-01 | 1.85E+00 | 7.19E-01 | $1.52 \mathrm{E}+00$ | $8.40 \mathrm{E}-01$ | 1.71E+00 | 6.24E-01 | $2.02 \mathrm{E}+00$ | 1.05E+00 | 8.60E-01 | 01 | 6.80 | 7.13E-01 | 0 | 8.50E-01 | 7.90E-01 | 7.78E-01 | 20\% |
| Pentac | 5.55 E | 5.90E-01 | 5.46 E | 6.80 E | 4.89E-01 | 2.15 | 5.00E-01 | 2.76 E | 8.14E-01 | $2.10 \mathrm{E}+\infty$ | 7.10 | 2.92E | 8.05E | $2.54 \mathrm{E}+0$ | 6.0 | $2.98 \mathrm{E}+00$ | 1.03E+00 | 2.30E-01 | 8.33E-01 | c | 6.71 | OE- | 8.06E-01 | 7.50E-01 | +00 | 16\% |
| Hexacosan | 3.49 E | c | 3.28 | 1.00E-02 | 2.91E-01 | 1.83E | 3.02E-01 | 2.54 E $^{\text {a }} 0$ | 4.96 | $2.02 \mathrm{E}+00$ | 4.42E-01 | $2.73 \mathrm{E}+00$ | 4.99E-01 | $3.20 \mathrm{E}+00$ | 01 | $3.63 \mathrm{E}+00$ | 6.66E-01 | 1.20 | 01 | c | $4.27 \mathrm{E}-01$ | E-01 | 01 | 8.10E-01 | $1.30 \mathrm{E}+00$ | \% |
| Heptacosane | 3.97E- | c | 3.45E-01 | c | 3.06E-01 | $3.25 \mathrm{E}+00$ | 2.54E-01 | $3.73 \mathrm{E}+00$ | 4.22E-01 | $3.52 \mathrm{E}+00$ | 4.17E-01 | $3.74 \mathrm{E}+00$ | 4.98E-01 | $4.40 \mathrm{E}+00$ | 4.12E-01 | $4.45 \mathrm{E}+00$ | 7.60E-01 | $1.28 \mathrm{E}+00$ | 7.16E-01 |  | 5.04E-01 | 1.57E+00 | 5.97E-01 | $1.33 \mathrm{E}+00$ | $1.41 \mathrm{E}+00$ | \% |
| Octacosane | 1.94E-01 | c | 1.75E-01 | c | 1.54E-01 | $1.21 \mathrm{E}+00$ | 1.24E-01 | $1.68 \mathrm{E}+00$ | 2.12E-01 | $1.36 \mathrm{E}+00$ | 2.01E-01 | $1.16 \mathrm{E}+00$ | 2.54E-01 | $7.90 \mathrm{E}-01$ | 2.06E-01 | $1.47 \mathrm{E}+00$ | 3.67E-01 | 2.20E-01 | 3.43E-01 |  | $2.48 \mathrm{E}-01$ | 6.20E-01 | 2.94E-01 | 5.00E-01 | 7.88E-01 | 13\% |
| Nona | 5.07E-01 | c | 3.80E-01 | E+ | 3.39E-01 | 4.77E+00 | 1.85E-01 | $4.81 \mathrm{E}+00$ | 2.84E-01 | 5.19E+00 | 4.17E-01 | $3.67 \mathrm{E}+00$ | 4.94E-01 | $3.61 \mathrm{E}+00$ | 5.00E-01 | $4.71 \mathrm{E}+00$ | $9.94 \mathrm{E}-01$ | $1.59 \mathrm{E}+00$ | 12E+0 | 0E-12 | 85E | $2.21 \mathrm{E}+00$ | 8.01E-01 | 0 | 1.36E+00 | 27\% |
| Triaconta | 1.48E-01 | c | 1.28E-01 |  | 1.11 | E+ | 9.41E-02 | 68E+ | 1.69E-01 | $2.21 \mathrm{E}+0$ | 1.53 F | 8.50E-0 | 1.83E | $6.50 \mathrm{E}-01$ | 1.48E-01 | 8.30E- | 2.85E--1 | 3.00E-22 | 2.45E-01 | c | 1.80 | 40E-2 | 2.14 | 0E- | 8.11E-01 | 40\% |
| Hentriacontane | 1.77 | c | 1.3 | 1.10E+00 | 1.16 | $1.37 \mathrm{E}+00$ | 6.66 | $1.49 \mathrm{E}+00$ | 1.05E-01 | $1.81 \mathrm{E}+00$ | 1.48E-01 | $1.13 \mathrm{E}+00$ | 1.70 | $1.44 \mathrm{E}+00$ | 1.71 | $1.51 \mathrm{E}+$ | 3.4 | 8.00E-01 | 3.83E-01 |  | 2.35E-01 | 5.80E-01 | 2.76E-01 | 01 | 4.06E-01 | 40\% |
| Dotriacontane | 9.09E-02 | c | 7.63E-02 | c | 6.55E-02 | c | 5.35E-02 | 8.70E-01 | 9.69E-02 | 1.07E+00 | 9.06E-02 | 3.20E-01 | 1.06E-01 | 1.30E-01 | 8.88E-02 | 3.90E-01 | 1.77E-01 | 3.10E-01 | 1.53E-01 | c | 1.10E-01 | 4.80E-01 | 1.32E-01 | 3.30E-01 | 3.40E-01 | 43\% |
| 22-29-30-trisnorhopane | 4.44E-02 |  | 4.27E-02 |  | 3.76E-02 |  | 4.11E-02 | c | 7.07E-02 | c | 5.68E-02 | 8.00E-02 | 6.28E-02 | $1.10 \mathrm{E}-01$ | 4.57E-02 | 1.00E-01 | 8.37E-02 | 7.00E-02 | 5.60E-02 |  | 4.82E-02 | c | 5.85E-02 | c | 1.37E-02 | 28\% |
| 17-a(H)-21b(H)-29-nortopane | 9.38E-02 | $2.50 \mathrm{E}-0$ | 9.08E-02 | ee-0 | 03E-0 | 10E-0 | 24E-02 | c | 66E-01 | c | 1.27E-01 | $2.80 \mathrm{E}-01$ | 1.34E-20 | 6.50E-01 | 9.70E-02 | 4.20E-01 | 1.79E-01 | 3.70E-01 | 1.17E-01 | 1.90E-01 | 1.02E-01 | $2.20 \mathrm{E}-01$ | 1.25E-01 | 1.70E-01 | 1.37E-02 | 14\% |
| 17-a(H)-21B(H)-hopane 22R\&S-17a(H)-21b(H)-30- | 1.15E-01 | 1.60E-01 | 1.11E-01 | 1.50E-01 | 9.75E-02 | 1.50E-01 | 1.09E-01 | c | 1.87E-01 | c | $1.51 \mathrm{E}-01$ | 1.60E-01 | 1.64E-01 | 3.80E-01 | 1.19 | 2.70 E | 2.19 E | 2.5 | 1.4 | 1.10E-01 | 1.2 | 2.70 E | 1.55E-01 | 1.00E-01 | .37 | 14\% |
| homohopane | 1.11 | 1.63E-01 | 1.06E-01 | 1.43E-01 | 9.30E-02 | 1.70E-01 | 1.00E-01 | c | 1.75E-01 | c | 1.40E-01 | 1.80E-01 | 1.56E-01 | 3.70E-01 | 1.13E-01 | $2.70 \mathrm{E}-01$ | 2.09E-01 | 1.90E-01 | 1.40E-01 | 1.70E-01 | 1.20E-01 | c | 1.46E-01 | c | 1.37E-02 |  |
| $22 R \& S-17 a(H)-21 \mathrm{~b}(\mathrm{H})-30-31-$ bishomohopane | 5.68E-02 |  |  |  |  |  |  | c | 10E-02 | c | 7.30E-02 | 1.10E-01 | 8.01E-02 | $2.20 \mathrm{E}-01$ | 5.82E-02 | 1.50E-01 |  |  |  |  | 6.24E-012 |  | , 3E-02 |  | 1.37E-02 | 14\% |
| 20R+S-abb-cholestane | 6.19E-02 | c | 6.01E-02 | c | $5.43 \mathrm{E}-02$ | c | 6.02E-02 | c | 9.88E-02 | c | 8.12E-02 | 6.00E-02 | 8.88E-02 | 1.70E-01 | 6.50E-02 | 1.20E-01 | 1.15E-01 |  | 7.82E-02 |  | 6.49E-02 | c | 7.78E-02 | c | 1.37E-02 | 32\% |
| 20R-aaa-cholestane | 5.13E-02 | c | 5.03E-02 | c | 4.57E-02 | c | 5.32E-02 | c | 8.49E-02 | c | $7.10 \mathrm{E}-02$ | 6.00E-02 | 7.47E-02 | 1.00E-01 | 5.44E-02 | 6.00E-02 | 9.50E-02 |  | 6.45E-02 |  | 5.37E-02 |  | 6.48E-02 |  | 1.37E-02 | \% |
| 20R + S-ab-ergostane | $6.28 \mathrm{E}-02$ |  | 6.10E-02 |  | 5.48E-02 |  | 6.00E-02 | c | 9.96E-02 | c | 8.13E-02 | 6.00E-02 | -02 | $1.20 \mathrm{E}-01$ | 6.58E-02 | 8.00E-02 | 1.16E-01 |  | 7.98E-02 |  | 6.64E-02 |  | 7.95 |  | 37E-02 | 18\% |
| 20R + S-ab-sitostane | $6.96 \mathrm{E}-12$ |  | 6.80E-02 |  | 6.17E-02 |  | 7.05E-0 | c | 1.14E-01 | c | $9.45 \mathrm{E}-02$ | 1.10E-01 | 1.01E-01 | 1.90E-01 | 7.36E-02 | 1.50E-0 | 1.29E-01 | c | 8.77E-02 |  | 7.29E-02 | c | 8.77E-02 | c | 1.37E-02 | 28\% |
| Fluoranthene | 7.16 | $2.90 \mathrm{E}-01$ | 7.11E-20 | $2.10 \mathrm{E}-01$ | 6.24 E | 1.40E-01 | 4.15E-01 | 1.50E-01 | 7.60E-01 | 1.80E-01 | 7.36 E | 1.60E-01 | 9.21 | 2.20E-01 | 7.81E-01 | 1.90 | $1.27 \mathrm{E}+00$ | 6.00E-02 | $1.49 \mathrm{E}+00$ | 1.00E-01 | $1.18 \mathrm{E}+00$ | 3.60E-01 | 1.34E+00 | 1.70E-01 | 2.73E-02 | 26\% |
| Acephenanthrylene | 1.13E-01 | c | 7.74E-02 | c | 6.90E-02 | c | 3.58E-02 | c | 5.39E-02 | c | 8.98E-02 | 8.00E-02 | 9.90E-02 | 1.10 E | 1.0 | 9.00E-02 | 2.29E-01 | c | 2.56E-01 | c | 1.49E-01 | c | 1.76E-01 | c | 2.73 E | 26\% |
| Benzo(ghi)fluoranthene | 3.25E-01 | c | 3.53E-01 | c | 3.08E-01 | c | 2.17E-01 | c | 4.10E-01 | c | 3.60E-01 | 1.60E-01 | 4.60E-01 | $2.70 \mathrm{E}-01$ | 3.68E-01 | 3.90E-01 | 5.53E-01 | 5.90E-01 | 6.50E-01 | 6.10E-01 | 5.66E- | $6.30 \mathrm{E}-01$ | 6.39E-01 | $4.20 \mathrm{E}-01$ | 3.00E-02 | 25\% |
| Cyclopenta(cd)pyrene | 1.44E-01 |  | 1.12E-01 | c | 1.03E-01 | c | 9.36E-02 | c | 1.32E-01 | c | $1.60 \mathrm{E}-01$ | 5.00E-02 | 1.54E-01 | c | 1.43E- | 60E-01 | 2.87E--1 | 3.40E-2 | 2.85 E | 2.20E-0 | 1.79E-0 | 3.00E-01 | 2.15E-0 | c | 2.73E-02 | 16\% |
| Benz(a)antrracene | 4.03E- | 7.00E-02 | 4.29E-01 |  | 3.73E-01 | 7.00E-02 | $2.38 \mathrm{E}-01$ | c | 4.62E-01 | c | $4.17 \mathrm{E}-01$ | 1.00E-02 | 5.51E-01 | $2.00 \mathrm{E}-02$ | 4.53E-01 | 3.00E-02 | 6.87E-01 | 1.20E-01 | 8.38E-01 | 7.00E-02 | $7.11 \mathrm{E}-01$ | 1.10E-01 | 7.98E-01 | 6.00E-02 | 2.73E-02 | 10\% |
| Chrysene/Triphenylene | 1.31 E | 1.90E-01 | 1.49E+00 | 1.40E-01 | 1.29E+00 | 5.00E-02 | 8.31E-01 | 8.00E-02 | $1.66 \mathrm{E}+00$ | c | $1.41 \mathrm{E}+00$ | 1.60E-01 | $1.91 \mathrm{E}+00$ | $2.00 \mathrm{E}-01$ | 1.51E+00 | 1.60E-01 | $2.16 \mathrm{E}+00$ | $2.00 \mathrm{E}-01$ | 2.68E | 1.60E-01 | $2.43 \mathrm{E}+00$ | $2.30 \mathrm{E}-01$ | $2.71 \mathrm{E}+00$ | 1.60E-01 | 2.73E-02 | 25\% |
| Retene | 1.39 E | c | 8.54E-01 | c | 7.73E-01 | 2.90E-01 | 2.13E-01 | c | $2.33 \mathrm{E}-01$ | c | $9.05 \mathrm{E}-01$ | c | $1.03 \mathrm{E}+00$ | c | 1.28E+00 | c | $2.84 \mathrm{E}+00$ | c | 3.50 E | $2.80 \mathrm{E}-01$ | $1.90 \mathrm{E}+0$ | 2.80E-01 | $2.21 \mathrm{E}+00$ | c |  | 29\% |
| Benzo(k)fluoranthen | $6.98 \mathrm{E}-01$ | EE-01 | 7.37E-01 | E-01 | 6.18E-01 | OE-0 | 4.44E-01 | c | 9.75E-01 | c | 7.42E-01 | 80E-01 | $1.51 \mathrm{E}+00$ | E-01 | 8.96E-01 | 1.40E-01 | $1.26 \mathrm{E}+00$ | ce-0 | $1.35 \mathrm{E}+00$ | 3.00E-02 | 1.2 | c | 1.38 |  | .73E-012 | 38\% |
| Benzo(b)fluoranthene | 8.13E-0 | $4.50 \mathrm{E}-01$ | 8.42E-01 | 2.90E-01 | 6.99E-01 | 1.90E-01 | 04E-01 | c | 15 E | c | 8.47E-01 | 4.00E-01 | $1.89 \mathrm{E}+0$ | 3.60E-01 | 1.07E | 6.00E-02 | 1.49E+0 | 1.60E-01 | 1.55E+ | 5.00E-02 | 1.39E+0 | 3.50E-0 | $1.59 \mathrm{E}+00$ | $2.30 \mathrm{E}-01$ | 2.73E-02 | \%\% |
| Benzo(i)fluoranthene | 2.35 |  | 1.79E-02 |  | 1.64E-02 |  | 1.29E-02 | c | 1.82E-02 | c | $2.39 \mathrm{E}-02$ |  | 2.41E-02 |  | 2.34E-02 |  | 4.75E-02 |  | 4.94E-02 |  | $2.99 \mathrm{E}-02$ | c | 3.56E-02 | c | 2.73E-02 | 38\% |
| Benzo()pyrene | $5.02 \mathrm{E}-0$ | $2.60 \mathrm{E}-01$ | 5.13E-2) | E-01 | 4.21E-01 | 1.30E-01 | 2.8 | c | $6.99 \mathrm{E}-01$ | c | 5.00E-01 | 2.50E-01 | $1.25 \mathrm{E}+00$ | $2.60 \mathrm{E}-01$ | 6.75E-01 | 1.80E-01 | 9.30E-0 | 30E-01 | 9.76 E | 1.40E-01 | 8.6 | c | $9.95 \mathrm{E}-01$ |  | 2.73E-02 | 25\% |
| Benzo(a)pyre | 5.90E-02 | 1.80E- | 4.35E-02 | OE-T | 3.96E-02 | c | 76E | c | 3.98E-02 | c | 5.45 | 1.40E-0 | 5.76 | 1.50E-01 | 5.74E- | 1.30E- | 1.17 E | 1.90E-II | 1.25E-01 | $1.20 \mathrm{E}-1$ | 7.48E | c | 8.85E-12 |  | 2.73E-02 | 25\% |
| Perylene | 3.44E-02 | 2.20E-0 | 3.26E-02 | 20E-01 | 3.03E-02 | 8.00E-02 | 4.11E-02 | 1.30E-01 | 5.92E-02 | 7.00E-02 | $5.61 \mathrm{E}-02$ | 90E-0 | 4.89E-02 | 1.40E-01 | 3.68E | 1.20E--1 | 6.67 | $1.20 \mathrm{E}-\mathrm{n}$ | 4.89E-02 | 1.40E- | 3.83E-02 | $2.80 \mathrm{E}-01$ | 4.83E-02 | 1.10E-01 | 2.73E-02 | 25\% |
| Indeno(cd) pryene | 5.16 |  | $5.16 \mathrm{E}-01$ |  | 4.18 | c | 2.93E-01 | c | 7.29E-01 | c | 5.10 E | 4.80E-01 | 1.37E+0 | $3.00 \mathrm{E}-01$ | 7.11E-01 | 2.30E-0 | 99-0 | 1.60 E | 9.95 E | 1.00E-02 | 8.80E-0 | 1.50E-01 | 1.01E+00 | 8.00E-02 | 2.73E-02 | 29\% |
| Benzo(ghi)perylene | $5.48 \mathrm{E}-01$ | 1.20E-01 | 5.52E-01 | 1.20E-01 | 4.67E-01 | c | 4.43E-01 | c | 8.75E-01 | c | 6.72E-01 | 3.80E-01 | $1.29 \mathrm{E}+00$ | $3.70 \mathrm{E}-01$ | 7.11E-01 | 3.50E-01 | 1.04E+00 | 3.80E-01 | $9.37 \mathrm{E}-01$ | $2.10 \mathrm{E}-01$ | 8.31E-01 | $2.60 \mathrm{E}-01$ | 9.78E-01 | 1.80E-01 | 2.73E-02 | , |
| Coronene | 2.59E-01 | c | 2.52E-01 | c | 2.08E-01 | c | 1.52E-01 | c | 3.51E-01 | c | $2.61 \mathrm{E}-01$ | 1.40E-01 | $6.32 \mathrm{E}-01$ | 1.20E-01 | 3.43E-01 | 1.60E-01 | 4.94E-01 | 1.20E-01 | 4.97E-01 | c | 4.23E-01 | 1.30E-01 | 4.89E-01 | 9.00E-02 | 3.41E-02 | 26\% |
| Tetradecanoi | 1.47E+00 | 04E+00 | 1.43E | 20E+00 | 1.30E+00 | 1.35E+00 | .06E+ | $1.94 \mathrm{E}+00$ | 1.67E+ | 7.70E-01 | 1.58E+00 | c | 1.88E+00 | c | 61E+0 | 5.36 E | 00 | c | 2.48E+00 | c | $1.80 \mathrm{E}+00$ | 5.88E+00 | 2.14 E | 0 | $2.17 \mathrm{E}+00$ | 47\% |
| Pentadecanoic acid | $4.32 \mathrm{E}-01$ | c | 4.16 E | 20E-01 | 3.76E | c | 03E | c | 4.77E-0 | 1.40E-01 | 4.59E-10 | c | 5.45E-01 | c | 4.71E-01 | 2.35 E | 7.91 E | c | 7.37E-01 | c | 5.31 | $2.99 \mathrm{E}+0$ | 6.30E-0 | $1.99 \mathrm{E}+00$ | 1.33E+6 | 50\% |
| Hexadecanoic acid | 8.65 | $1.05 \mathrm{E}+01$ | 8.59E+00 | 8.04E+00 | 7.78E+00 | $1.52 \mathrm{E}+01$ | 6.45E+00 | $1.14 \mathrm{E}+01$ | 1.01E+01 | 8.39E+00 | $9.47 \mathrm{E}+00$ | c | 1.12E+01 | c | $9.58 \mathrm{E}+00$ | 3.38E | 1.57E+ | c | 1.43 |  | 1.06 | $2.67 \mathrm{E}+01$ | 1.26E+01 | $1.75 \mathrm{E}+01$ | $66 \mathrm{E}+00$ | 53\% |
| Heptadecanoic acid | $6.27 \mathrm{E}-01$ | 3.90E-01 | 6.51E-01 | 3.90E-01 | 5.88E-01 | c | 5.13E-01 | c | 8.09E-01 | c | 7.23E-01 | c | 8.55E-01 | c | 7.08E-01 | 8.50E-01 | $1.13 \mathrm{E}+00$ | c | 9.74E-01 | c | 7.56E-01 | 5.10E-01 | 9.06E-01 | 2.00E-01 | 3.03E-01 | 7\% |
| Octadecanoic acid | $4.41 \mathrm{E}+00$ | 6.89E+00 | 4.52E+00 | 4.95E+00 | 4.07E+00 | $4.23 \mathrm{E}+00$ | $3.50 \mathrm{E}+00$ | 5.80E+00 | 5.59E+00 | 4.54E+00 | 5.00E+00 | 1.10E+00 | 5.94E+00 | $2.60 \mathrm{E}-01$ | 4.94E+00 | $1.35 \mathrm{E}+01$ | $7.96 \mathrm{E}+00$ | c | $6.91 \mathrm{E}+00$ | c | 5.33E+00 | 6.86E+00 | 6.38E+00 | $3.65 \mathrm{E}+00$ | 4.56E+00 | \% |
| Eicosanoic acid | 3.6 | OE-O | 2.54E-0 | 3.50E-01 | 2.27E-0 | 2.70E-01 | 1.02E-1 | 5.50E-01 | 1.48 E | 8.00E-01 | 2.74E-01 | c | 3.17E-01 | c | 3.51 E | $1.24 \mathrm{E}+00$ | 7.37E-0 | c | 8.49E- | c | 4.89E-7 | 8.70E-01 | 5.74E-01 | EE-01 | 8.22E-01 | 48\% |
| Heneicosanoic acid | 8.0 | $4.10 \mathrm{E}-01$ | 4.99E-02 |  | 4.50E-02 | c | 1.34 E | c | 1.52E-20 | c | 5.32E-02 | 3.00E-02 | 6.03E-02 | c | $7.43 \mathrm{E}-02$ | $2.00 \mathrm{E}-0$ | $1.63 \mathrm{E}-01$ | 4.40E-01 | $2.01 \mathrm{E}-01$ | $3.90 \mathrm{E}-01$ | 1.09E-01 | 3.00E-02 | 1.27E-01 |  | 8.22E-01 | $36 \%$ |
| Docosanoic acid | 4.9 | $5.90 \mathrm{E}-01$ | 3.12E-01 | 6.70E-01 | 2.82E-01 | c | 8.94E-02 | c | 1.05 E | 3.20E-01 | 3.32E-01 | 7.40E-01 | 3.78E-01 | 3.00E-02 | 4.61E-01 | $1.70 \mathrm{E}+00$ | $1.00 \mathrm{E}+00$ | 5.20E-01 | 1.22E+00 | c | 6.70E-01 | 1.19E+00 | 7.82E-01 | 8.00E-01 | 2.23E-01 | 25\% |
| Tricosanoic acid | 1.96E-01 | 2.30E-01 | 1.21E-01 | 2.90E-01 | 1.09E-01 | c | 3.11E-02 | c | 3.46E-02 | c | 1.29E-01 | 1.60E-01 | 1.46E-01 | c | 1.81E-01 | 5.00E-01 | 4.00E-01 | 2.50E-01 | 4.92E-01 | 8.00E-02 | 2.67E-01 | 3.70E-01 | 3.11E-01 | $2.60 \mathrm{E}-01$ | 1.50E-01 | 24\% |
| Tetracosanoic acid | $1.08 \mathrm{E}+00$ | 8.70E-01 | 6.64E-01 | 1.04E+00 | 6.00E-01 | 4.20E-01 | 1.69E-01 | 6.80E-01 | 1.87E-01 | $9.50 \mathrm{E}-01$ | 7.04E-01 | 3.70E-01 | 8.00E-01 | c | $9.96 \mathrm{E}-01$ | $2.73 \mathrm{E}+00$ | 2.20E+00 | 2.10E-01 | 2.71E+00 | c | 1.47E+00 | $2.02 \mathrm{E}+00$ | 1.71E+00 | $1.25 \mathrm{E}+00$ | 6.29E-01 | 23\% |
| Pentacosanoic acid | 1.03 | 3.30E-01 | 6.34E-02 | 3.80E-01 | 5.73E-02 | c | 1.65E-12 | c | 1.84E-02 | c | 6.74E-02 | 8.00E-02 | 7.65E-02 | c | 9.48E-02 | 6.40E-01 | 2.09E-01 | 6.00E-02 | 2.57E-01 | c | 1.40E-01 | 3.40E-01 | 1.63E-01 | 1.90E-01 | 3.72E-01 | 35\% |
| Hexacosanoic acid | 6.7 | 6.30E- | 4.19E-21 | 7.60E-01 | 3.78E-01 | 3.00E-02 | 1.08E-01 | $2.50 \mathrm{E}-01$ | 1.22E-01 | 5.60E-01 | $4.44 \mathrm{E}-01$ | 4.20E-01 | 5.05E-01 | 3.00E-02 | 6.25E-01 | $1.47 \mathrm{E}+00$ | 1.38E+00 | 2.90E-01 | 1.69E+00 |  | 9.22E-01 | OE-0 | 1.07E+00 | OE-0 | 4.60E-01 | 35\% |
| Heptacosanoic acid | 5.51 E | OE-01 | 3.42E-02 | 3.40E-0 | 3.09E-02 | c | 15E-0 | c | 1.04E-02 | c | 3.64E-02 | 1.40E-01 | 4.14E-02 | 5.00E-02 | 5.10E-02 | $2.20 \mathrm{E}-01$ | 1.12E-01 | 8.90E-0 | 1.38E-01 | 8.30E-01 | 7.49E-02 | c | 8.73E-02 | c | 3.05E-02 | 35\% |
| Octacosanoic acid | 3.61E-01 | 6.60E-01 | $2.26 \mathrm{E}-01$ | $1.16 \mathrm{E}+00$ | 2.03E-01 | c | 6.07E-02 | 1.70E-01 | 6.99E-02 | 4.60E-01 | $2.40 \mathrm{E}-01$ | 5.00E-01 | 2.73E-01 | $2.60 \mathrm{E}-01$ | 3.35E-01 | 9.70E-01 | 7.34E-01 | 3.50E-01 | 9.02E-01 | D0E-02 | 4.93E-01 | 1.74E+ | 5.74E-01 | 1.62E+0 | 2.34E-01 | 47\% |
| Nonacosanoic acid | 5.15E-02 | c | 3.24E-02 | c | 2.91E-02 | c | 9.25E-03 | c | 1.08E-02 | c | 3.47E-02 | c | 3.95E-02 | c | 4.79E-02 | c | 1.04E-01 | $9.50 \mathrm{E}-01$ | 1.27E-01 | c | 6.98E-02 | c | 8.15E-02 | c | $2.34 \mathrm{E}-01$ | 32\% |
| Triacontanoic acid | 4.15 | c | 2.58E-01 | 5.00E-01 | 2.33E-01 | c | 6.80E-02 | c | 7.67E-02 | c | 2.74E-01 | 3.10E-01 | 3.11E-01 | c | 3.84E-01 | 7.50E-01 | 8.45E-01 | $1.31 \mathrm{E}+00$ | 1.04E+00 | $1.15 \mathrm{E}+00$ | 5.65E-01 | c | 6.59E-01 | c | 2.34E-01 | 17\% |
| Butanedioic acid | $3.56 \mathrm{E}-01$ | $8.20 \mathrm{E}-01$ | $3.33 \mathrm{E}-01$ | $2.29 \mathrm{E}+00$ | 3.03E-01 | $4.29 \mathrm{E}+00$ | $2.33 \mathrm{E}-01$ | 5.57E+00 | 3.53E-01 | $4.96 \mathrm{E}+00$ | $3.65 \mathrm{E}-01$ | $1.00 \mathrm{E}+01$ | $4.28 \mathrm{E}-01$ | $6.55 \mathrm{E}+00$ | 3.87E-01 | 8.00E-01 | 6.58E-01 | $4.77 \mathrm{E}+00$ | $6.44 \mathrm{E}-01$ | $4.60 \mathrm{E}-01$ | 4.42E-01 | 6.90E-01 | 5.26E-01 | $1.01 \mathrm{E}+00$ | $1.28 \mathrm{E}+00$ | 42\% |
| Pentanedioic acid | 1.62E-01 | 8.30E-01 | 1.64E-01 | $1.31 \mathrm{E}+00$ | 1.49E-01 | $1.28 \mathrm{E}+00$ | 1.26E-01 | 8.50E-01 | 1.93E-01 | 7.20E-01 | 1.81E-01 | $2.08 \mathrm{E}+00$ | 2.13E-01 | $1.20 \mathrm{E}+00$ | 1.82E-01 | c | 2.91E-01 | $1.06 \mathrm{E}+00$ | 2.64E-01 | 4.00E-02 | 1.96E-01 | c | $2.35 \mathrm{E}-1$ | c | 1.52E+6 | 42\% |
| Hexanedioic acid | 1.66E-01 | -01 | 1.81E-01 | 0E-01 | 1.64E-01 | 30E-01 | 48E-0 | c | 01 | c | 2.00E-01 | $2.10 \mathrm{E}-0$ | 2.36E-01 | c | 93E-0 | c | $2.91 \mathrm{E}-01$ | c | 2.44E-01 | c | 1.97E-01 | c | 2.36E-01 | c | 1.31E+00 | 42\% |
| Heptanedioic acid | $6.08 \mathrm{E}-03$ |  | 3.73E-03 | c | 3.38E-03 |  | $9.31 \mathrm{E}-04$ | c | 1.02E-03 | c | $3.96 \mathrm{E}-03$ | 5.80E-01 | 4.49E-03 | c | $5.62 \mathrm{E}-03$ | c | 1.24E-02 | c | 1.53E-02 | c | 8.29E-03 | c | $9.66 \mathrm{E}-03$ | c | $1.32 \mathrm{E}+00$ | 42\% |
| Octanedioic acid | 4.46 |  | 4.18E |  | 3.57E-01 | 3.50E-01 | 2.92E-01 | 4.70E-01 | 5.53E-01 |  | 4.55E-01 | 7.00E-02 | 5.66E-0 |  | 4.56E-01 |  | 8.50E-01 | 1.80E-01 | 6.75E-01 | 3.10E-01 | 5.40E-0 |  | 6.52E-0 |  | $1.32 \mathrm{E}+00$ | 42\% |
| Nonanedioic acid | $4.17 \mathrm{E}-01$ | 7.90E-01 | 3.43E-01 | $1.03 \mathrm{E}+00$ | 2.82E-01 | $1.34 \mathrm{E}+00$ | 1.99E-01 | $5.50 \mathrm{E}-01$ | $4.32 \mathrm{E}-01$ | 4.90E-01 | 3.69E-01 | 1.6 | 4.70E-01 | $1.58 \mathrm{E}+00$ | 3.92E-01 | $9.00 \mathrm{E}-01$ | 8.32E-01 | $1.06 \mathrm{E}+00$ | 6.92E-01 | 2.00E-01 | 7E | 3.70E-01 | 6.24E-01 | 4.90E-01 | $1.18 \mathrm{E}+00$ | 42\% |


| trac | March04 |  | April04 |  | May04 |  | June04 |  | July04 |  | August04 |  | September04 |  | October04 |  | November04 |  | December04 |  | Janucry05 |  | February05 |  | MDL ${ }^{\text {a }}$ | UNC ${ }^{\text {b }}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1-2-benzenedicarboxylic acid | 2.56E-03 | 6.30E-01 | 1.57E-03 | 1.04E+00 | 1.42E-03 | 1.81E+00 | 3.91E-04 | $2.36 \mathrm{E}+00$ | 4.28E-04 | 2.66E+00 | 1.66E-03 | 4.91E+00 | 1.89E-3 | 4.90E+ | 2.3 | c | $5.22 \mathrm{E}-03$ | 00 | 6.44E | 8.00E-02 | 3.48E-03 | 1.00 | 6E-03 | 1.40E-01 | 0 | 38\% |
| 1-3-benzenedicarboxylic acid | 4E-0 | 1.40E-01 | 1.20E-03 | 2.00E-01 | 9.43E-04 |  | 88E-04 | 10E-01 | 2.05E-03 |  | 84E-2 |  | 1.04E-13 |  | -04 |  | 1.22E-3 | 50E-01 | 2.25-03 | 5.00E-02 | 1.71E-0 |  | 1.74E-03 |  | 1.34 | 38\% |
| 1-4-benzenedicarboxylic acid | 2.05E-03 | 3.50--01 | 1.81E-03 | 4.40E-01 | 1.53E-03 | 6.70E-01 | 89E-04 | 10E-01 | 1.70E-03 | 4.80E-01 | 1.50E-03 | 5.80E-01 | 1.89E | 8.90E-01 | 2.13 | c | 4.33E-3 | $1.266+00$ | 5.52E-1 | 2.80E-01 | 3.34E-03 | OE-1 | 3.71E-03 | 0e-01 | 1.27E+00 | 38\% |
| Nonadecanoic acid | 1.12E-01 | 7.00E-02 | 8.51E-02 | 7.00E-02 | 7.65E-02 | c | 4.43E-02 | c | 6.66E-02 | c | 9.35E-02 | 4.00E-02 | 1.08E-01 | c | 1.11--01 | $2.50 \mathrm{E}-01$ | 2.19E-01 | c | 2.39E-01 | c | 1.45E-01 | c | 1.70E-01 | c | 1.45E-01 | 73\% |
| 1-8-naphthalic anhydride | 5.69E-03 | 3.50E-01 | 3.49E-03 | 5.60E-01 | 3.16E-03 | c | 8.71E-04 | c | 9.53E-04 | c | 3.70E-03 | 9.90E-01 | 4.20E-03 | 1.25E+00 | 5.25E-03 | 6.10E-01 | 1.16E-02 | c | 1.43E-02 | c | 7.75E-03 |  | 9.03E-03 |  | 2.78 E | 16\% |
| 1 H -phenalen-1--one | 4.62E-01 | c | 4.9 | 5.70E-01 | 4.3 | c | 2.63E-01 | c | 5.24E-01 | ${ }^{\text {c }}$ | 4.71E-01 | 40E-0 | 6.35E-01 | OE- | 5.22E | c | 7.80 |  | 9.80E- | 4.90 E | 8.39 |  | 9.38E-01 |  | 1.74E | 16\% |
| Anthracen-9-10-dione | 1.37E+00 | 7.20E-01 | 1.56E+00 | .10E-01 | 1.36E+00 | c | 24E-01 | c |  | c | 1.52E+00 | 4.30E-01 | 2.03E+00 | 4.30E-01 | 1.58E+00 | 4.60E-01 | 2.25E+00 | 5.90E-01 | $2.72 \mathrm{t}+00$ | 6.20E-0 | 2.50E+00 | 1.70E-0 | 2.80E+00 | 1.20E-01 | 7.41 E | 16\% |
| Benz(a)antracene-7 12-dione | 7.75E-02 | c | $9.04 \mathrm{E}-12$ | c | 7.81E-02 | c | 5.04E-02 | c | 1.02E-01 | c | 8.45E-02 | 4.90E-01 | 1.16E-01 | $5.40 \mathrm{E}-01$ | 9.07E-02 | 3.90E-01 | 1.25E-01 | c | 1.58E-01 | c | 1.47E-01 | c | 1.64E-01 | c | 7.06E-01 | 16\% |
| Levoglucosan | 4.4 | 3.70E+01 | 1 | 2.52E+01 | $2.45 \mathrm{E}+01$ | $3.78 \mathrm{E}+01$ | 75E+00 | 90E+01 | 39E+00 | $4.32 \mathrm{E}+01$ | $2.87 \mathrm{E}+01$ | 6.03E+01 | 3.25E+01 | $3.98 \mathrm{E}+01$ | 4.07E+01 | $5.88 \mathrm{E}+01$ | $9.00 \mathrm{E}+01$ | 1.64E+02 | 1.11E+02 | 8.03E+01 | 6.01E+01 | 1.03E+02 | 7.00E+01 | 7.81E+01 | 2.70E+00 | 37\% |
| 3-Acetylpentanedioic acid | 1.64-01 | c | 2.68E-01 | 1 | 2.73E-01 | $4.40 \mathrm{E}+00$ | 1.25E-01 | OE+0 | 4.55E-01 | $2.60 \mathrm{E}+00$ | 7.49E-01 | $2.20 \mathrm{E}+00$ | 4.69E-01 | 3.20E+00 | 1.74E-01 | c | 2.31--01 | 6.00E-01 | 9.45E-02 | c | 4.88E-02 | c | 2.76E-02 | c | 1.00E-01 |  |
| 2-Hydroxy-4-isopropyladipic acid | 3.00E-01 | 00 | 4.88E-01 | 1 | 4.97E-01 | 3.55E+01 | 2.28E-01 | 5.70E+01 | 8.29E-01 | $4.62 \mathrm{E}+01$ | 1.36E+00 | $2.23 \mathrm{E}+01$ | 8.55E-01 | 3.69E+01 | 3.18E-01 | c | 4.21E-01 | 1.93E+01 | 1.72E-01 | 9.00E+00 | 8.90E-02 | 3.30E+00 | 5.03E-02 | 0 | 1.0 |  |
| 3 -Acetyl hexanedioic acid | $2.07 \mathrm{E}+00$ | 4.00E-01 | 3.36E+00 | 200E-01 | 3.43E+00 | $2.30 \mathrm{E}+00$ | $1.58 \mathrm{E}+0$ | 4.00E-01 | 5.72E+0 | 2.40E+0 | 9.41E+0 | $9.00 \mathrm{E}-01$ | 5.9 | $2.60 \mathrm{E}+00$ | 2.19E+00 | 2.00E-01 | 2.91E+00 | .00E-01 | 1.19E+0 | 5.00E-01 | 6.14E-01 | c | 3.47 | c | 1.00E-01 |  |
| 3-Hydroxyglutaric acid | 2.32E-01 | OE+0 | E-01 | 1.23E+01 | 3.84 | 8E+0 | 1.77E-01 | 4.05E+01 | 6.42E | 4.08E+ | 1.06E+ | 2.03E+ | 6.61E- | 3.27E+01 | 2.4 |  | 3.26 | $9.10 \mathrm{E}+0$ | 1.33 | 5.20E+00 | 6.88E-02 | 5.90E+ | 3.89E-02 | 0 | 1.00E-01 |  |
|  | 1E-01 | 2.00E-01 | 8E-01 | 9.00E-01 | 3-01 | .30E +0 | 0E-01 | 80E+0 | 3E-0 | $3.90 \mathrm{E}+0$ | 8E-0 | 2.00E+0 | 878-01 | $2.70 \mathrm{E}+0$ | 1E-0 | c | 0E-01 | OE+ + | 9.82E-02 | .00e-01 | 5.0 | c | 2.87E- | 1.00E- | . $.00 \mathrm{E}-$ |  |
| 3-(2-Hydroxy-ethyl)-2-2-dimethyl- | 1.14E+00 | c | 1.85E+00 | 1.00E-01 | 1.89E+00 | 5.00E-01 | 8.68E-01 | $2.70 \mathrm{E}+00$ | 3.15E+00 | 2.00E-01 | 5.19E+00 | c | 3.25E+00 | 3.00E-01 | 1.21E+00 |  | 1.60E+00 | c | 6.55E-01 | c | 3.38E-01 |  | 1.91E-01 | c | 1.00E-01 |  |
| Pinic acid | 8.37E-01 | c | 1.36E+00 | 6.00E-01 | $1.39 \mathrm{E}+00$ | 00E-01 | 6.38E-01 | 3.00E-01 | 2.32E+00 | 4.00E-01 | 3.81E+00 | 4.00E-0 | 2.39E+00 | 2.00E-01 | 8.88E-01 | c | BE+00 | c | 4.81-01 | 3.00E-01 | 2.49E-01 | 1.00E | 1.41E-01 | c | 1.00E-01 |  |
| Pinonic | E-01 | c | E-01 | D.0E-01 | E-01 | c | E-01 | c | $2 \mathrm{~F}+00$ | c | $1.84 E+00$ | c | 1.15E+00 | c | 4.28E-01 | c | 5.67E-01 | OE-02 | 2.32-01 | 7.00E-0 | 1.20 E | c | 6.77 | c | 1.00E |  |
| acid | 2.36E-01 | 2.00E-01 | 2.80E-01 | 7.00E-01 | 2.36E-01 | $3.00 \mathrm{E}+00$ | 4.05E-01 | 3.20E+00 | 5.21E-01 | $2.40 \mathrm{E}+00$ | 5.27E-01 | 1.20E+00 | 4.55E-01 | $2.50 \mathrm{E}+00$ | 2.52E-01 | c | 2.36E-01 | 6.00E-01 | 2.87E-01 | 4.00E-01 | 1.14E-01 | c | 3.11E-01 | 2.00E-01 | 1.00E-01 |  |
| 2-Methylglyceric acid | 1.19E+ | 01 | 9.5 | 2.50E+00 | 2.19E+0 | 2.40E+0 | $1.36 \mathrm{E}+00$ | 4.63E+0 | 2.85E+00 | $5.60 \mathrm{E}+01$ | 4.58E+00 | 1.50E+01 | 3.84E+00 | 3.89E+01 | 8.83E-01 | 6.80E+00 | 6.49E-01 | 2.10E+00 | 9.84-01 | 6.00E-01 | 7.19E-01 | 1.40E+00 | 7.92E-01 | 1.00E+00 | 1.00E-01 |  |
| 2-Methyltrreitol | $2.011+00$ |  | 1E+00 | $2.00 E+00$ | 3.69E+00 | 5.64E+01 | 2.29E+00 | 8.58E+01 | 81E+00 | $5.99 E+01$ | 3E+00 | $2.89 \mathrm{E}+01$ | 6.47E+00 | 7.12E+01 | 1.49E+00 | . $100 \mathrm{E}+00$ | 1.10E+00 | 2.00E-01 | 1.66E+00 | c | 1.21E+0 | c | $1.34 \mathrm{E}+00$ | c | 1.00E-01 |  |
| 2-Methylerythritol | 3.30E+00 | 3.00E-01 | 2.65E+00 | 4.60E+00 | 6.07E+00 | 1.04E+02 | 3.77E+00 | $1.44 \mathrm{E}+02$ | $7.91 \mathrm{~F}+00$ | 9.22E+01 | 1.27E+01 | 6.32E+01 | 1.06E+01 | $1.17 \mathrm{E}+02$ | 2.45E+00 | 1.69E+01 | 1.80E+00 | 7.00E-01 | 2.73E+00 | c | 2.00E+00 | c | 2.20E+00 |  | 1.00E-01 |  |
| b-Caryophyllinic ac |  | 1.60E+00 |  |  |  | $2.10 \mathrm{E}+00$ | 4.95E-01 | $4.40 \mathrm{E}+00$ | 2.29E+00 | 4.1 | 3.02E+00 | 1.70E+00 | 1.51E+00 | 9.20E+00 | 3.46E-01 | c | 3.34--01 | $4.40 \mathrm{E}+00$ | 5.87E-02 | $2.00 E+00$ | 1.53E-02 | 1.90E+00 | 1.13E-02 | 5.90E+00 | 1.00E-01 |  |

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Table S5. Paired model and observation quantities of each organic tracer at Detroit, MI in units of ( $\mathbf{n g} / \mathrm{m}^{\mathbf{3}}$ ) in the context of measurement detection limit (MDL ${ }^{\mathrm{a}}$ ) and measurement uncertainty ( $\mathrm{UNC}^{\mathrm{b}}$ ). Observations below the detection limit are denoted by ${ }^{\mathrm{c}}$.

| tracer | March04 |  | April04 |  | May04 |  | June04 |  | July04 |  | August04 |  | September04 |  | October04 |  | November04 |  | December04 |  | Janucry05 |  | February05 |  | MDL ${ }^{\text {a }}$ | $\mathrm{UNC}^{\text {b }}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | model | obs | model | bs | model | obs | model | obs | model | obs | model | obs | model | obs | model | obs | model | obs | model | obs | model | obs | model | obs |  |  |
| Tetracosane | 1.72 E | 5.00E-01 | 1.25E+00 | 5.20E-01 | 1.67E+00 | $5.22 \mathrm{E}+00$ | $1.56 \mathrm{E}+00$ | $4.38 \mathrm{E}+00$ | $1.32 \mathrm{E}+00$ | $4.72 \mathrm{E}+00$ | $1.99 \mathrm{E}+00$ | $1.08 \mathrm{E}+00$ | $1.74 \mathrm{E}+00$ | $1.54 \mathrm{E}+00$ | $2.07 \mathrm{E}+00$ | $1.94 \mathrm{E}+00$ | $2.33 \mathrm{E}+00$ | 5.30E-01 | 1.83E+00 | , 7E+00 | 2.19E+00 | [ 4 +00 | E+00 | $1.72 \mathrm{E}+00$ | .78E-01 | 20\% |
| Pentac | $1.18 \mathrm{E}+00$ | OE- | 9.03E-01 | 8.50 | 19E | 24 E | 17 E | 2.67 E | $88 \mathrm{E}-$ | 06E | 150 E | 1.84 | $1.32 \mathrm{E}+00$ | $3.09 E+00$ | 1.5 | 2.6 | $1.74 \mathrm{E}+00$ | c | 1.37E+00 | 6.20 E | 00 | 8.00E-01 | $1.98 \mathrm{E}+00$ | 1.44 E | $1.02 \mathrm{E}+00$ | 16\% |
| Hexacosane | $6.77 \mathrm{E}-01$ | 7.00E-01 | 5.06E-01 | 5.1 | 6.67E-01 | 3.61 | 6.62E-01 | 2.67 E | 5.65E-01 | $3.52 \mathrm{E}+00$ | $8.48 \mathrm{E}-01$ | $2.30 \mathrm{E}+00$ | 7.64E-01 | $2.85 \mathrm{E}+00$ | 8.52E-01 | $4.24 \mathrm{E}+00$ | $1.02 \mathrm{E}+00$ |  | 7.91E-01 | $1.73 \mathrm{E}+00$ | 9.18E-01 | 8.50E-01 | 1.15E+00 | $1.51 \mathrm{E}+00$ | 1.30E+00 | 16\% |
| Heptacosane | $8.91 \mathrm{E}-01$ | $9.10 \mathrm{E}-01$ | 5.93E-01 | 1.10E+00 | 7.82E-01 | 5.11E+00 | 6.77E-01 | $4.10 \mathrm{E}+00$ | 5.64E-01 | 5.46E+00 | 8.36E-01 | $3.98 \mathrm{E}+00$ | 8.07E-01 | $4.36 \mathrm{E}+00$ | 9.85E-01 | $5.51 \mathrm{E}+00$ | 1.18E+00 |  | 9.39E-01 | 1.74E+00 | 1.18E+00 | 1.54E+00 | 1.39E+00 | $1.68 \mathrm{E}+0$ | 1.41E+00 | 16\% |
| Octaco | 4.03 | 4.10 E | 2.77E-01 |  | 3.65 | $2.26 \mathrm{E}+00$ | 3.17E | $1.69 \mathrm{E}+00$ | 2.67E-01 | $2.65 \mathrm{E}+00$ | 3.99 | 9.80 | 3.8 | $1.29 \mathrm{E}+00$ | 4.6 | $1.97 \mathrm{E}+00$ | 5.52E-01 |  | $4.41 \mathrm{E}-01$ | $7.80 \mathrm{E}-01$ | 5.3 | 5.20E-01 | 6.491 | 8.10E-01 | 7.8 | 13\% |
| Nonacos | $1.37 \mathrm{E}+00$ | $1.01 \mathrm{E}+00$ | 7.79E-01 | $1.83 \mathrm{E}+00$ | 1.02E+00 | $6.58 \mathrm{E}+00$ | 7.13E-01 | $5.77 \mathrm{E}+00$ | 5.45E-01 | $6.53 \mathrm{E}+00$ | 7.90E-01 | $4.17 \mathrm{E}+00$ | $9.21 \mathrm{E}-01$ | 5.35E+00 | 1.24E+00 | $6.92 \mathrm{E}+00$ | 1.48E+00 | 1.64E+00 | $1.23 \mathrm{E}+00$ | 3.27E+00 | 1.84E+00 | $3.14 \mathrm{E}+00$ | 1.93E+00 | $2.93 \mathrm{E}+00$ | 1.36E+00 | 27\% |
| Tria | $2.76 \mathrm{E}-01$ | c | 1.91 E |  | $2.55 \mathrm{E}-0$ | . $65 \mathrm{E}+$ | 2.34E-01 | 17E+00 | 2.08E-01 | $2.71 \mathrm{E}+\infty$ | 2.98E-01 | 7.30E-4 | E-01 | 1.1 | 4E-1 | $1.27 \mathrm{E}+00$ | 4.23E-01 |  | 3.26E-01 | OE | 01 | 6.40E-01 | -01 | 9.40E-01 | 8.11E-01 | 40\% |
| Hent | 4.68E-01 |  | $2.66 \mathrm{E}-01$ | 80E-01 | 3.51 | $2.19 \mathrm{E}+00$ | 2.50E-01 | 184E+00 | .96E-M | $1.97 \mathrm{E}+00$ | 2.79E-01 | $1.34 \mathrm{E}+00$ | 3.18E-01 | $1.74 \mathrm{E}+00$ | E-01 | $2.27 \mathrm{E}+0$ | 5.21E-01 | $1.06 \mathrm{E}+00$ | 4.26E-01 | $7.90 \mathrm{E}-1$ | BE-0 | OE- | 5E-2 | 7.80E-01 | 4.06E-01 | 40\% |
| Dotriacontan | 1.47E-01 |  | 9.98E-02 |  | 1.32 | $1.12 \mathrm{E}+00$ | 1.20 |  | 1.09E-01 | c | 1.53E-01 | 3.60E-01 | 1.38E-01 | $3.60 \mathrm{E}-01$ | 1.78E-01 | $4.60 \mathrm{E}-01$ | 2.34E-01 | 3.20E-01 | 1.79E-01 | 6.80E-01 | $2.05 \mathrm{E}-01$ | 4.50E-0 | $2.60 \mathrm{E}-01$ | 5.20E- | 3.40E-01 | 43\% |
| 22-29-30-trisnorhopane | $5.02 \mathrm{E}-02$ | 9.00 E | 4.71E-02 | 5.00E-02 | $6.17 \mathrm{E}-02$ |  | 7.30 | 7.00E-02 | 6.73E-02 |  | $9.97 \mathrm{E}-02$ | 8.00E-02 | 7.67E-02 | 1.20E-01 | 8.83E-02 | 8.00E-02 | 1.13E-01 | 1.60E-01 | 8.3 |  | $6.91 \mathrm{E}-02$ |  | 1.07E-01 |  | 1.37E-02 | 28\% |
| 17-a(H)-21b(H)-29-nortopane | 1.04E-01 | 2.80E-01 | 9.90E-02 | $2.20 \mathrm{E}-01$ | 1.29E-01 | OE-1 | 1.58E-01 | 1.40E-01 | 1.44E-01 | 1.20E-01 | 2.15E-01 | 3.20E-01 | 1.66E-01 | 5.30E-01 | 1.84E-01 | 3.10E-01 | 2.35E-01 | 5.30E-01 | 1.74E-01 | $2.50 \mathrm{E}-01$ | 1.49 E | $4.10 \mathrm{E}-01$ | 2.29E- | $3.70 \mathrm{E}-01$ | 1.37E-02 | 14\% |
| ${ }^{17}$ 17-a(H)-218(H)-hopane | 1.31E-01 | 1.80E-01 | 1.23E-01 | 1.20E-01 | 1.61E-01 | 1.70E-01 | -01 | $2.40 \mathrm{E}-01$ | E-01 | 1.10E-01 | 2.61E-01 | 2.10E-01 | 20-01 | $4.30 \mathrm{E}-01$ | 2.28E-01 | 2.50E-01 | . $933 \mathrm{E}-$ | 3.70E-01 | -01 | 2.10E-01 | 1.85E-01 | $2.00 \mathrm{E}-01$ | -01 | 2.00E-01 | 1.37E-02 | 14\% |
| hor |  |  |  | 1.15E-01 | 1.54E-01 |  | 1.81E-01 |  | EE-01 | c | $2.48 \mathrm{E}-01$ | $2.30 \mathrm{E}-01$ | 1.90E-01 | $3.10 \mathrm{E}-01$ | $2.21 \mathrm{E}-01$ | $2.60 \mathrm{E}-01$ | $2.84 \mathrm{E}-01$ | $5.60 \mathrm{E}-01$ | $2.10 \mathrm{E}-01$ | $2.40 \mathrm{E}-01$ |  |  |  |  | 1.37E-02 | 14\% |
| $22 \mathrm{R} \mathrm{\& S}-17 \mathrm{a}(\mathrm{H})-$ bishomohopane | 6.49E-02 |  | $6.04 \mathrm{E}-02$ |  | 7.96E-02 |  | 9.40E-02 |  | 8.73E-02 |  | $1.28 \mathrm{E}-01$ | EE- | $9.90 \mathrm{E}-02$ | 1.80 E | 1.13E-01 | 1.40 E | 1.46 E |  | 1.07E-01 |  | E-02 |  | 1.42E-01 |  | 1.3 |  |
| 20R+S-abb-cholestane | 6.64E-02 |  | 6.51E-02 |  | 8.32E-02 |  | 1.00E-01 |  | $8.97 \mathrm{E}-02$ |  | 1.37E-01 | OE- | 1.06 | 80E | 1.21E- | 60E | 1.49E- | .00E-2 | 1.13E-01 | 7.00E-02 | 8.72E-02 |  | $1.32 \mathrm{E}-01$ | 10 E | 1.37E | 32\% |
| 20R-aaa-cholestane | $5.34 \mathrm{E}-02$ |  | 5.37E-02 |  | 6.79 E |  | 8.39E-02 |  | 7.39E-02 |  | 1.14E-01 | 5.00E-02 | 8.95 | 00E | 9.77E-02 | .00E | 1.19E- | 1.10 E | 9.03E-02 | OOE-02 | 7.22E-02 |  | 1.06E-01 | OE- | 1.3 | 28\% |
| 20R+S-ab-ergostane | $6.81 \mathrm{E}-02$ | c | 6.62E-02 | c | 0E-02 | c | 1.01E-01 | c | 9.13E-02 | c | $1.38 \mathrm{E}-01$ | 9.00E-02 | 1.07E-01 | 1.00E- | 1.23E--1 | OE-20 | 1.52E-01 | 8.00E | 1.15 E | c | 8.96E |  | 1.36E-01 | c | 1.37 E | 18\% |
| 20R+S | 7.32E-02 | c | 7.30E-02 |  | 9.27E-02 | c | 1.14E-01 | c | 1.01E-01 | c | 1.55E-01 | 1.40E-01 | 1.21E-01 | 2.10E-01 | 1.34E-01 | E-01 | E-01 | $2.10 \mathrm{E}-01$ | 1.24E-01 | E-02 | 9.78E-02 |  | 1.45E-01 | 1.20E-01 | 1.37E-02 | 28\% |
| Fluoranthene | $7.34 \mathrm{E}+0$ | ce-0 | 4.61E+00 | $2.20 \mathrm{E}-01$ | 6.35E+00 | 90E-0 | $5.10 \mathrm{E}+00$ | 1.80E-01 | 4.19E+00 | 2.00E-01 | 6.11E+00 | 2.10E-01 | 5.69E+00 | 1.60E-01 | $7.32 \mathrm{E}+00$ | 1.80E-01 | 7.78E+00 | 1.80E-01 | 6.22E+00 | 3.10E-01 | 8.93E+00 | 4.20E-01 | 1.04E+01 | 3.00E-01 | 2.73E-02 | 26\% |
| Acephenantrylene | 2.14 E | 1.40E-0 | 1.07E-1 | 1.50E-01 | 1.37E |  | .38E-01 |  | 5.90 E | c | 8.13E-12 | 1.00E- | 1.23E-0 | 8.00E-02 | 1.73E-10 | 1.00E-01 | 2.34E-01 | c | 1.94E-01 | c | 3.08E-01 | 1.00E-02 | 3.04E-01 | c | 2.73E-9 | 26\% |
| Benzo(ghi)fluoranthene | $4.08 \mathrm{E}+$ | 6.30E-01 | 2.59E+00 | $4.40 \mathrm{E}-01$ | 3.58E+00 | 5.60E-01 | $2.90 \mathrm{E}+00$ | $4.20 \mathrm{E}-01$ | 2.40E+00 | c | 3.50E+00 | 2.50E-u | 3.21E+00 | 2.70E-0 | 4.11E+00 | 2.90E-12 | 4.34E+00 | 9.10E-01 | 3.46E+00 | $1.13 \mathrm{E}+00$ | 4.93E+00 | $1.50 \mathrm{E}+00$ | 5.78E+00 | $1.10 \mathrm{E}+0$ | 3.00E-02 | 25\% |
| Cyclopenta(cd)pyrene | 2.31E-01 | c | 1.3 | c | 1.72 | c | 1.48E-01 | c | 1.08E-01 | c | 1.66E-01 | 1.30E-01 | 1.93E-01 | c | 2.21 | c | 2.82 E | 5.30E-1 | 2.31 E | 3.10E | 3.43E-01 | $2.30 \mathrm{E}-01$ | 3.49E-01 | 3.4 | 2.73E-02 | 16\% |
| Benz(a)antrracen | 5.13E+00 | 3.00E-02 | 3.24E+00 |  | $4.47 \mathrm{E}+00$ | 1.10E-01 | 3.59E+00 | 9.00E-02 | $2.96 \mathrm{E}+00$ | 1.20E-01 | $4.32 \mathrm{E}+00$ | 8.00E-02 | 3.98E+00 | c | 5.14E+00 | 5.00E-02 | $5.41 \mathrm{E}+00$ | $2.10 \mathrm{E}-01$ | 4.32E+00 | 1.40E-01 | 6.19E+00 | 1.60E-01 | 7.23E+00 | 1.70E-01 | 2.73E-02 | 10\% |
| Chrysene/Triphenylene | $1.94 \mathrm{E}+01$ | 1.70E-01 | 1.2 | EE-01 | 1.70E+01 | 10E-01 | 1.37E+01 | 10E-01 | 1.13E+01 | 00E-01 | 1.65E+01 | 20E-01 | $1.51 \mathrm{E}+01$ | 1.60E-0 | 1.95E+01 | $2.20 \mathrm{E}-01$ | $2.04 \mathrm{E}+0$ | 3.00E-01 | $1.63 \mathrm{E}+0$ | $2.70 \mathrm{E}-01$ | 2.33E | $3.30 \mathrm{E}-0$ | 2.73E+01 | $10 \mathrm{E}-0$ | $2.73 \mathrm{E}-02$ | 25\% |
| Retene | 2.88 | 3.00E-01 | 1.28E+0 | 2.80E-01 | 1.61E+00 | c | $6.81 \mathrm{E}-01$ |  | 3.38E-01 | c | 4.24E-01 | 3.00E-01 | $1.25 \mathrm{E}+00$ | 2.70E-01 | 1.97E | $2.70 \mathrm{E}-01$ | $2.67 \mathrm{E}+00$ | 2.90E-01 | 2.32E+00 | 2.90E-01 | $4.10 \mathrm{E}+00$ | 3.00E-0 | 3.69E+00 | $2.90 \mathrm{E}-\mathrm{t}$ |  | 29\% |
| Benzo(k)fluoranthene | 4.82 E | 1.60E-0 | 3.14E+00 | 1.50E-01 | $4.41 \mathrm{E}+00$ |  | 3.60E+00 | 1.00E-01 | 3.05E+00 | 1.20E-01 | $4.45 \mathrm{E}+00$ | 1.70E-01 | 4.36E+00 | 1.30E-01 | 4.99E+00 | 1.60E-01 | $5.43 \mathrm{E}+00$ | 1.00E-01 | 4.34E+00 | 9.00E-02 | 5.78E+00 |  | $6.90 \mathrm{E}+00$ |  | 2.73E-02 | 38\% |
| Benzo(b)fluoranthene | 4.09 | 4.00E-01 | 2.72 E | $2.60 \mathrm{E}-01$ | 3.85E+00 | 4.70E-01 | $3.17 \mathrm{E}+00$ | 3.70E-01 | 2.72E+00 | 1.80E-01 | $3.98 \mathrm{E}+00$ | $2.70 \mathrm{E}-01$ | 4.05E+00 | 1.80E-01 | 4.34E+00 | 1.60E-01 | 4.83E+00 | 1.80E-01 | 3.86E+00 | $2.30 \mathrm{E}-01$ | 4.89E+00 | 4.10E-01 | 5.93E+00 | 4.30E-01 | 2.73E-02 | 38\% |
| Benzo(j)fluoranthene | 4.01E-02 |  | 2.29E-02 |  | 2.85E-02 | c | 2.20E-02 |  | 1.58E-02 | c | 2.39E-02 | c | 2.97E-02 | c | 3.67E-02 | c | 4.71E-02 | c | 3.91E-02 |  | 5.82E-02 |  | 5.80E-02 |  | 2.73E-02 | 38\% |
| Benzo()Pyrene | $2.04 \mathrm{E}+00$ | $2.10 \mathrm{E}-01$ | 1.37E+00 | 1.60E-01 | 1.97E+00 | c | 1.61E+00 | $2.20 \mathrm{E}-01$ | 1.40E+00 | OE-1 | 2.05E+00 | $2.40 \mathrm{E}-01$ | 2.18E+00 | OE- | 2.18E+00 | 00E | $2.49 \mathrm{E}+00$ | 40E | $2.00 \mathrm{E}+00$ | OOE | 2.42E+00 | 6.40E-01 | 2.97E+00 | 40 E | 2.73 | 25\% |
| Benzo(a)pyren | 1.02 | 1.20E-0 | 5.65E-6 | 1.30E-0 | 7.09E-12 | c | 5.11 E | $1.40 \mathrm{E}-01$ | 3.68E-20 | c | 5.47E | 1.90E-0 | 7.01 E | 1.20E-01 | 9.13 E | $1.30 \mathrm{E}-0$ | 1.188 | $2.30 \mathrm{E}-0$ | 9.84E-0 | 1.60E-01 | 1.46E-01 |  | 1.46 | 5.20 E | $2.73 \mathrm{E}-02$ | 25\% |
| Perylene | 3.80 E | 1.70E-01 | 3.46E-20 | 1.60E-01 | 4.20E-02 | 1.70E-01 | 5.45E-02 | $1.20 \mathrm{E}-01$ | 4.35E-02 | 1.40E-01 | 6.99E-02 | $2.40 \mathrm{E}-01$ | $6.23 \mathrm{E}-02$ | $2.20 \mathrm{E}-01$ | 5.61E | $1.90 \mathrm{E}-01$ | 6.70E-02 | 2.30E-01 | 5.14E- | $3.70 \mathrm{E}-01$ | 6.22 E | 4.20E-01 | 7.41 | $2.70 \mathrm{E}-1$ | $2.73 \mathrm{E}-02$ | 25\% |
| Indeno(cl) pyrene | 1.06 | c | 7.70 | E-01 | 1.14 E | c | 9.49E-01 | $7.50 \mathrm{E}+00$ | 8.73E-01 | 9.00E-02 | 1.28E+00 | 3.40E-01 | $1.54 \mathrm{E}+00$ | $2.60 \mathrm{E}-01$ | 1.23E+00 | $2.70 \mathrm{E}-01$ | 1.53E+00 | 1.60E-01 | $1.23 \mathrm{E}+00$ | 1.20E-01 | 1.25 E | 2.30E-01 | 1.61E+00 | $2.20 \mathrm{E}-\mathrm{t}$ | 2.73E-02 | 29\% |
| Benzo(ghi)perylene | $9.44 \mathrm{E}-01$ |  | 7.45E-01 | 3.20E-01 | 1.06E+00 | .40E-01 | 1.01E+00 | 40E-01 | 8.98E-01 | 30E-0 | $1.35 \mathrm{E}+00$ | 20E-2 | 1.48 | 3.50E-0 | 1.20 | 3.30E-01 | 1.47E+00 | 4.50E-01 | 1.17E+00 | 3.30E-01 | 1.18E+00 | 3.70E-01 | 1.54E+00 | 3.50E-01 | 2.73E-02 | 12\% |
| Coronene | 5.14E-01 | ce-ot | 3.67E-01 | 1.00E-01 | 5.36 | c | 4.49E-01 | c | 07E | c | 98E | 2.00E-01 | 7.14E-01 | 1.50E-0 | 5.88E | 1.60E-0 | 7.32E | $2.60 \mathrm{E}-01$ | 5.91E-0 | 1.00E-01 | 6.18E-0 | $2.70 \mathrm{E}-0$ | 7.80E-01 | 1.80E-0 | 3.41 | 26\% |
| Tetradecanoic acid | 2.45 E | $1.63 \mathrm{E}+0$ | 1.87E+00 | $1.43 \mathrm{E}+00$ | $2.33 \mathrm{E}+00$ | $3.10 \mathrm{E}+01$ | $2.09 \mathrm{E}+00$ | $2.88 \mathrm{E}+00$ | 1.70E+00 | $2.53 \mathrm{E}+00$ | 2.71E+00 | c | 2.45E+ | c | 3.10 | c | 3.51E+ | c | $2.90 \mathrm{E}+00$ | c | $3.32 \mathrm{E}+00$ | 7.40E-01 | 4.10 E | c | 2.17 | 47\% |
| Pentadecanoic acid | 7.01E-01 | 6.80E-01 | 5.29E-01 | $6.30 \mathrm{E}-01$ | 6.60E-01 | $1.73 \mathrm{E}+01$ | 5.87E-01 | c | 4.77E-01 | 6.90E-01 | 7.58E-01 | c | 6.92 E | c | 8.81E-01 | c | 1.01E+00 | c | 8.30E-01 | c | $9.57 \mathrm{E}-01$ | c | 1.17E+00 | c | $1.33 \mathrm{E}+0$ | 50\% |
| Hexadecanoic acid | 1.37E+01 | $5.20 \mathrm{E}+00$ | 1.08E+01 | $4.45 \mathrm{E}+00$ | 1.34E+01 | $9.64 \mathrm{E}+01$ | 1.22E+01 | 48E+01 | 9.93E+00 | 9.16E+00 | 1.60E+01 | c | 1.42E+01 | c | +01 | c | 2.02 E | c | 1.67E+01 | c | E+01 | 1E+ | 2.34E+01 | OE- | 8.66E+00 | 53\% |
| Heptadecanoic acid | 8.49E-01 | 3.8 | 7.36 | 3.20E-01 | 9.02E | $2.42 \mathrm{E}+0$ | 8.7 | c | 7.24 | c | 1.18E | c | 1.00 | c | 1.24 |  | 1.38 | c | 1.14E+00 | c | 1.18E+00 |  | 1.58E+00 | c | 3.03E-01 | 76\% |
| Octadecanoic aci | 6.02 | 4.56E+0 | 5.14E+ | $3.35 \mathrm{E}+00$ | 6.32E+00 | $3.19 \mathrm{E}+01$ | 6.10E+00 | 6.13E+00 | $5.06 \mathrm{E}+00$ | 3.77E+0 | $8.18 \mathrm{E}+00$ | 1.50E-01 | 6.98E+00 | 8.10E-01 | 8.68E+00 | $4.40 \mathrm{E}-01$ | 9.80E+ | c | 8.03E | c | 8.39E+ | $2.61 \mathrm{E}+00$ | 1.12E+ | 1.90E-u1 | 4.56E+00 | 99\% |
| Eicosanoic acid | 7.00E-01 | $5.30 \mathrm{E}-01$ | 3.51 | 4.30E-01 | 4.42E-01 | $4.12 \mathrm{E}+00$ | $2.47 \mathrm{E}-01$ | 8.80E-0 | 1.65E-01 | 1.79E+00 | $2.30 \mathrm{E}-01$ |  | 3.79 |  | 5.5 | c | 7.38 E |  | 6.26 E |  | $9.97 \mathrm{E}-01$ | $4.00 \mathrm{E}-01$ | 9.68E-01 | $1.80 \mathrm{E}-01$ | 8.22E-01 | 48\% |
| Heneicosanoic acid | $1.65 \mathrm{E}-01$ | 1.40E-01 | 7.42E-02 | 3.00E-02 | 9.33E-02 | c | 4.04E-02 | c | 2.10E-02 | c | 2.64E-02 | 4.00E-02 | 7.34E-02 | 1.10E-01 | 1.14E-01 | c | 1.54E-01 | 4.70E-01 | 1.34E-01 | 4.70E-01 | 2.35E-01 | 5.00E-02 | 2.12E--10 | $2.00 \mathrm{E}-12$ | 8.22E-01 | 36\% |
| Docosanoic acid | $1.01 \mathrm{E}+00$ | 5.60E-01 | 4.58E-01 | $6.30 \mathrm{E}-01$ | 5.75E-01 | $1.44 \mathrm{E}+00$ | 2.57E-01 | $6.60 \mathrm{E}-01$ | 1.37E-01 | $1.51 \mathrm{E}+00$ | 1.78E-01 | $1.27 \mathrm{E}+00$ | 4.57E-01 | 8.90E-01 | 7.07E-01 | 5.50E-01 | 9.48E-01 | 6.80E-01 | 8.24E-01 | 8.00E-01 | 1.43E+00 | 9.90E-01 | 1.30 E+00 | 8.20E-0 | 2.23E-01 | 25\% |
| Tricosanoic acid | $4.05 \mathrm{E}-$ | 2.40E-01 | 1.81E-0 | $2.60 \mathrm{E}-01$ | 2.27E-01 | c | 9.71E-0 | c | 4.93E-02 | 2.00E-02 | 6.18E-12 | $2.90 \mathrm{E}-0$ | 1.78E | 3.10E-0 | 2.78E-910 | 1.80E-01 | 3.76E-01 | 2.90E-01 | 3.27E-01 | 2.70E-01 | 5.77E-0 | 3.10E-01 | 5.20E | $2.60 \mathrm{E}-10$ | 1.50E-01 | 24\% |
| Tetracosanoic acid | $2.23 \mathrm{E}+0$ | 8.40E-01 | 9.93E-01 | $9.00 \mathrm{E}-01$ | 1.25E+00 | $4.75 \mathrm{E}+00$ | 5.31E-01 | $1.64 \mathrm{E}+00$ | $2.68 \mathrm{E}-01$ | 1.77E+00 | 3.36E-01 | $1.14 \mathrm{E}+00$ | 9.74E-0 | $9.60 \mathrm{E}-01$ | 1.53E+00 | $4.40 \mathrm{E}-01$ | 2.07E+00 | 3.50E-01 | 1.80E+00 | 6.60E-01 | $3.17 \mathrm{E}+00$ | $1.10 \mathrm{E}+00$ | $2.86 \mathrm{E}+00$ | 7.80E-0 | 6.29E-01 | 23\% |
| Pentacosanoic acid | 2.11 E | 3.50E-0 | 9.46E-02 | 3.60E-01 | 1.19E-01 | 2.60E-01 | 5.10E-02 |  | 2.61E-02 | 2.00E-02 | 3.27E-02 | 1.30E-0 | 9.31E-02 | 1.80E-01 | 1.46E-01 | 7.00E-02 | 1.97E-01 | 4.00E-02 | 1.71E-01 | 1.70E-01 | 3.01E-01 | 1.30E-0 | 2.72E-01 | 8.00E-012 | 3.72E-01 | 35\% |
| Hexacosanoic acid | 1.44E+00 | 50E-01 | 6.53E-01 | 6.70E-01 | 8.26E-01 | $1.72 \mathrm{E}+00$ | 3.70E-01 | 9.40E-01 | 2.00E-01 | 9.20E-01 | 2.57E-01 | 8.20E-01 | $6.50 \mathrm{E}-01$ | 8.30E-01 | $1.01 \mathrm{E}+00$ | $6.50 \mathrm{E}-01$ | $1.35 \mathrm{E}+00$ | 2.90E-01 | 1.17E+00 | 3.10E-01 | 2.04E+00 | 5.60E-01 | 1.86E+00 | 3.70E | 4.60E- | 35\% |
| Heptacosanoic acid | $1.13 \mathrm{E}-0$ | 3.20E-01 | 5.10E-02 |  | 6.41E-02 |  | 2.77E-02 |  | 1.45E-02 | c | 1.81E-02 | 1.10E-01 | 5.04E-02 | 1.40E-01 | 7.84E-02 | 1.40E-01 | 1.06E-01 | 9.20E-01 | 9.18E-02 | 8.50E-01 | 1.61E-01 | $1.10 \mathrm{E}+00$ | 1.46E-01 |  | 3.05E-02 | 35\% |
| Octacosanoic acid | 7.78E-01 | 5.60E-01 | 3.57E-01 | 8.50E-01 | 4.52E-01 | 3.10E-01 | 2.08E-01 | 5.70E-01 | $1.17 \mathrm{E}-01$ | 5.80E-01 | 1.51E-01 | 5.50E-01 | 3.59E-01 | 8.10E-01 | 5.50E-01 | 9.80E-01 | 7.30E-01 | 4.20E-01 | 6.32E-01 | 2.80E-01 | 1.10E+00 | $1.68 \mathrm{E}+00$ | 1.00E+00 | 1.55E+ | 2.34E-01 | 47\% |
| Nonacosanoic acid | 1.0 |  | 4.80E-02 |  | $6.03 \mathrm{E}-02$ |  | $2.67 \mathrm{E}-02$ | c | 1.46E-02 | c | 3E-12 |  | 4.80E-02 |  | 7.36E-02 |  | $9.88 \mathrm{E}-02$ | 9.40E-01 | 8.56E-02 |  | 1.50E-01 | c | $1.35 \mathrm{E}-$ |  | $2.34 \mathrm{E}-01$ | 32\% |
| Triacontanoic acid | $8.67 \mathrm{E}-01$ | 4.10E-01 | 3.92E-01 | 4.90E-01 | 4.94E-01 | c | $2.17 \mathrm{E}-01$ | c | 1.15E-01 | c | 1.46E-01 | 1.30E-01 | 3.88E-01 | 8.00E-01 | 6.03E-01 | $1.23 \mathrm{E}+00$ | 8.09E-01 | $1.41 \mathrm{E}+00$ | 7.02E-01 | 1.23E+00 | $1.23 \mathrm{E}+00$ | c | 1.12E+0 | $1.89 \mathrm{E}+0$ | 2.34 E | 17\% |
| Butanedioic acid | $4.95 \mathrm{E}-01$ | $3.41 \mathrm{E}+00$ | 3.64E-01 | $2.09 \mathrm{E}+00$ | 4.39E-01 | $2.42 \mathrm{E}+00$ | 3.75E-01 | $7.88 \mathrm{E}+00$ | 2.88E-01 | 7.03E+00 | 4.76E-01 | $2.52 \mathrm{E}+0$ | 4.64E-01 | $6.75 \mathrm{E}+00$ | 5.98E-01 | $3.98 \mathrm{E}+00$ | $6.90 \mathrm{E}-01$ | 3.80E-0 | 5.84E-01 | 4.70E-01 | 7.08E-01 | 5.90E-01 | 8.28E-0 | 5.67E+0 | 1.28E+ | 42\% |
| Pentanedioic acid | E-01 | E+00 | 1.70E-01 | $1.25 \mathrm{E}+00$ | 2.03E-01 | 5.40E-01 | 1.92E-01 | $2.72 \mathrm{E}+00$ | 53E-01 | $2.48 \mathrm{E}+00$ | $2.57 \mathrm{E}-01$ | c | 2.27E-01 | $2.20 \mathrm{E}+00$ | 2.82E-01 | $4.10 \mathrm{E}-01$ | 3.14E-01 | c | $2.64 \mathrm{E}-01$ | c | 23E-0 | c | 3.63E-01 | 40 E | 1.52E | 42\% |
| Hexanedioic acid | $1.77 \mathrm{E}-01$ | 4.40E-01 | 1.78E-01 | 3.20E-01 | 2.11E-01 | 1.40E-01 | 2.19E-01 | $3.50 \mathrm{E}-01$ | 1.79E-01 | $2.30 \mathrm{E}-01$ | 3.04E-01 | c | 2.48E-01 | 5.50E-01 | 2.99E-01 | c | 3.23E-01 | c | $2.70 \mathrm{E}-01$ | c | $2.53 \mathrm{E}-01$ | c | $3.60 \mathrm{E}-01$ | 1.30E-01 | $1.31 \mathrm{E}+00$ | 42\% |
| Heptanedioic acid | $1.26 \mathrm{E}-02$ |  | 5.60 | c | 7.04E-03 |  | $2.98 \mathrm{E}-03$ |  | 1.48E-03 |  | 1.85E-03 | c | 5.47E-03 | $1.03 \mathrm{E}+00$ | 8.62E-03 | c | 1.17E-02 |  | 1.02E-02 | c | 1.79E-02 | c | 1.62E-02 | 1.00E-02 | 1.32E+00 | 42\% |
| Octanedioic acid | 6.03E-01 | c | 4.75E-01 | c | $6.26 \mathrm{E}-01$ | 1.80E-01 | 6.15E-01 | $3.00 \mathrm{E}-01$ | 5.73E-01 | 6.40E-01 | 8.31E-0 | c | 6.71E-01 | 1.20E-01 | 8.75E-0 | c | 1.14E+0 | 4.00E-02 | 8.64E-0 | c | $8.58 \mathrm{E}-1$ | c | 1.26E+0 | $2.00 \mathrm{E}-2$ | 1.32E+ | 42\% |
| Nonanedioic acid | 6.59E-0 | E- | 35E-01 | $5.90 \mathrm{E}-0$ | $6.00 \mathrm{E}-01$ | $1.01 \mathrm{E}+0$ | 41E-01 | $1.21 \mathrm{E}+0$ | 4E-1 | 8.60E-01 | . $04 \mathrm{E}-0$ | 6.00E-02 | 5.98E-0 | $2.09 E+$ | 8.22E-0 | 8.00E-01 | $1.16 \mathrm{E}+$ | 3.50E-0 | 8.58E-01 | 3.00E-01 | 9.36E-01 | 3.30E-01 | 1.30E+ | 9.10 E | 1.18E | 42\% |


| trace | March04 |  | April04 |  | May04 |  | June04 |  | July04 |  | August04 |  | September04 |  | October04 |  | November04 |  | December04 |  | Janucry05 |  | February05 |  | MDL ${ }^{\text {a }}$ | $\mathrm{UNC}^{\text {b }}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1-2-benzened | 5.30E-03 | $1.50 \mathrm{E}+00$ | $2.33 \mathrm{E}-03$ | $1.00 \mathrm{E}+00$ | 2.96E-03 | $1.01 \mathrm{E}+00$ | 1.25E-03 | $2.92 \mathrm{E}+00$ | 6.21E-04 | $3.17 \mathrm{E}+00$ | 7.79E-04 | $1.00 \mathrm{E}+00$ | $2.30 \mathrm{E}-03$ | $7.32 \mathrm{E}+00$ | 3.62E-03 | $2.24 \mathrm{E}+00$ | 4.90E-03 |  | 4.27E-03 |  | 7.54E-03 | 1.00E-02 | 6.79E-03 | 0 | 0 | 38\% |
| 1-3-benzenedicarboxylic acid | $3.98 \mathrm{E}-04$ | $2.90 \mathrm{E}-01$ | 2.87E-04 | 1.80E-01 | 4.21E-04 |  | 2.73E-04 |  | 1.92E-04 | 3.70E-0 | 2.65E-04 |  | 4.88E-04 |  | 4.15 E |  | $9.66 \mathrm{E}-04$ |  | 5.03 E | c | 7.30 E |  | 7.05 E | 6.20E- | 34 | 38\% |
| 1-4-benzenedicarboxylic acid | 3.52E-03 | 4.30 E | 1.6 | 3.60E-01 | 2.11 | 6.80E-01 | $9.57 \mathrm{E}-04$ | $1.23 \mathrm{E}+00$ | 5.15E-04 | $9.30 \mathrm{E}-01$ | $6.63 \mathrm{E}-04$ | 4.00E-02 | 1.75 | $1.40 \mathrm{E}+00$ | $2.51 \mathrm{E}-03$ | 6.80E-01 | 3.68E-03 | 1.20E-01 | 2.97E-03 | 1.00E-01 | 5.13E-03 | 1.20E-01 | 4.65E-03 | $7.30 \mathrm{E}-01$ | 1.27E+00 | 38\% |
| Nonadecanoic acid | E-0 | 7.00E-02 | 1.09E-01 | 1.00E-01 | 1.36E-01 | c | 02 | c | 6.50E-02 | c | . 02 | 1.00E-02 | 1.26E-01 | 5.00E-02 | 01 |  | $2.25 \mathrm{E}-01$ | c | -01 | c | -01 | c | 2.83E-01 | c | 1.45E-01 | 73\% |
| 1-8-naphthalic anhydride | 1.18E-02 |  | 5.23E-03 | $1.20 \mathrm{E}+00$ | 6.58E-03 | c | 2.78E-03 | c | $1.38 \mathrm{E}-03$ | c | 1.73E-03 | 9.80E-01 | 5.12E-03 | 8.70E-01 | 8.06E-03 | 7.90E-01 | 1.09E-02 | ${ }^{\text {c }}$ | $9.50 \mathrm{E}-03$ |  | 1.68E-02 |  | 1.51E-02 |  | 2.78E+00 | 16\% |
| 1 H -phenalen-1-one | $32 \mathrm{E}+00$ | e-o | 3.98E+00 | 5.70E-01 | 51E+00 | 7.20E-01 | .11E+00 | c | 54E+00 | c | -00 |  | 00 |  | $6.31 \mathrm{E}+00$ | 80E-01 | 6.65E+00 | 6.20E-0 | 5.30E+ | 20 E | $7.63 \mathrm{E}+0$ |  | 8.89E+0 |  | 00 | 16\% |
| Anthracen-9-10-dione | $1.99 \mathrm{E}+01$ | 7.00E-01 | $1.26 \mathrm{E}+01$ | 7.40E-01 | 1.75E+01 | c | 1.42E+01 | 6.70E-01 | 1.17E+01 | $7.70 \mathrm{E}-01$ | $1.71 \mathrm{E}+01$ | 2.90E-01 | 1.56E+01 | $2.60 \mathrm{E}-01$ | $2.01 \mathrm{E}+01$ | 3.30E-01 | 2.111+01 | 6.10E-01 | $1.68 \mathrm{E}+0$ | 6.60E-01 | $2.39 \mathrm{E}+01$ | 3.00E-0 | $2.81 \mathrm{E}+01$ | 2.00E-01 | 7.41E-01 | 16\% |
| Benz()antriracene-7 12-dione | 1.23 |  | 7.83 E |  | 1.09E+00 |  | 8.75E-01 |  | $7.25 \mathrm{E}-01$ |  | 1.06E+00 | 4.80E-01 | 9.65E | 4.40E-1 | 1.24E+00 | $4.20 \mathrm{E}-1$ | 1.30E+00 |  | $1.04 \mathrm{E}+00$ |  | 1.48E+ |  | 1.74E+00 |  | 7.06E-01 | 16\% |
| Levoglucosan | +01 | 5.26E+ | 4.05E+01 | 5.84E | $5.10 \mathrm{E}+01$ | 23E+01 | $2.16 \mathrm{E}+01$ | 31E+01 | 207E+01 | 5.58E+01 | $1.34 \mathrm{E}+01$ | $1.48 \mathrm{E}+02$ | 3.96E+01 | $1.03 \mathrm{E}+02$ | 6.24E+01 | $6.76 \mathrm{E}+01$ | 8.45E+01 | $1.19 \mathrm{E}+02$ | $7.36 \mathrm{E}+01$ | E+02 | 1.30E+0 | $1.38 \mathrm{E}+02$ | 1.17E+02 | $1.25 \mathrm{E}+02$ | 0E+00 | 37\% |
| 3-Acetylpentanedioic acid | $8.08 \mathrm{E}-02$ | $1.00 \mathrm{E}+00$ | 2.24E-01 | $2.20 \mathrm{E}+00$ | 1.17E-01 | 0 | $2.37 \mathrm{E}-01$ | $4.50 \mathrm{E}+00$ | 5.55E-01 | 1.65E+01 | 4.24E-01 | $8.40 \mathrm{E}+00$ | 4.29E-01 | $6.60 \mathrm{E}+00$ | 1.46E-01 | 3.30E+00 | $1.73 \mathrm{E}-01$ | 1.40E+00 | 8.45E-02 | 3.00E-01 | 1.46E-01 | c | 1.42E-01 | c | 1.00E-01 |  |
| 2-Hydroxy-4-isopropyladipic acid | 1.4 | $5.80 \mathrm{E}+00$ | 4.09E-01 | $1.98 \mathrm{E}+01$ | 2.14E-01 | 97E+01 | $4.33 \mathrm{E}-01$ | $2.36 \mathrm{E}+01$ | 1.01E+00 | 5.78E+01 | $7.73 \mathrm{E}-01$ | $3.99 \mathrm{E}+01$ | 7.82E-01 | 3.78E+01 | 2.67E-01 | $1.69 \mathrm{E}+01$ | 3.15E-01 | $1.41 \mathrm{E}+01$ | 1.54E-1 | 5.50E+00 | 2.65E-01 | E-01 | 2.59E-01 | 1 | 1.00E |  |
| 3-Acetyl hexanedioic acid | $1.02 \mathrm{E}+00$ | $1.00 \mathrm{E}+00$ | $2.82 \mathrm{E}+00$ | $1.40 \mathrm{E}+00$ | 1.48E+00 | $1.30 \mathrm{E}+00$ | $2.99 \mathrm{E}+00$ | $1.80 \mathrm{E}+00$ | 6.98E+00 | $6.30 \mathrm{E}+00$ | 5.34E+00 | $5.30 \mathrm{E}+00$ | 5.40E+00 | $2.30 \mathrm{E}+00$ | 1.84E+00 | $1.60 \mathrm{E}+00$ | 2.18E+00 | $1.20 \mathrm{E}+00$ | $1.06 \mathrm{E}+00$ | 8.00E-01 | $1.83 \mathrm{E}+00$ | $1.10 \mathrm{E}+00$ | 179E+00 | 1.00E+00 | 1.00E-01 |  |
| 3-Hydroxyglutari acid | 1.14E-01 | $1.22 \mathrm{E}+01$ | $3.16 \mathrm{E}-01$ | $1.97 \mathrm{E}+01$ | $1.66 \mathrm{E}-01$ | $3.16 \mathrm{E}+01$ | 3.35E-01 | $3.36 \mathrm{E}+01$ | $7.82 \mathrm{E}-01$ | $6.81 \mathrm{E}+01$ | 5.98E-01 | $3.96 \mathrm{E}+01$ | $6.05 \mathrm{E}-01$ | $4.65 \mathrm{E}+01$ | $2.06 \mathrm{E}-01$ | $1.72 \mathrm{E}+0$. | $2.44 \mathrm{E}-01$ | $1.04 \mathrm{E}+0$ | $1.19 \mathrm{E}-01$ | 6.70E+00 | $2.05 \mathrm{E}-0$ | $4.10 \mathrm{E}+0$ | $2.01 \mathrm{E}-01$ | $3.70 \mathrm{E}+00$ | 1.00E-01 |  |
| acid | 8.39E-02 | 5.00E-01 | $2.33 \mathrm{E}-01$ | 1.40E+00 | -01 | +00 | $2.47 \mathrm{E}-01$ | 1.70E+00 | 5.77E-01 | 5.20E+0 | 4.41E-0 | $3.60 \mathrm{E}+0$ | 4.46 | $2.80 \mathrm{E}+0$ | 1.52E-01 | $1.60 \mathrm{E}+00$ | 1.30E-0 | .00E-0 | 8.78E-02 | $2.00 \mathrm{E}-01$ | 1.51E-01 |  | 1.48E-01 |  | 1.00E-01 |  |
| cyclobutane-carboxylic acid | 5.60E-01 | $3.30 \mathrm{E}+00$ | 1.55E+00 | $4.50 \mathrm{E}+00$ | 8.13E-01 | $3.70 \mathrm{E}+00$ | 1.64E+00 | $3.40 \mathrm{E}+00$ | 3.84E+00 | 1.04E+01 | $2.94 \mathrm{E}+00$ | $8.30 \mathrm{E}+00$ | $2.97 \mathrm{E}+00$ | 7.50E+00 | 1.01E+00 | $3.10 \mathrm{E}+00$ | $1.20 \mathrm{E}+00$ | $1.70 \mathrm{E}+00$ | 5.86E-01 | $9.00 \mathrm{E}-01$ | 1.01E+00 | 4.00E-01 | 9.86E-01 | 3.00E-01 | 1.00E-01 |  |
| Pinic acid | $4.11 \mathrm{E}-01$ | $1.40 \mathrm{E}+00$ | $1.14 \mathrm{E}+00$ | $1.80 \mathrm{E}+00$ | 5.98E-01 | 6.00E-01 | $1.21 \mathrm{E}+00$ | $1.00 \mathrm{E}+00$ | $2.83 \mathrm{E}+00$ | 2.10E+00 | 2.16E+00 | 1.00E+00 | 2.19E+00 | $1.60 \mathrm{E}+00$ | 7.45E-01 | $1.50 \mathrm{E}+00$ | 8.81E-01 | $1.50 \mathrm{E}+00$ | 4.31E-01 | $1.30 \mathrm{E}+00$ | 7.42E-01 | 1.10E+ | 7.25E-01 | c | 1.00E-01 |  |
| Pinonic ac | 1.98E-01 | 0E-01 | 5.50E-01 | $1.70 \mathrm{E}+00$ | 88E-01 | 2E+00 | 5.82E-01 | 70E+00 | 36E+00 | 50E+00 | 1.04E+00 | 90E+00 | 1.05E+00 | 2.00E+00 | 59E-01 | 30E+0 | 4.25E-01 | $1.00 \mathrm{E}+0$ | 2.07E-0 | OE- | 3.57E-0 | c | 3.49E- | c | OOE |  |
| acid | -01 | 1.10E+00 | 1.77E-01 | 1.50E+00 | E-01 | 10E+00 | 3.05E-01 | $1.70 \mathrm{E}+00$ | 3.34E-01 | $2.90 \mathrm{E}+00$ | 3.88E-01 | $3.10 \mathrm{E}+00$ | 6.06E-01 | $2.10 \mathrm{E}+00$ | 2.11E-01 | $1.30 \mathrm{E}+00$ | 1.67E-01 | $9.00 \mathrm{E}-01$ | 1.56E-01 | 5.00E-0 | 1.53E-01 | $6.00 \mathrm{E}-01$ | 2.99E-01 | 6.00E-01 | 1.00E-01 |  |
| 2-Methylglyceric acid | 8.01E-01 | 1.60E+ | 9.69E-01 | $4.30 \mathrm{E}+00$ | 9.92E-01 | $8.50 \mathrm{E}+00$ | 2.13E+00 | $1.78 \mathrm{E}+01$ | 2.88E+00 | $3.02 \mathrm{E}+01$ | 2.86E+00 | $2.67 \mathrm{E}+01$ | $2.65 \mathrm{E}+00$ | $2.74 \mathrm{E}+01$ | 9.36E-01 | $4.50 \mathrm{E}+00$ | 7.45E-01 | $2.00 \mathrm{E}+00$ | $9.54 \mathrm{E}-01$ | 0E-01 | 1.03E+00 | c | 1.17E+00 | 9.00E-01 | 1.00E-01 |  |
| 2-Methyltrreitol | $1.35 \mathrm{E}+00$ | c | $1.63 \mathrm{E}+00$ | $1.80 \mathrm{E}+00$ | 1.67E+00 | $3.20 \mathrm{E}+00$ | 3.59E+00 | $1.80 \mathrm{E}+01$ | $4.85 \mathrm{E}+00$ | $2.68 \mathrm{E}+01$ | $4.82 \mathrm{E}+00$ | $2.67 \mathrm{E}+01$ | 4.46E+00 | $1.80 \mathrm{E}+01$ | 1.58E+00 | $2.50 \mathrm{E}+00$ | 1.26E+00 | 2.00E-01 | $1.61 \mathrm{E}+00$ | c | $1.74 \mathrm{E}+0$ | c | $1.98 \mathrm{E}+00$ | c | 1.00E-01 |  |
| 2-Methylerythritol | 2.22E+00 |  | $2.69 \mathrm{E}+00$ | 5.50E+00 | $2.75 \mathrm{E}+00$ | 8.50E+00 | 5.90E+00 | $4.04 \mathrm{E}+01$ | 7.98E+00 | $6.63 \mathrm{E}+01$ | 7.93E+00 | $6.98 \mathrm{E}+01$ | $7.34 \mathrm{E}+00$ | 4.52E+01 | 2.60E+00 | 5.90E+00 | 2.07E+00 | 4.00E-01 | $2.65 \mathrm{E}+00$ |  | 2.86E+00 | c | 3.25E+0 |  | 1.00E-01 |  |
| b-Caryophyllinic acid | -02 | +00 | 2.77E-01 | 4.00 E | 3.58E-01 | 6.50 | $1.03 \mathrm{E}+00$ | 5.30 | 1.83E+00 | 6.10 | $1.20 \mathrm{E}+00$ | 1.0 | $1.71 \mathrm{E}+00$ | 1.21E+0 | $2.84 \mathrm{E}-01$ | $5.60 \mathrm{E}+00$ | $1.84 \mathrm{E}-01$ | $1.03 \mathrm{E}+01$ | 2.17E-02 | $4.90 \mathrm{E}+00$ | 2.28E-02 | 5.10E+00 | 1.04E-02 |  | 1.00E-01 |  |

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## Alternate Method for Model-Derived Isoprene Tracers

Laboratory experiments are often conducted at artificially high organic aerosol concentrations in order to provide sufficient mass for analysis. As a result, a highly volatile species may be present in the aerosol phase in a chamber while preferentially partitioned to the gas phase in the ambient. This partitioning behavior could bias the estimated ratio of individual tracers to total isoprene aerosol low compared to the ambient atmosphere.

A second approach for calculating model estimates of isoprene tracers, which attempts to account for differences in laboratory vs. ambient mass-based partitioning, is implemented. Tracers are assumed to be nonvolatile and form at the same rate as Odum 2-product surrogates in both the ambient and laboratory. The Odum 2-product representation of isoprene SOA, with saturation concentrations of 116 and $0.6 \mu \mathrm{~g} / \mathrm{m}^{3}$ for products 1 and 2 respectively (Carlton et al., 2010), is assumed to accurately represent all the laboratory generated aerosol mass. Since laboratory aerosol is expected to have significant contributions from both products, while the ambient will be dominated by product 2 , the second isoprene SOA semivolatile with a $\mathrm{C}^{*}$ of 0.6 $\mu \mathrm{g} / \mathrm{m}^{3}$ is assumed to be a more atmospherically relevant surrogate. The gas+aerosol amount of the second product and the ratio of each isoprene tracer to total product 2 (AISO2+SV_ISO2) is calculated for four laboratory experiments with measured tracer concentrations (Kleindienst et al., 2007). This method results in revised tracer fraction estimates (fTR1, fTR2, and fTR3 for 2methylglyceric acid, 2-methylthreitol, and 2-methylerythritol respectively) expressed relative to total product 2. CMAQ model output is processed with these fractions and total ISO2 (AISO2 +SV_ISO2). SV_ISO2 is converted from ppm to $\mu \mathrm{g} / \mathrm{m}^{3}$ using standard temperature and pressure.

Note that since total gas+aerosol model estimates are used along with the tracer fractions, errors in partitioning due to the influence of temperature should also be minimized. However, partitioning biases in the model could lead to differences in deposition thus affecting the total product 2 (AISO2+SV_ISO2), which are not accounted for.

A major difference between this method and the standard method is that this method does not depend on model predictions of isoprene oligomers since isoprene oligomers (unless already in the Odum 2-product fit) are not present in the chamber.

Table S6. Revised tracer fraction estimates calculated based on four laboratory experiments performed by Kleindienst et al. (2007).

| 箴 |  |  |  | 旊 | $\underset{\sim}{\underset{\sim}{\underset{\sim}{x}}}$ | $\underset{\sim}{\mathbb{N}}$ | $\stackrel{m}{E}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 99.94 | 1.11 | 1.56 | 1.72 | 21.2 | 0.052 | 0.074 | 0.081 |
| 45.47 | 0.38 | 1.06 | 2.26 | 14.0 | 0.027 | 0.076 | 0.162 |
| 77.36 | 1.13 | 1.85 | 2.24 | 18.4 | 0.061 | 0.101 | 0.122 |
| 15.58 | 0.19 | 0.22 | 0.50 | 8.1 | 0.023 | 0.028 | 0.061 |
|  |  |  |  | average: | 0.041 | 0.070 | 0.106 |

Figure S2(a) shows the resulting modeled to observed concentration ratios for the revised method (compare to Figure 4(a) in main manuscript). Ratios are even lower than in the standard method implying that accounting for the influence of partitioning cannot account for model discrepancies. The seasonality of the bias is somewhat dampened as a result of degraded wintertime performance in the new method.

Figure S2(b) replaces the standard temperature (298K) with 250 K in the conversion of gas-phase SV_ISO2 from ppm to $\mu \mathrm{g} / \mathrm{m}^{3}$. While it slightly improves model performance, it does not increase model predictions by the factor of 2 needed to explain the summertime underestimate.

Figure S2(c) assumes that all of the aerosol from the second Odum product (AISO2) consists entirely of methylglyceric acid (25\%), methylthreitol (25\%), and methylerythritol (50\%) (an upper limit). The tracers are still underestimated, but the measurement/model gap in summer is improved. Chamber experiments indicate the sum of these three species makes up only $23 \%$ of total AISO2.


Figure S2. Model to observation ratios of isoprene secondary organic aerosol tracers using (a) the revised method, (b) the revised method and $\mathrm{T}=250 \mathrm{~K}$, and (c) a third method assuming all AISO2J mass corresponds to the sum of the three tracers. Compare to Figure 4(a) of the main manuscript.


Figure S3. Tetracosane ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S4. Pentacosane ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S5. Hexacosane ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S6. Heptacosane ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S7. Octacosane ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S8. Nonacosane ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S9. Triacontane ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S10. Hentriacontane ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S11. Dotriacontane ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S12. 22-29-30-trisnorhopane ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S13. 17-a(H)-21b(H)-29-norhopane ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S14. 17-a(H)-21B(H)-hopane ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S15. 22R\&S-17a(H)-21b(H)-30-homohopane ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S16. $22 R \& S-17 a(H)-21 b(H)-30-31-$ bishomohopane ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S17. 20R+S-abb-cholestane ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S18. 20R-aaa-cholestane ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S19. 20R+S-abb-ergostane ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S20. 20R+S-abb-sitostane ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S21. Fluoranthene ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S22. Acephenanthrylene ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S23. Benzo(ghi)fluoranthene ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S24. Cyclopenta(cd)pyrene ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S25. Benz(a)anthracene ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S26. Chrysene/Triphenylene ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S27. Retene ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S28. Benzo(k)fluoranthene ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S29. Benzo(b)fluoranthene ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S30. Benzo(j)fluoranthene ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S31. Benzo(e)pyrene ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S32. Benzo(a)pyrene ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S33. Perylene ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S34. Indeno(cd)pyrene ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S35. Benzo(ghi)perylene ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S36. Coronene ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S37. Tetradecanoic acid ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S38. Pentadecanoic acid ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S39. Hexadecanoic acid ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S40. Heptadecanoic acid ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S41. Octadecanoic acid ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S42. Eicosanoic acid ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S43. Heneicosanoic acid ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S44. Docosanoic acid ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S45. Tricosanoic acid ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S46. Tetracosanoic acid ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S47. Pentacosanoic acid ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S48. Hexacosanoic acid ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S49. Heptacosanoic acid ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S50. Octacosanoic acid ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S51. Nonacosanoic acid ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S52. Triacontanoic acid ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S53. Butanedioic acid ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S54. Pentanedioic acid ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S55. Hexanedioic acid ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S56. Heptanedioic acid ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S57. Octanedioic acid ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S58. Nonanedioic acid ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S59. 1-2-benzenedicarboxylic acid ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S60. 1-3-benzenedicarboxylic acid ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S61. 1-4-benzenedicarboxylic acid ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S62. Nonadecanoic acid ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S63. 1-8-naphthalic anhydride ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S64. 1H-phenalen-1-one ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S65. Anthracen-9-10-dione ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S66. Benz(a)anthracene-7 12-dione ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S67. Levoglucosan ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S68. 3-Acetylpentanedioic acid ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S69. 2-Hydroxy-4-isopropyladipic acid ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S70. 3-Acetyl hexanedioic acid ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S71. 3-Hydroxyglutaric acid ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


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Figure S72. 2-Hydroxy-4-4-dimethylglutaric acid ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S73. 3-(2-Hydroxy-ethyl)-2-2-dimethyl-cyclobutane-carboxylic acid ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S74. Pinic acid ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S75. Pinonic acid ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S76. 2-3-Dihydroxy-4-oxopentanoic acid ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S77. 2-Methylglyceric acid ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S78. 2-Methylthreitol ratio of model to observations. "Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S79. 2-Methylerythritol ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


Figure S80. b-Caryophyllinic acid ratio of model to observations.
"Mean" denotes geometric mean for all points in which the species was quantified in the ambient sample. Dashed lines bound all comparisons that agree within a factor of two. For open symbols, observations were below minimum detection limit (MDL) and MDL was used to calculate the ratio (these points are not included in the mean calcuation)


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Figure S81. CMAQ-CA attributed sources of 22-29-30-trisnorhopane (in picograms of carbon per meter^3).


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Figure S82. CMAQ-CA attributed sources of 17-a(H)-21b(H)-29-norhopane (in picograms of carbon per meter^3).


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Figure S83. CMAQ-CA attributed sources of 17-a(H)-21B(H)-hopane (in picograms of carbon per meter^3).


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Figure S84. CMAQ-CA attributed sources of $22 R \& S-17 a(H)-21 b(H)-30$-homohopane (in picograms of carbon per meter^3).


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Figure S85. CMAQ-CA attributed sources of 22R\&S-17a(H)-21b(H)-30-31-bishomohop (in picograms of carbon per meter^3).


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Figure S86. CMAQ-CA attributed sources of 20R+S-abb-cholestane (in picograms of carbon per meter^3).


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Figure S87. CMAQ-CA attributed sources of 20R-aaa-cholestane (in picograms of carbon per meter^3).


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Figure S88. CMAQ-CA attributed sources of 20R+S-abb-ergostane (in picograms of carbon per meter^3).


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Figure S89. CMAQ-CA attributed sources of 20R+S-abb-sitostane (in picograms of carbon per meter^3).


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Figure S90. CMAQ-CA attributed sources of Levoglucosan
(in picograms of carbon per meter^3).


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Figure S91. CMAQ-CA attributed sources of 1 H -phenalen-1-one (in picograms of carbon per meter^3).


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Figure S92. CMAQ-CA attributed sources of Anthracen-9-10-dione (in picograms of carbon per meter^3).


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Figure S93. CMAQ-CA attributed sources of Benz(a)anthracene-7 12-dione (in picograms of carbon per meter^3).


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Figure S94. CMAQ-CA attributed sources of Indeno(cd)pyrene (in picograms of carbon per meter^3).


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Figure S95. CMAQ-CA attributed sources of Coronene (in picograms of carbon per meter^3).
a) $\underset{\substack{\infty}}{\substack{0}}$ ○ 2-Methylglyceric acid

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## b) <br> 



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c)
$\begin{array}{llllllllllll}\text { Mar 04 } & \text { Apr } 04 & \text { May } 04 & \text { Jun } 04 & \text { Jul } 04 & \text { Aug } 04 & \text { Sep } 04 & \text { Oct } 04 & \text { Nov } 04 & \text { Dec } 04 & \text { Jan } 05 & \text { Feb } 05\end{array}$


Figure S96. Comparison of model predicted total isoprene SOC (left axis) and measurements of isoprene organic tracers (right axis) at the four sites.
a)

b)

c)

d)


Figure S97. Comparison of model predicted total monoterpene SOC (left axis) and measurements of isoprene organic tracers (right axis) at the four sites.

○ 2-3-Dihydroxy-4-oxopentanoic acid | 0.00 | 0.05 | 0.10 | 0.15 |
| :--- | :--- | :--- | :--- |



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