

Electronic Supplementary Information (ESI) for:

Oxidation by Ozone of Linoleic Acid Monolayers at the Air–Water

Interface in Multi-Component Films at 21 °C and 3 °C.

Ben Woden,^a Yizhou Su,^b Max Skoda,^c Adam Milsom^b and Christian Pfrang.^{b,d,*}

^aUniversity of Reading, Department of Chemistry, Reading, UK.

^bUniversity of Birmingham, School of Geography, Earth and Environmental Sciences, Birmingham, UK.

^cISIS Neutron and Muon Source, Didcot, UK.

^dUniversity of Reading, Department of Meteorology, Reading, UK

*Corresponding author: Prof. Christian Pfrang (c.pfrang@bham.ac.uk)

Section S1: Multilayer-Py model fits for pure d-LOA monolayers

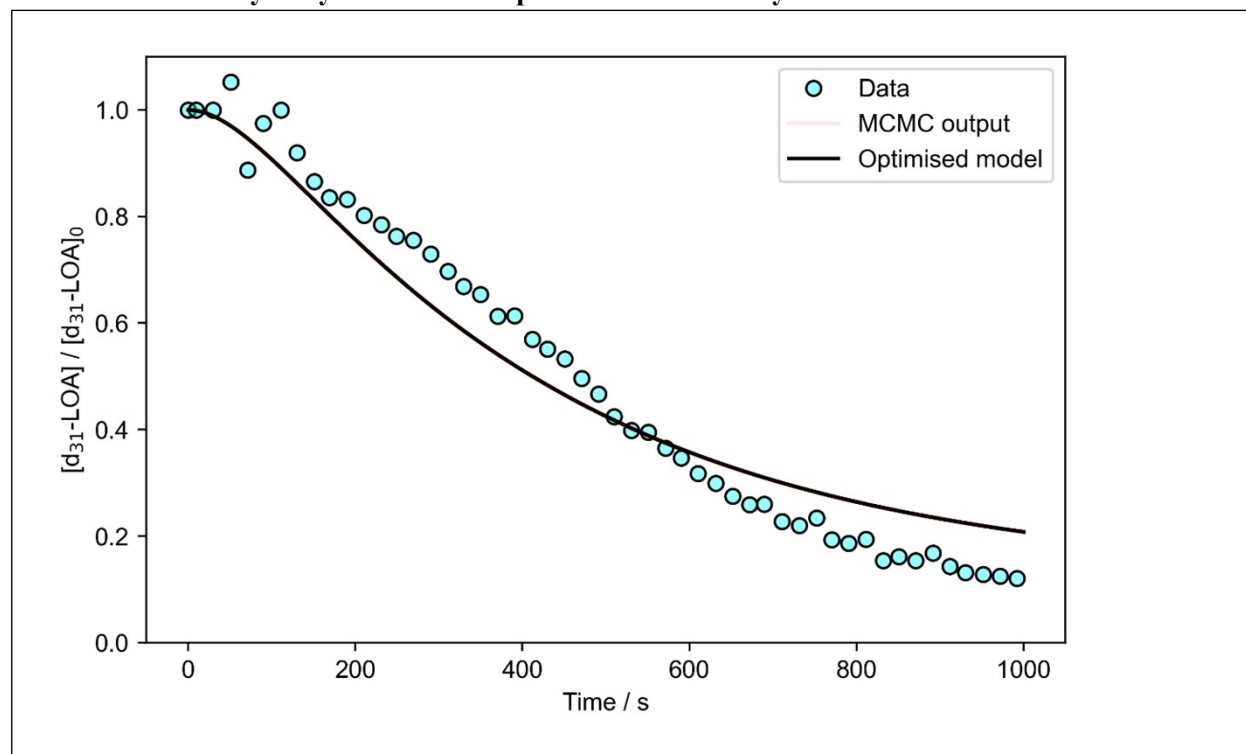


Figure S1 – Multilayer-Py modelling fits for *d*-LOA. The figure displays the normalised decay of *d*-LOA as a function of time with experimental data (blue circles), the results of the global optimisation using Markov chain Monte Carlo (MCMC) sampling (pink lines close to the best fit) and the optimised model fit (solid black line) for 98 ppb & 21 ± 1 °C.

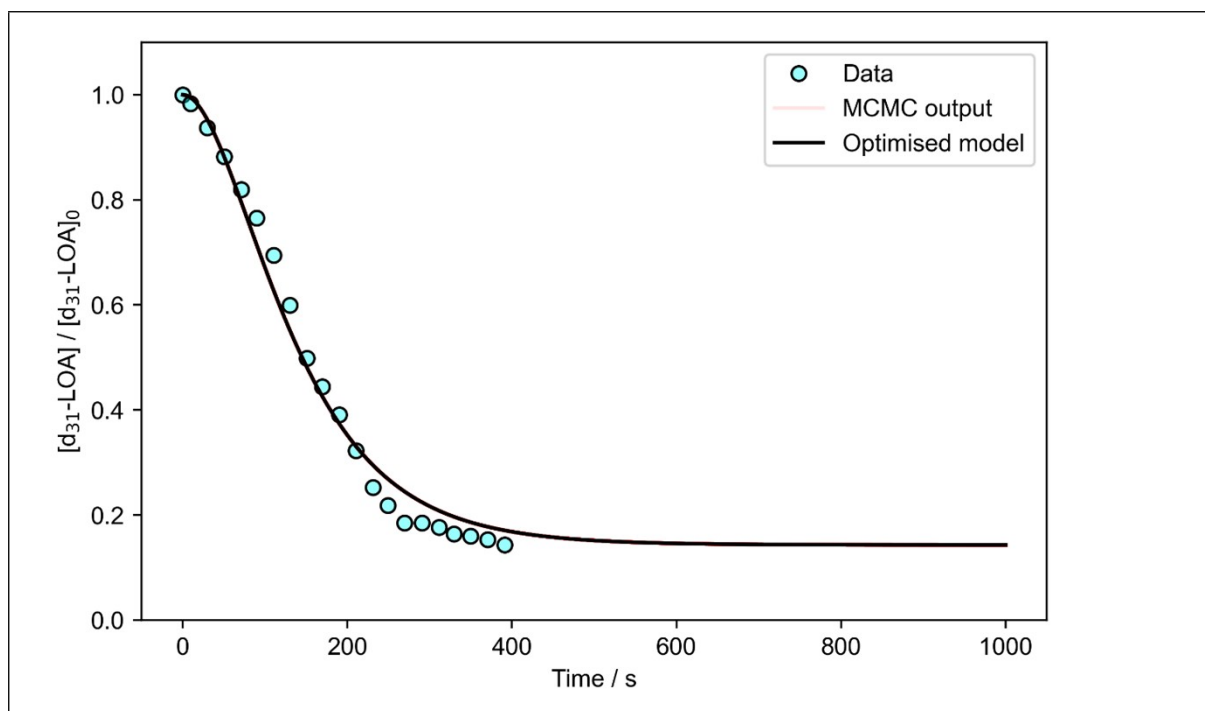


Figure S2 – Multilayer-Py modelling fits for *d*-LOA. The figure displays the normalised decay of *d*-LOA as a function of time with experimental data (blue circles), the results of the global optimisation using Markov chain Monte Carlo (MCMC) sampling (pink lines close to the best fit) and the optimised model fit (solid black line) for 246 ppb & 21 ± 1 °C.

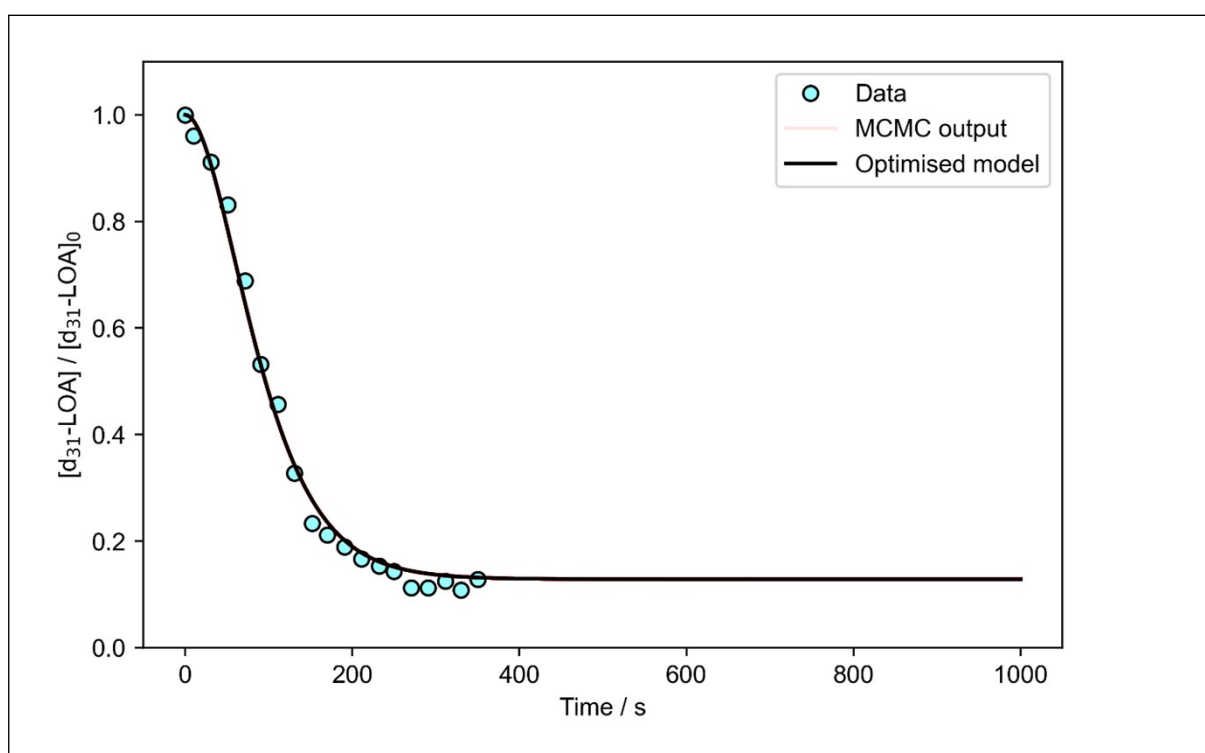


Figure S3 – Multilayer-Py modelling fits for *d*-LOA. The figure displays the normalised decay of *d*-LOA as a function of time with experimental data (blue circles), the results of the global optimisation using Markov chain Monte Carlo (MCMC) sampling (pink lines close to the best fit) and the optimised model fit (solid black line) for 492 ppb & 21 ± 1 °C.

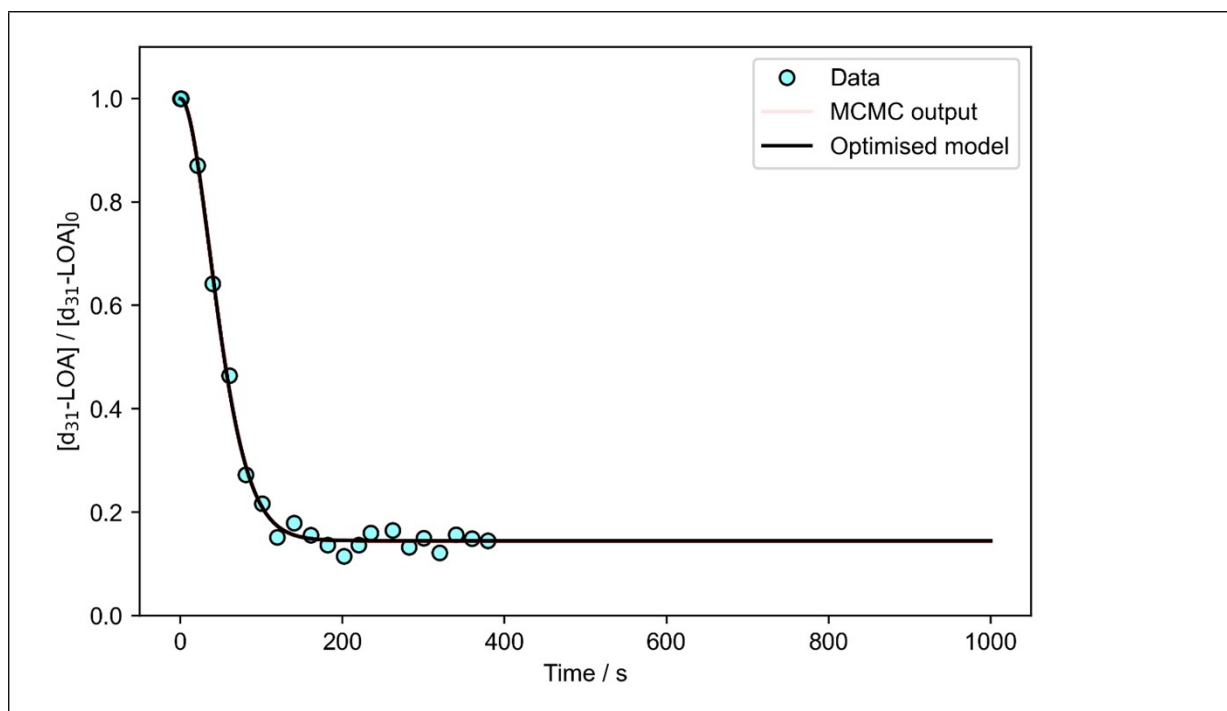


Figure S4 – Multilayer-Py modelling fits for *d*-LOA. The figure displays the normalised decay of *d*-LOA as a function of time with experimental data (blue circles), the results of the global optimisation using Markov chain Monte Carlo (MCMC) sampling (pink lines close to the best fit) and the optimised model fit (solid black line) for 983 ppb & 21 ± 1 °C.

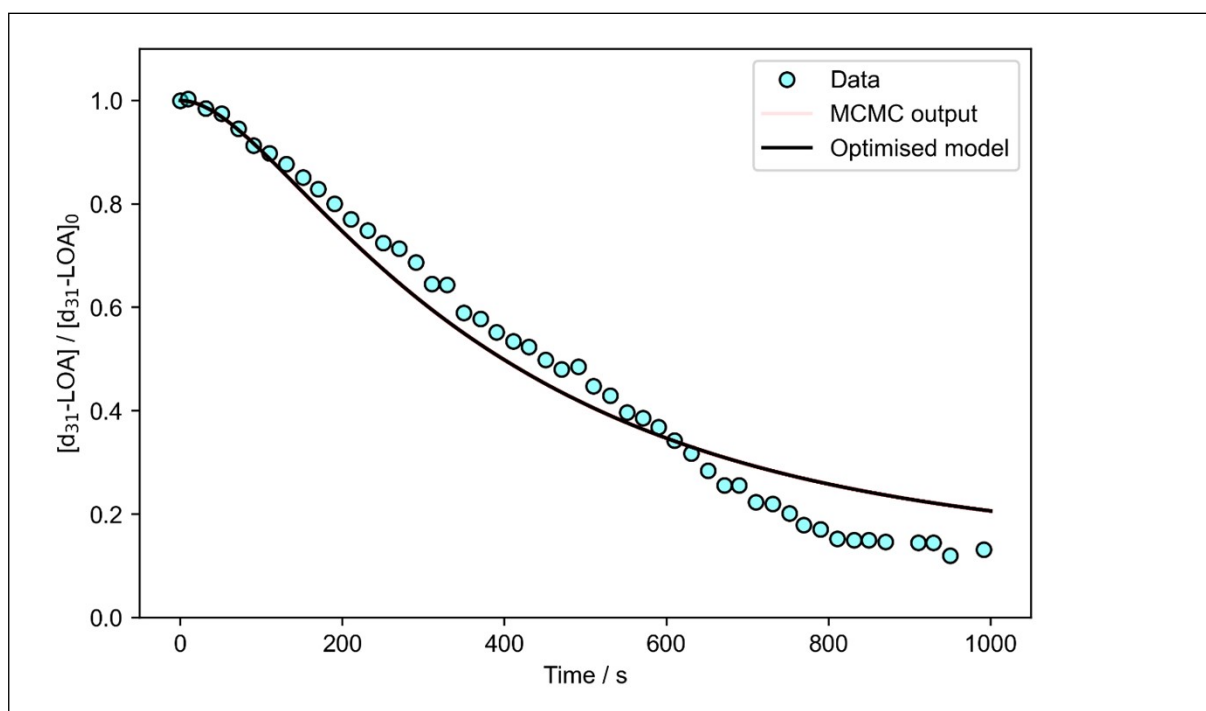


Figure S5 – Multilayer-Py modelling fits for *d*-LOA. The figure displays the normalised decay of *d*-LOA as a function of time with experimental data (blue circles), the results of the global optimisation using Markov chain Monte Carlo (MCMC) sampling (pink lines close to the best fit) and the optimised model fit (solid black line) for 98 ppb & 3 ± 1 °C.

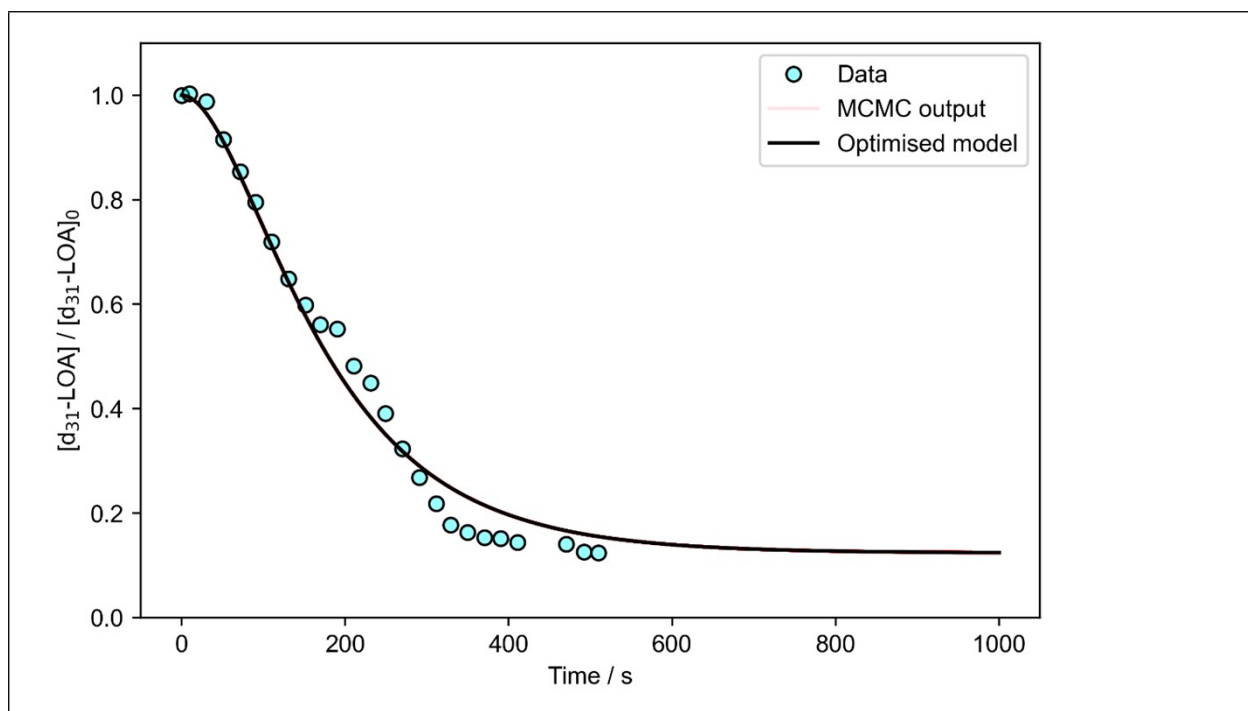


Figure S6 – Multilayer-Py modelling fits for *d*-LOA. The figure displays the normalised decay of *d*-LOA as a function of time with experimental data (blue circles), the results of the global optimisation using Markov chain Monte Carlo (MCMC) sampling (pink lines close to the best fit) and the optimised model fit (solid black line) for 246 ppb & 3 ± 1 °C.

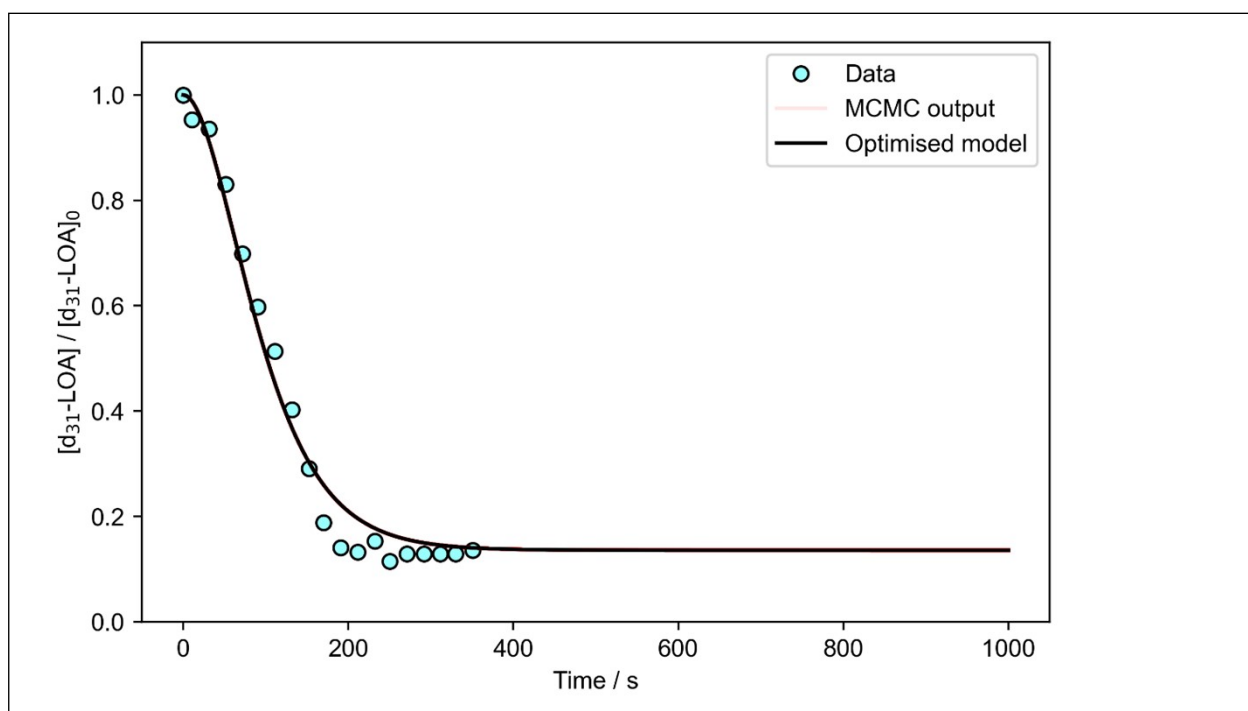


Figure S7 – Multilayer-Py modelling fits for *d*-LOA. The figure displays the normalised decay of *d*-LOA as a function of time with experimental data (blue circles), the results of the global optimisation using Markov chain Monte Carlo (MCMC) sampling (pink lines close to the best fit) and the optimised model fit (solid black line) for 492 ppb & 3 ± 1 °C.

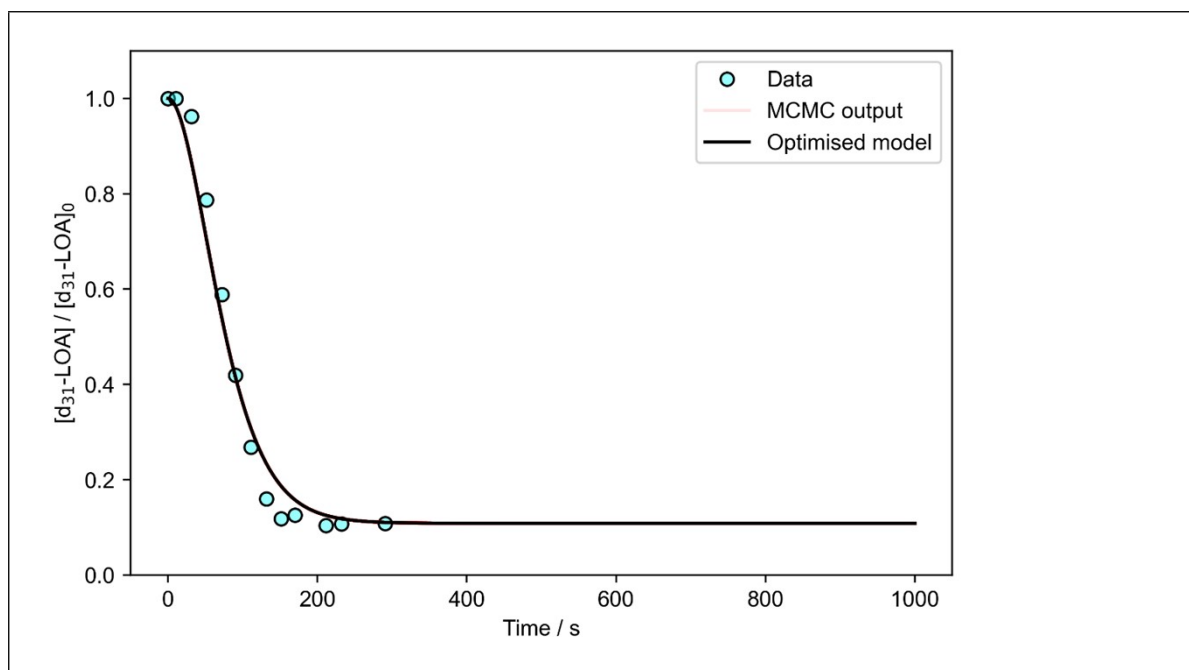


Figure S8 – Multilayer-Py modelling fits for *d*-LOA. The figure displays the normalised decay of *d*-LOA as a function of time with experimental data (blue circles), the results of the global optimisation using Markov chain Monte Carlo (MCMC) sampling (pink lines close to the best fit) and the optimised model fit (solid black line) for 983 ppb & 3 ± 1 °C.

Section S2: Multilayer-Py model fits for d-LOA/h-OA mixed monolayers

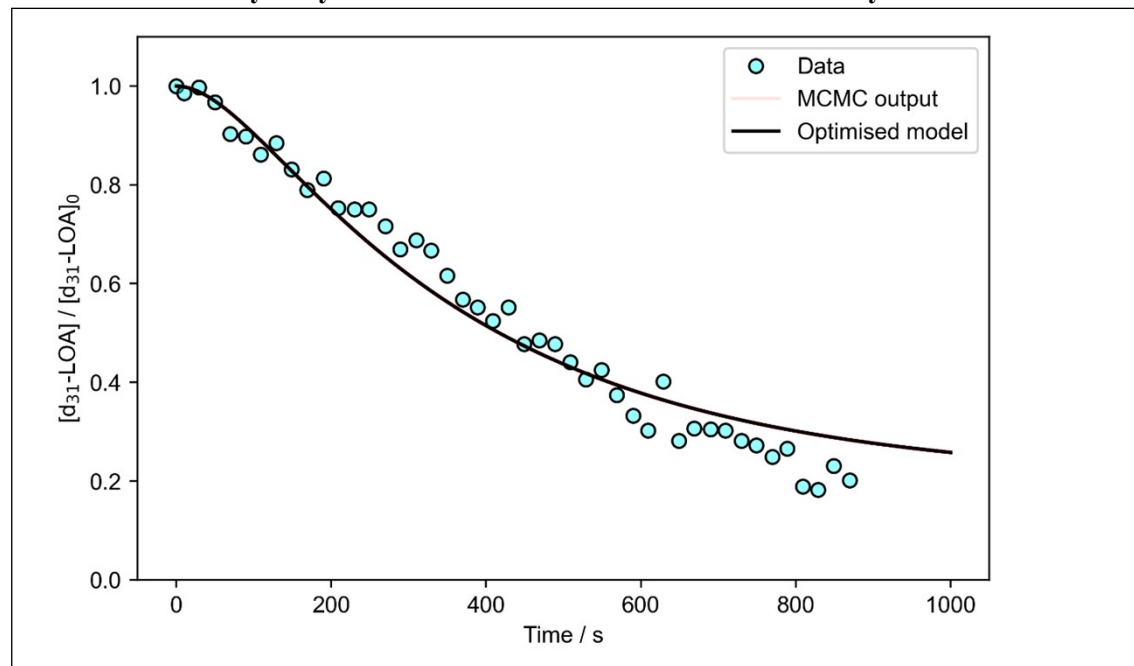


Figure S9 – Multilayer-Py modelling fits for *d*-LOA/*h*-OA mixture. The figure displays the normalised decay of *d*-LOA as a function of time with experimental data (blue circles), the results of the global optimisation using Markov chain Monte Carlo (MCMC) sampling (pink lines close to the best fit) and the optimised model fit (solid black line) for 98 ppb & 21 ± 1 °C.

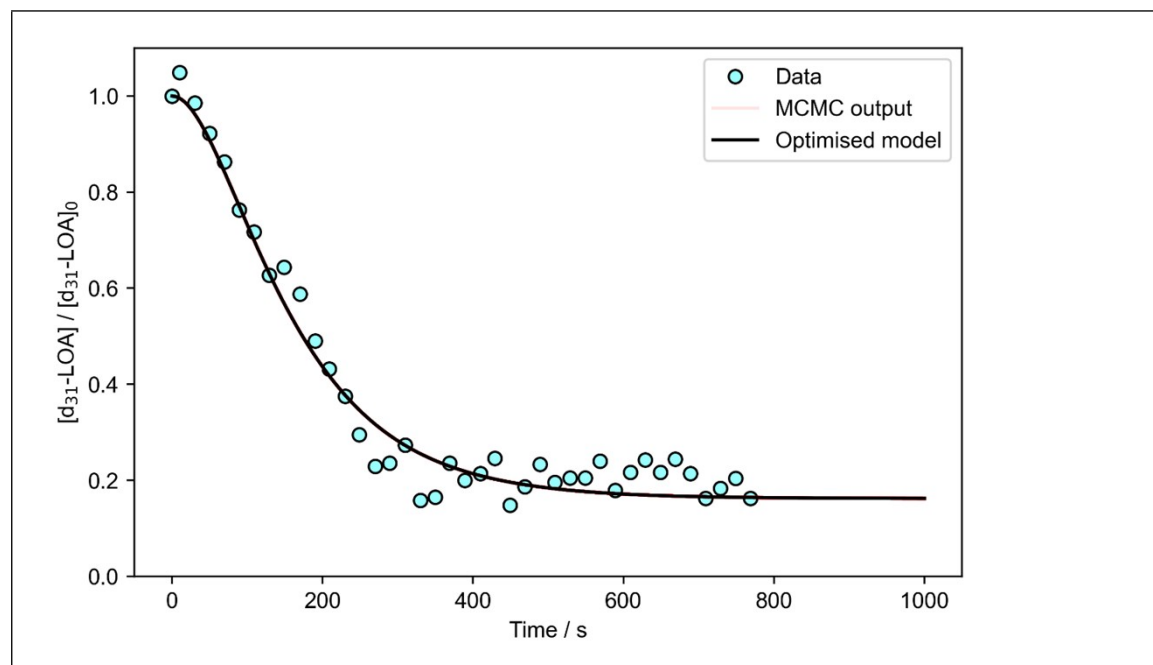


Figure S10 – Multilayer-Py modelling fits for *d*-LOA/*h*-OA mixture. The figure displays the normalised decay of *d*-LOA as a function of time with experimental data (blue circles), the results of the global optimisation using Markov chain Monte Carlo (MCMC) sampling (pink lines close to the best fit) and the optimised model fit (solid black line) for 246 ppb & 21 ± 1 °C.

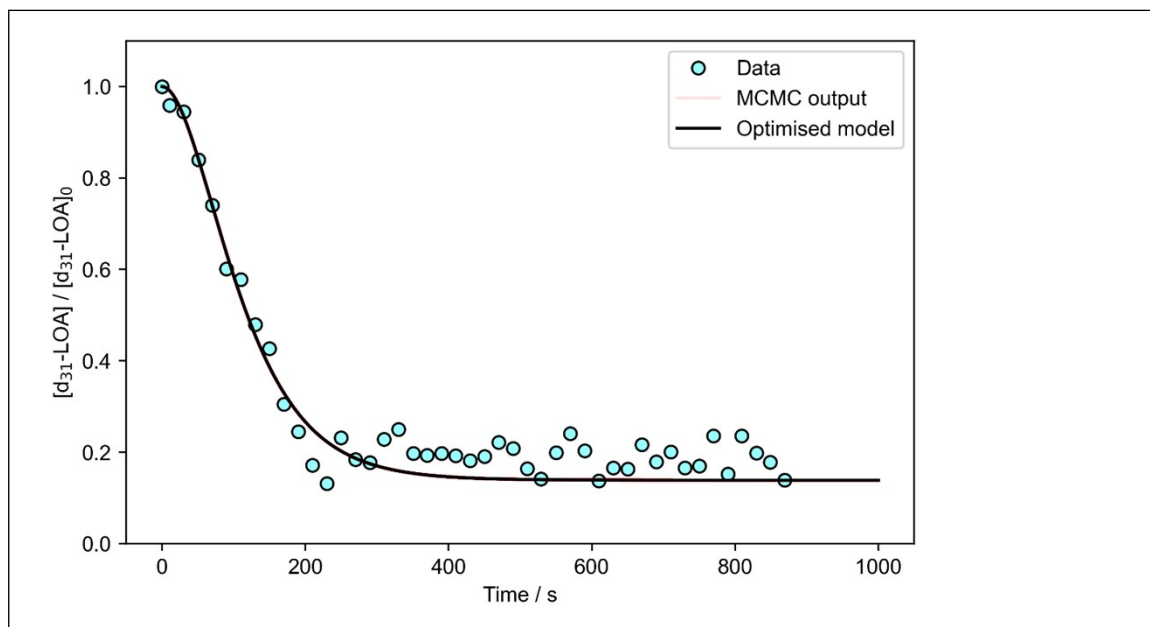


Figure S11 – Multilayer-Py modelling fits for *d*-LOA/*h*-OA mixture. The figure displays the normalised decay of *d*-LOA as a function of time with experimental data (blue circles), the results of the global optimisation using Markov chain Monte Carlo (MCMC) sampling (pink lines close to the best fit) and the optimised model fit (solid black line) for 492 ppb & 21 ± 1 °C.

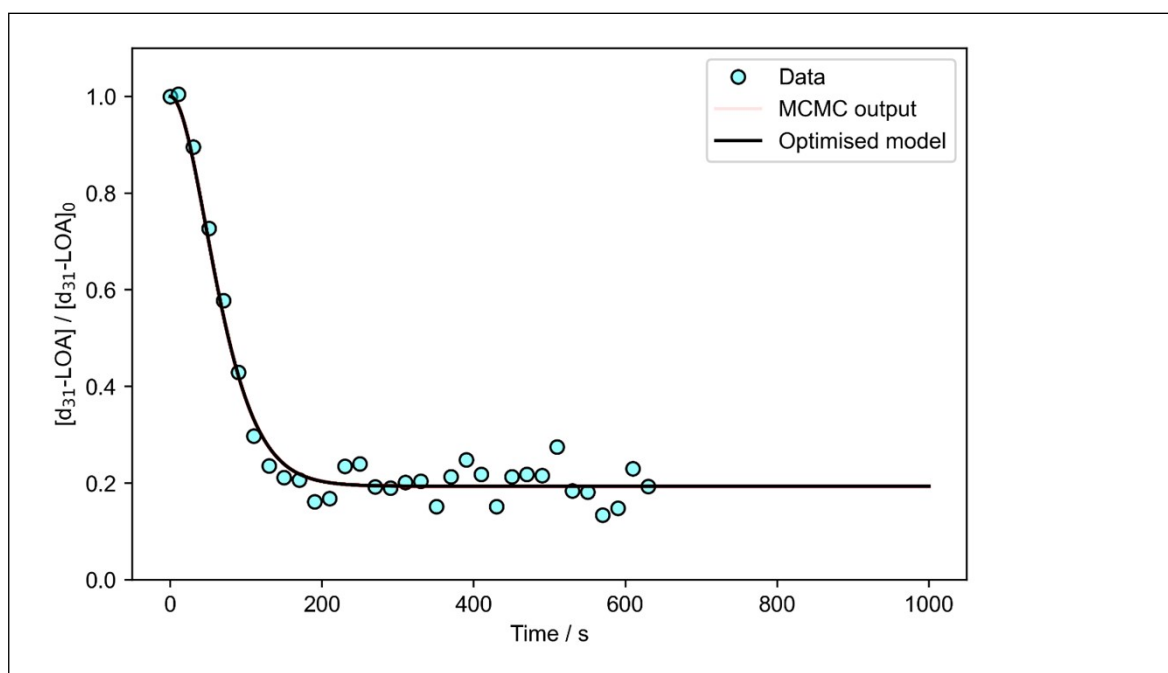


Figure S12 – Multilayer-Py modelling fits for *d*-LOA/*h*-OA mixture. The figure displays the normalised decay of *d*-LOA as a function of time with experimental data (blue circles), the results of the global optimisation using Markov chain Monte Carlo (MCMC) sampling (pink lines close to the best fit) and the optimised model fit (solid black line) for 983 ppb & 21 ± 1 °C.

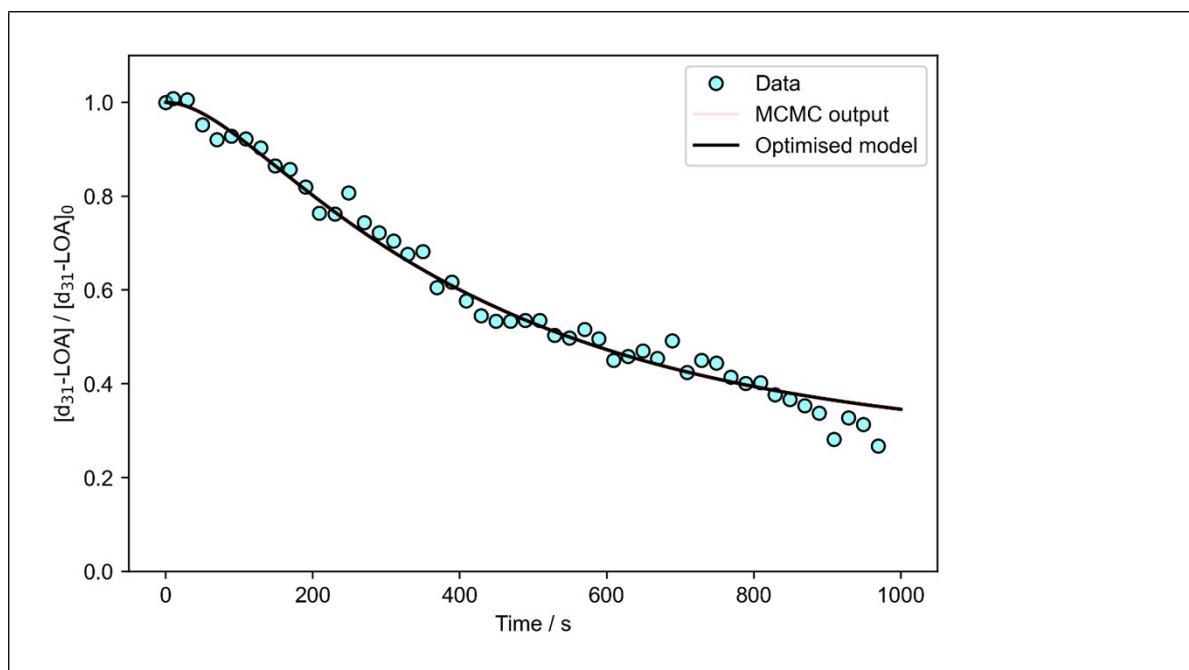


Figure S13 – Multilayer-Py modelling fits for *d*-LOA/*h*-OA mixture. The figure displays the normalised decay of *d*-LOA as a function of time with experimental data (blue circles), the results of the global optimisation using Markov chain Monte Carlo (MCMC) sampling (pink lines close to the best fit) and the optimised model fit (solid black line) for 98 ppb & 3 ± 1 °C.

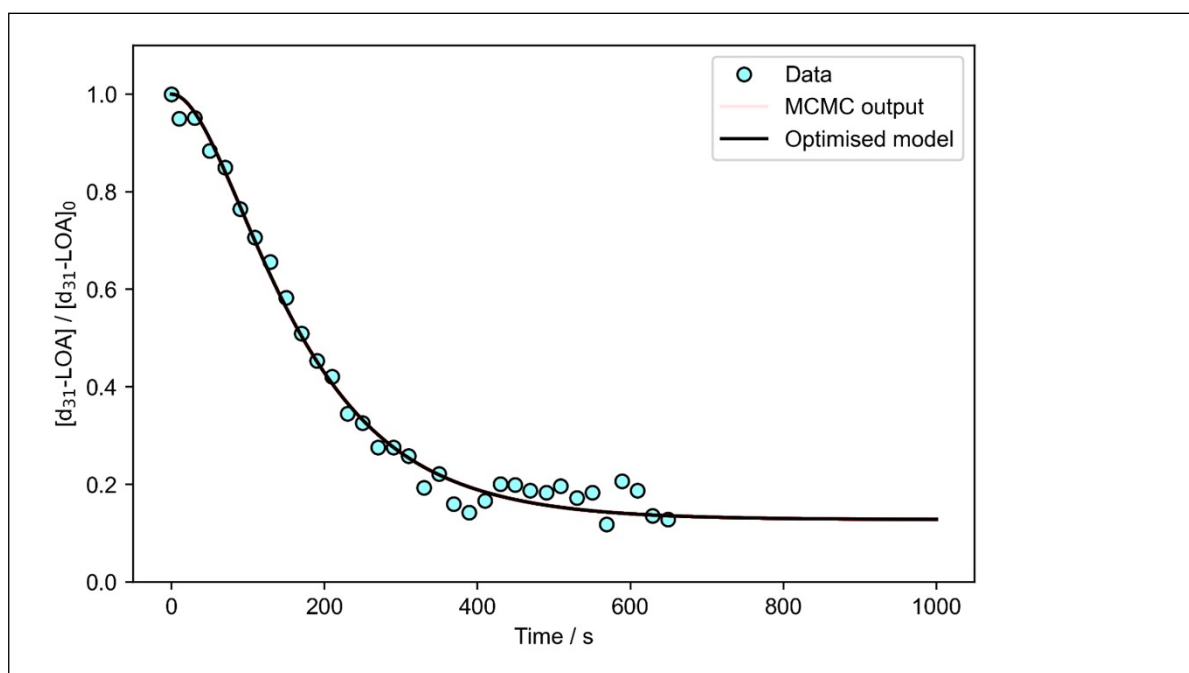


Figure S14 – Multilayer-Py modelling fits for *d*-LOA/*h*-OA mixture. The figure displays the normalised decay of *d*-LOA as a function of time with experimental data (blue circles), the results of the global optimisation using Markov chain Monte Carlo (MCMC) sampling (pink lines close to the best fit) and the optimised model fit (solid black line) for 246 ppb & 3 ± 1 °C.

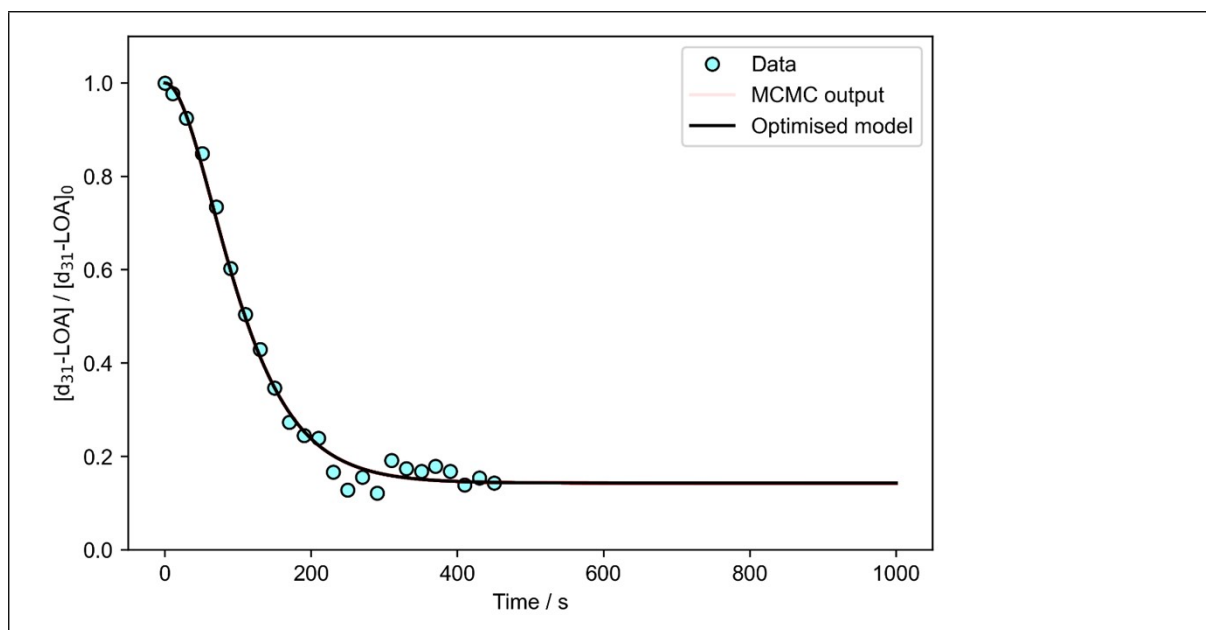


Figure S15 – Multilayer-Py modelling fits for *d*-LOA/*h*-OA mixture. The figure displays the normalised decay of *d*-LOA as a function of time with experimental data (blue circles), the results of the global optimisation using Markov chain Monte Carlo (MCMC) sampling (pink lines close to the best fit) and the optimised model fit (solid black line) for 492 ppb & 3 ± 1 °C.

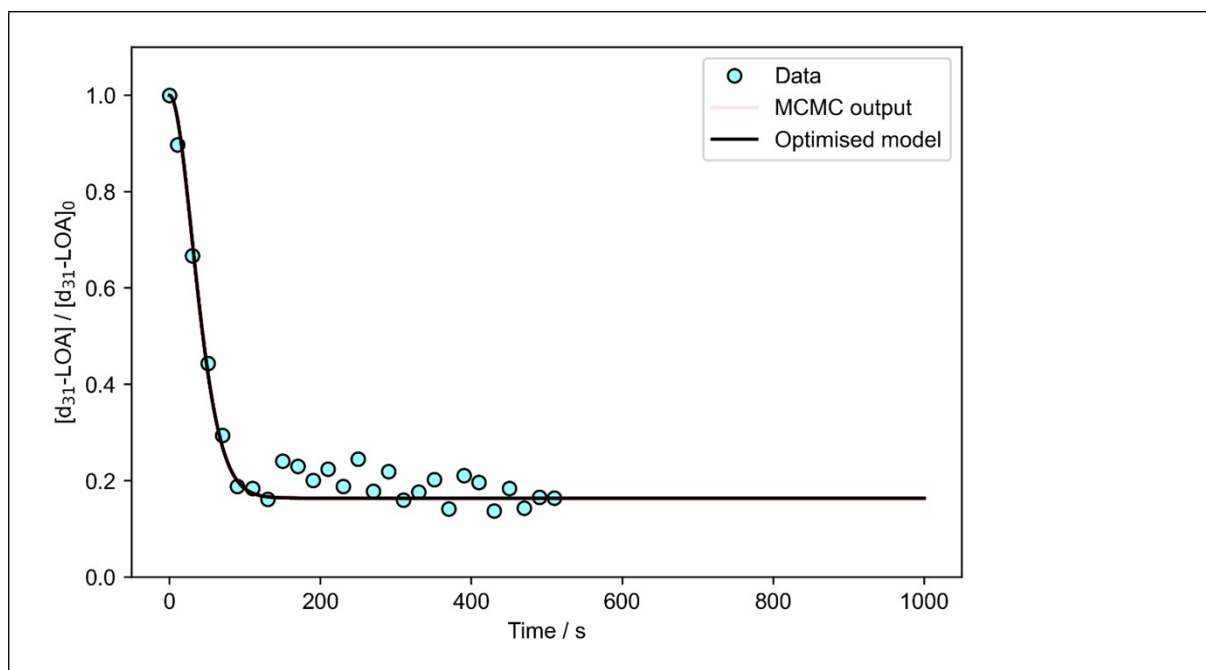


Figure S16 – Multilayer-Py modelling fits for *d*-LOA/*h*-OA mixture. The figure displays the normalised decay of *d*-LOA as a function of time with experimental data (blue circles), the results of the global optimisation using Markov chain Monte Carlo (MCMC) sampling (pink lines close to the best fit) and the optimised model fit (solid black line) for 983 ppb & 3 ± 1 °C.

Section S3: Multilayer-Py model fits for d-LOA/h-MO mixed monolayers

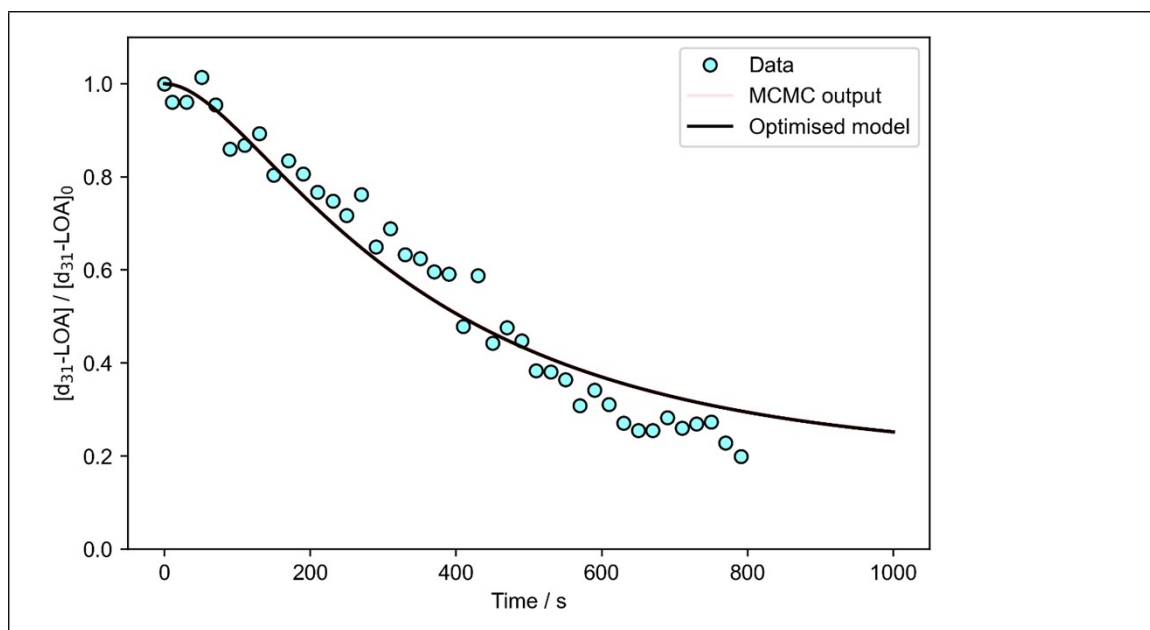


Figure S17 – Multilayer-Py modelling fits for *d*-LOA/*h*-MO mixture. The figure displays the normalised decay of *d*-LOA as a function of time with experimental data (blue circles), the results of the global optimisation using Markov chain Monte Carlo (MCMC) sampling (pink lines close to the best fit) and the optimised model fit (solid black line) for 98 ppb & 21 ± 1 °C.

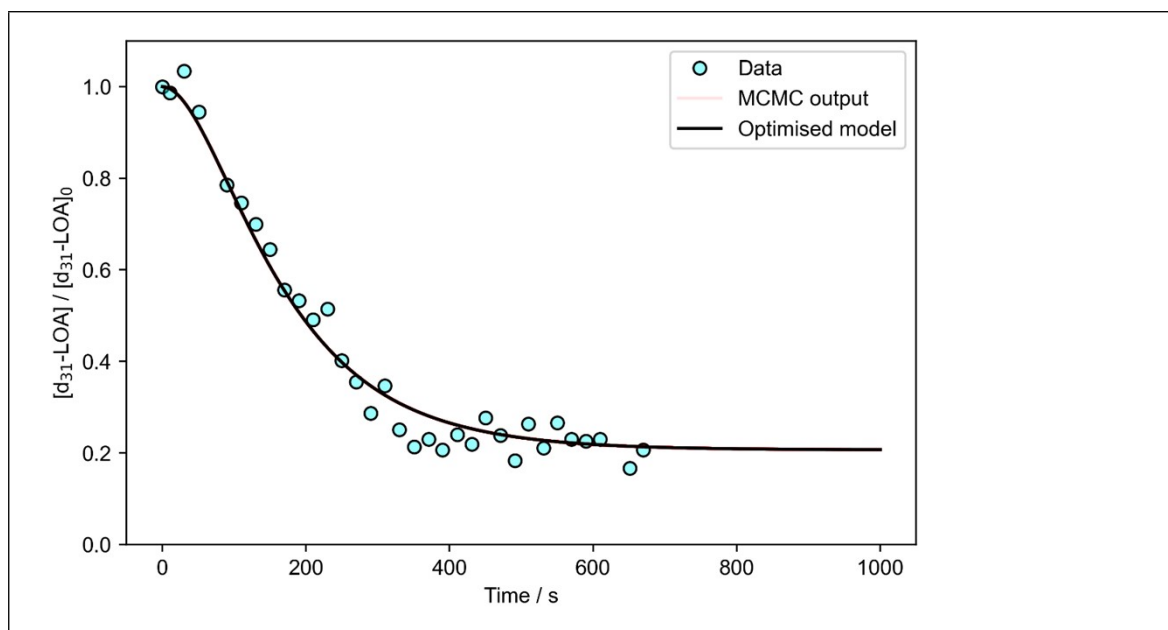


Figure S18 – Multilayer-Py modelling fits for *d*-LOA/*h*-MO mixture. The figure displays the normalised decay of *d*-LOA as a function of time with experimental data (blue circles), the results of the global optimisation using Markov chain Monte Carlo (MCMC) sampling (pink lines close to the best fit) and the optimised model fit (solid black line) for 246 ppb & 21 ± 1 °C.

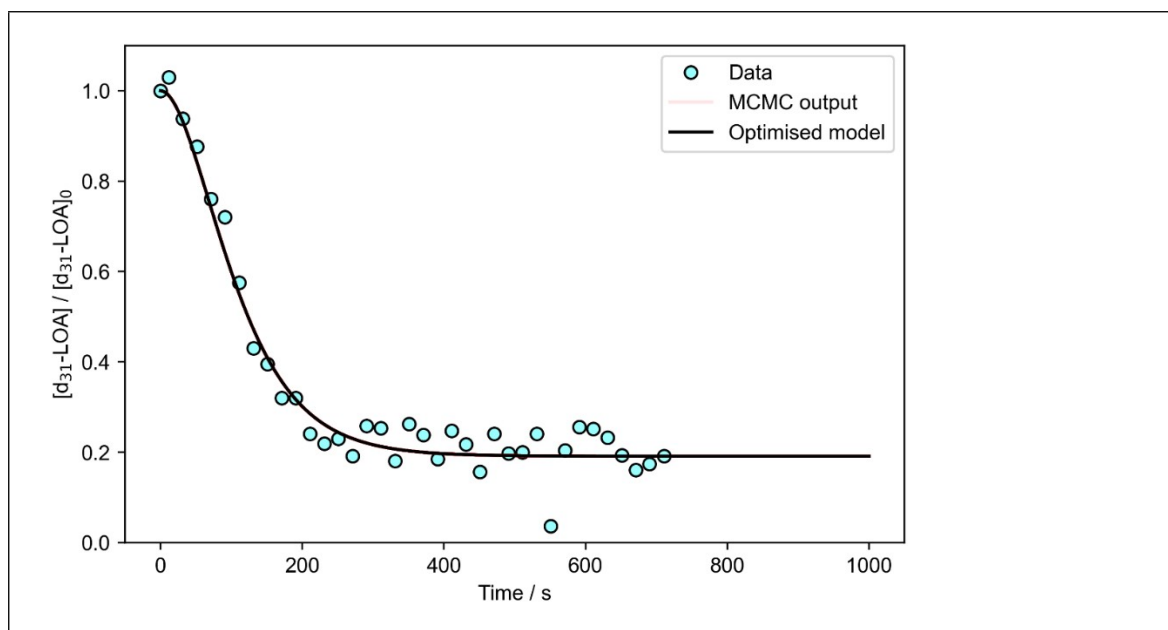


Figure S19 – Multilayer-Py modelling fits for *d*-LOA/*h*-MO mixture. The figure displays the normalised decay of *d*-LOA as a function of time with experimental data (blue circles), the results of the global optimisation using Markov chain Monte Carlo (MCMC) sampling (pink lines close to the best fit) and the optimised model fit (solid black line) for 492 ppb & 21 ± 1 °C.

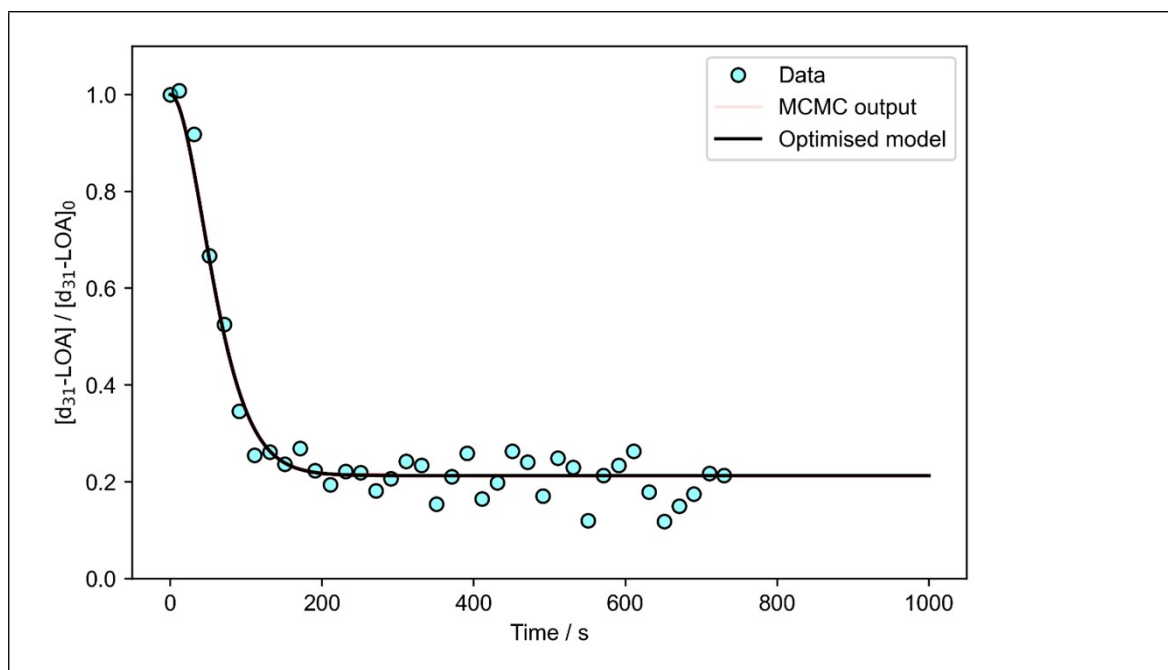


Figure S20 – Multilayer-Py modelling fits for *d*-LOA/*h*-MO mixture. The figure displays the normalised decay of *d*-LOA as a function of time with experimental data (blue circles), the results of the global optimisation using Markov chain Monte Carlo (MCMC) sampling (pink lines close to the best fit) and the optimised model fit (solid black line) for 983 ppb & 21 ± 1 °C.

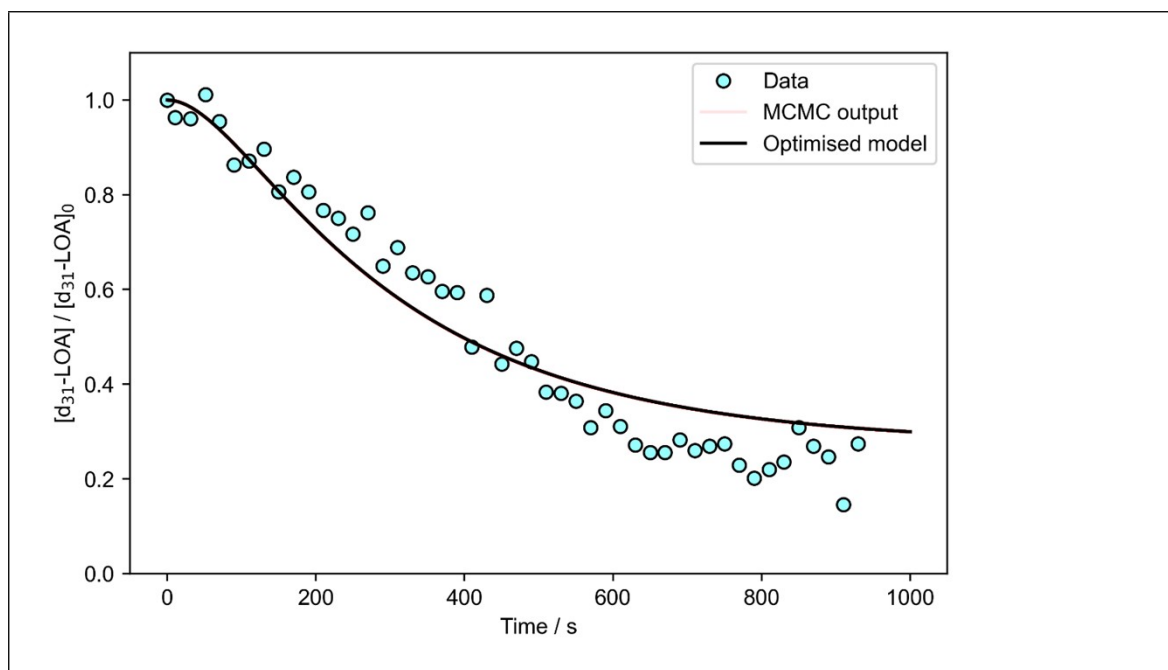


Figure S21 – Multilayer-Py modelling fits for *d*-LOA/*h*-MO mixture. The figure displays the normalised decay of *d*-LOA as a function of time with experimental data (blue circles), the results of the global optimisation using Markov chain Monte Carlo (MCMC) sampling (pink lines close to the best fit) and the optimised model fit (solid black line) for 98 ppb & 3 ± 1 °C.

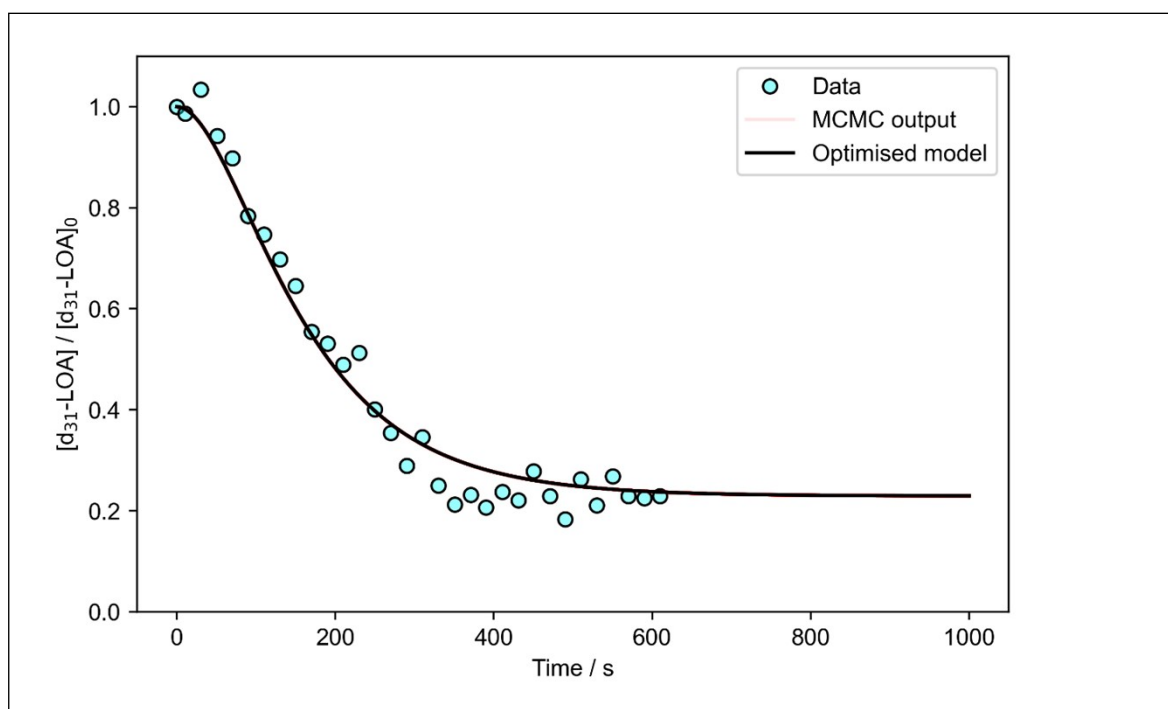


Figure S22 – Multilayer-Py modelling fits for *d*-LOA/*h*-MO mixture. The figure displays the normalised decay of *d*-LOA as a function of time with experimental data (blue circles), the results of the global optimisation using Markov chain Monte Carlo (MCMC) sampling (pink lines close to the best fit) and the optimised model fit (solid black line) for 246 ppb & 3 ± 1 °C.

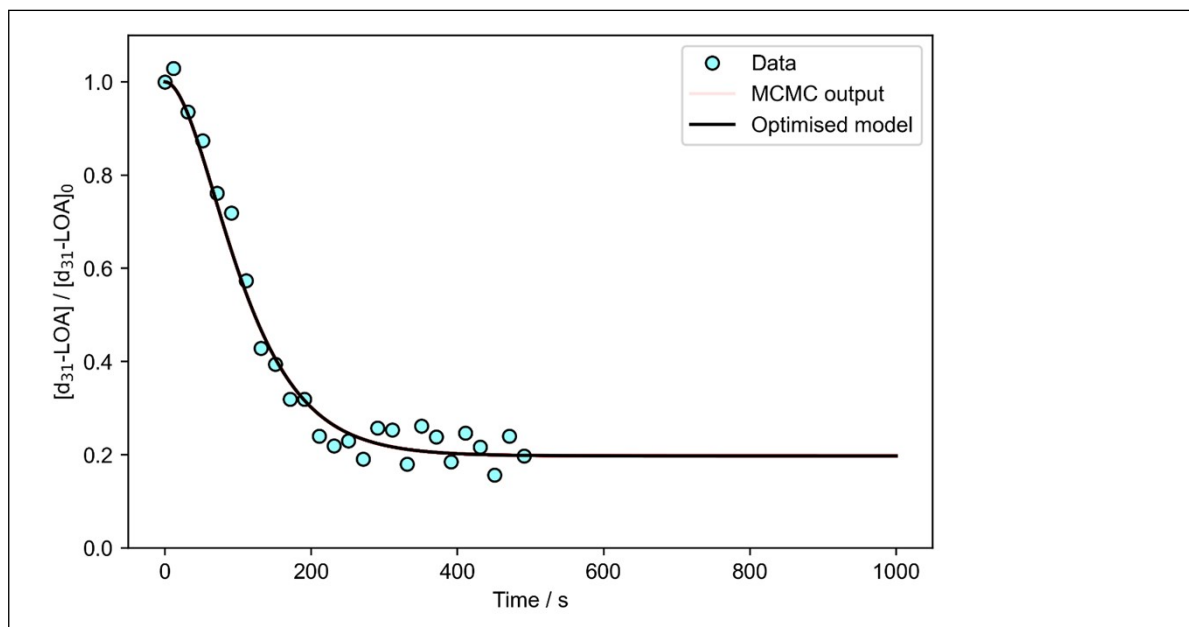


Figure S23 – Multilayer-Py modelling fits for *d*-LOA/*h*-MO mixture. The figure displays the normalised decay of *d*-LOA as a function of time with experimental data (blue circles), the results of the global optimisation using Markov chain Monte Carlo (MCMC) sampling (pink lines close to the best fit) and the optimised model fit (solid black line) for 492 ppb & 3 ± 1 °C.

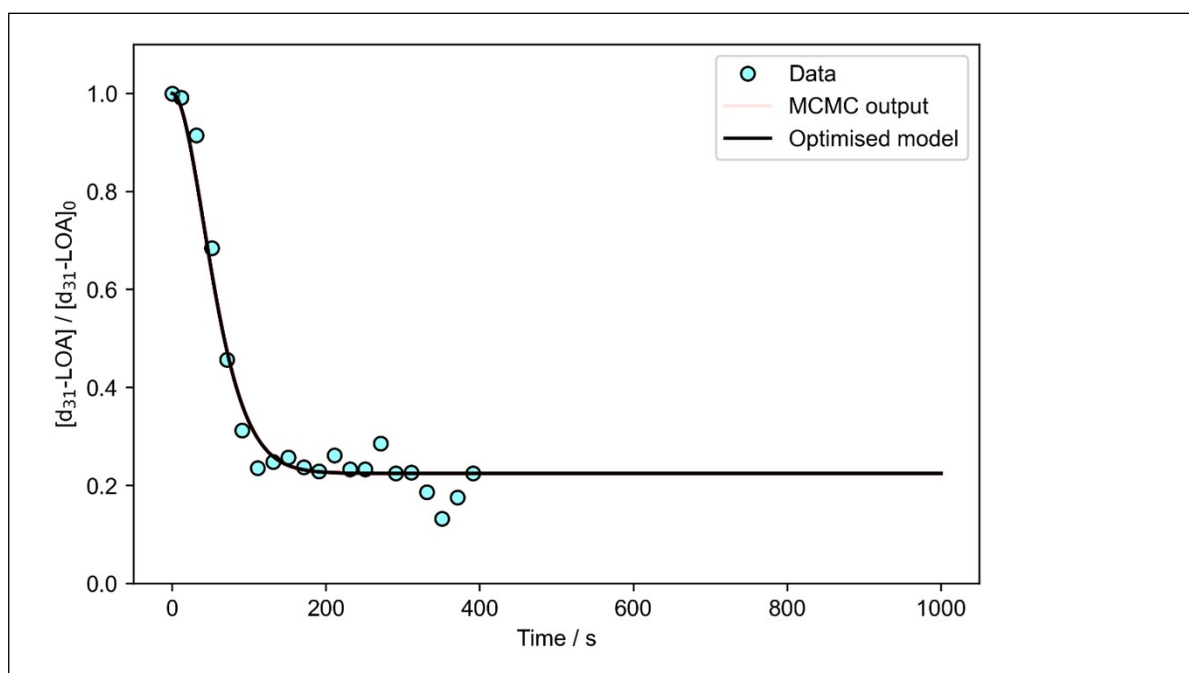


Figure S24 – Multilayer-Py modelling fits for *d*-LOA/*h*-MO mixture. The figure displays the normalised decay of *d*-LOA as a function of time with experimental data (blue circles), the results of the global optimisation using Markov chain Monte Carlo (MCMC) sampling (pink lines close to the best fit) and the optimised model fit (solid black line) for 983 ppb & 3 ± 1 °C.

Section S4: Multilayer-Py model fit comparison for low ozone levels

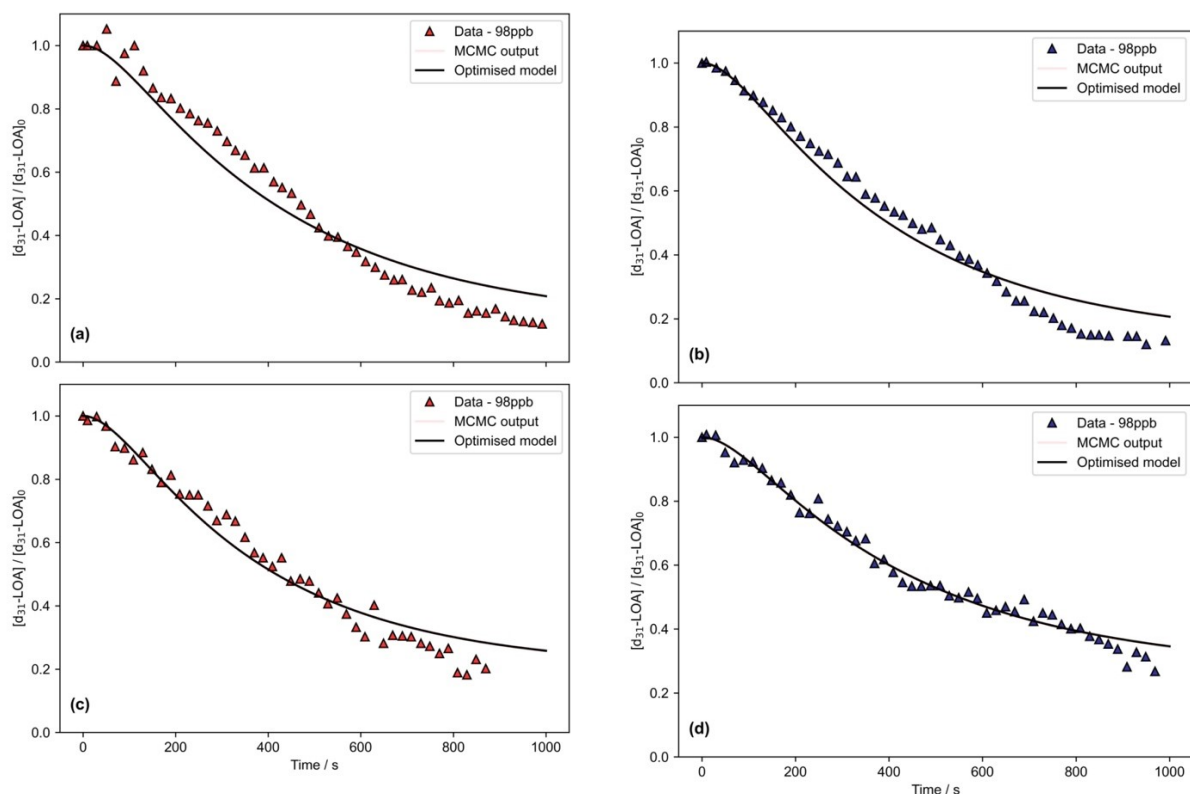


Figure S25 – Multilayer-Py modelling fits to lowest $[O_3]$ for pure *d*-LOA oxidation and *d*-LOA/*h*-OA mixtures (the model runs presented here consider ozone build-up in the reaction chamber, a single-stage oxidation process and residue formation). The figures display the normalised decay of *d*-LOA as a function of time with experimental data (symbols), the results of the global optimisation using Markov chain Monte Carlo (MCMC) sampling (pink lines close to the best fit) and the optimised model fit (solid black line). (a) 98 ppb & 21 ± 1 °C for pure *d*-LOA; (b) 98 ppb & 3 ± 1 °C for pure *d*-LOA; (c) 98 ppb & 21 ± 1 °C for *d*-LOA/*h*-OA; and (d) 98 ppb & 3 ± 1 °C for *d*-LOA/*h*-OA.