

Supplementary Material for:

Development of a new smog chamber for studying the impact of different UV lamps on SAPRC chemical mechanism predictions and aerosol formation

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Table S1. List of CSIRO smog chamber experiments.

Exp ID	Type	Purpose	Length (hr)	Lights	VOC (ppbv)	NO (ppbv)	NO ₂ (ppbv)
NR007	NO ₂ photo	Photolysis	-	Variable	-	-	471
NR009	NO ₂ photo	Photolysis	-	Variable	-	-	259
NR016	Clean air	Characterisation	6	Mixed	-	-	-
NR018	Ozone	Wall loss	24	-	133	-	-
NR019	Ozone	Wall loss	75	-	188	-	-
NR027	m-Xylene/NOx	Aerosol wall loss	28	Mixed	104	29	0.5
NR028	Clean air	Characterisation	6	Mixed	-	-	-
NR029	Clean air	Characterisation	6	Mixed	-	-	-
NR030	Clean air	Characterisation	6	350B	-	-	-
NR031	Clean air	Characterisation	6	BLB	-	-	-
NR034	CO	Characterisation	6	Mixed	21,700	-	-
NR035	CO/NOx	Characterisation	6	Mixed	24,200	94	<0.5
NR036	CO/NOx	Characterisation	6	Mixed	24,400	26	0.7
NR037	CO	Characterisation	6	Mixed	15,600	-	-
NR038	NO ₂	Wall loss	51	-	-	-	225
NR039	NOx	Characterisation	6	Mixed	-	80	0.8
NR049	NOx	Characterisation	7	Mixed	-	19	0.6
NR050	NO	Wall loss	73	-	-	262	-
NR051	Isopentane/NOx	Characterisation	6	Mixed	252	26.5	0.6
NR052	NO ₂ photo	Photolysis	-	Variable	-	-	233
NR053	NO ₂ photo	Photolysis	-	Variable	-	-	250
NR058	Propene/NOx	Modelling	6	Mixed ^a	90	27	<0.5
NR060	Propene/NOx	Modelling	6	350B	90	26	<0.5
NR062	Propene/NOx	Modelling	6	BLB	94	26	<0.5
NR064	Propene/NOx	Modelling	6	Mixed ^a	146	28	<0.5
NR065	Propene/NOx	Modelling	6	350B	146	29	<0.5
NR067	Clean air	Characterisation	6	Mixed ^a	-	-	-
NR068	Propene/NOx	Modelling	6	BLB	146	28	<0.5
NR070	Propene/NOx	Modelling	6	Mixed	113	28	<0.5
NR071	Propene/NOx	Modelling	6	Mixed	180	28	<0.5
NR073	Propene/NOx	Modelling	6	Mixed	113	28	<0.5
NR074	Propene/NOx	Modelling	6	Mixed	180	28	<0.5
NR075	Propene/NOx	Modelling	6	Mixed	150	29	<0.5
NR089	Propene/NOx	Modelling	6	350B	180	26	<0.5
NR091	CO	Characterisation	6	350B	22,100	-	-
NR092	CO	Characterisation	6	BLB	25,200	-	-
NR093	CO/NOx	Characterisation	6	350B	25,400	28	<0.5
NR094	CO/NOx	Characterisation	6	BLB	25,200	28	<0.5
NR095	p-Xylene/NOx	Modelling	7	Mixed ^a	125	30	0.7
NR096	p-Xylene/NOx	Modelling	7	BLB	123	30	0.6
NR097	p-Xylene/NOx	Modelling	7	350B	126	30	<0.5
NR098	p-Xylene/NOx	Modelling	6	Mixed ^a	83	13	4.5
NR099	p-Xylene/NOx	Modelling	8	350B	83	13	4.5
NR100	p-Xylene/NOx	Modelling	8	BLB	83	13	4.5
NR102	NO ₂ photo	Photolysis	-	Variable	-	-	235
NR103	m-Xylene/NOx	Aerosol wall loss	32	Mixed	228	64	0.8
NR152	o-Xylene/NOx	Modelling	8	Mixed ^a	53	22	0.7
NR153	o-Xylene/NOx	Modelling	7	350B	51	23	<0.5
NR154	o-Xylene/NOx	Modelling	7	BLB	52	22	<0.5

Exp ID	Type	Purpose	Length (hr)	Lights	VOC (ppbv)	NO (ppbv)	NO₂ (ppbv)
NR155	NO ₂ photo	Photolysis	-	Variable	-	-	238
NR169	p-Xylene/NOx	Modelling	9	Mixed	50	49	6
NR170	p-Xylene/NOx	Modelling	7	Mixed	58	18	3
NR171	o-Xylene/NOx	Product ID	6	Mixed	50	49	5
NR201	o-Xylene/NOx	Aerosol wall loss	30	Mixed	231	61	6
NR230	o-Xylene/NOx	Aerosol wall loss	30	Mixed	235	59	4
NR279	Hydrocarbons	Wall loss	23	-	750	-	-

^a Experiments were performed at half light intensity

The following experiments were undertaken in the previous CSIRO smog chamber, following the method described in Azzi et al. (2010):

Table S2. Experiments undertaken in Lucas Heights (LH) CSIRO smog chamber

Exp ID	Type	Purpose	Length (hr)	Lights	VOC (ppbv)	NO (ppbv)	NO₂ (ppbv)
LH586	p-Xylene/NOx	Modelling	6	BLB	63	64	2
LH588	p-Xylene/NOx	Modelling	6	BLB	61	44	2
LH589	p-Xylene/NOx	Modelling	6	BLB	65	34	1
LH590	p-Xylene/NOx	Modelling	6	BLB	37	44	2
LH591	p-Xylene/NOx	Modelling	6	BLB	35	67	2
LH592	p-Xylene/NOx	Modelling	6	BLB	36	33	1
LH593	p-Xylene/NOx	Modelling	6	BLB	93	64	2
LH595	p-Xylene/NOx	Modelling	6	BLB	90	43	2
LH596	p-Xylene/NOx	Modelling	6	BLB	88	32	1

The raw maximum particle number and mass observed in each experiment, for observed concentrations not corrected for wall partitioning, are shown in Table S.3. Where particles were observed, the nucleation time (Nucl.time) was calculated based on the appearance of particles at the lower diameter end of the differential mobility analyser (DMA). For experiments with number less than NR184, measurements were taken using the long-DMA (TSI 3081) with lowest observable aerosol diameter of 13 nm. For experiments with identifier number greater than NR184, nucleation measurements were taken with the nano-DMA (TSI 3085) with lowest observable diameter around 3 nm, although the final aerosol numbers may have been taken using the long DMA depending on average aerosol diameter at the end of the experiment. The pace of nucleation and the appearance of particles typically across a wide range (5-25 nm) between 5min scan increments is such that it is not expected that the difference in DMA will have any appreciable change on these numbers, with the exception of experiments with very slow or delayed nucleation.

Table S3. Maximum particle mass and number observed in chamber experiments

Exp ID	Type	Purpose	Lights	Nucl.time (min)	Max PN (# cm⁻³)	Max mass (µg m⁻³)
NR007	NO ₂ photo	Photolysis	Variable	-	<20	-
NR009	NO ₂ photo	Photolysis	Variable	-	<20	-
NR016	Clean air	Characterisation	Mixed	~200	1.1e3	<0.02
NR018	Ozone	Wall loss	-	b	b	b
NR019	Ozone	Wall loss	-	b	b	b
NR027	m-Xylene/NO _x	Aerosol wall loss	Mixed	35	7.6e4	29
NR028	Clean air	Characterisation	Mixed	~100	7.4e3	0.4
NR029	Clean air	Characterisation	Mixed	~260	3.0e3	<0.1
NR030	Clean air	Characterisation	350B	-	<20	-
NR031	Clean air	Characterisation	BLB	-	<20	-
NR034	CO	Characterisation	Mixed	-	<20	-
NR035	CO/NO _x	Characterisation	Mixed	-	<20	-
NR036	CO/NO _x	Characterisation	Mixed	-	<20	-
NR037	CO	Characterisation	Mixed	-	<20	-
NR038	NO ₂	Wall loss	-	-	<20	-
NR039	NO _x	Characterisation	Mixed	-	<20	-
NR049	NO _x	Characterisation	Mixed	-	<20	-
NR050	NO	Wall loss	-	-	<50	-
NR051	Isopentane/NO _x	Characterisation	Mixed	-	<20	-
NR052	NO ₂ photo	Photolysis	Variable	-	<20	-
NR053	NO ₂ photo	Photolysis	Variable	-	<20	-
NR058	Propene/NO _x	Modelling	Mixed ^a	b	b	b
NR060	Propene/NO _x	Modelling	350B	b	b	b
NR062	Propene/NO _x	Modelling	BLB	b	b	b
NR064	Propene/NO _x	Modelling	Mixed ^a	b	b	b
NR065	Propene/NO _x	Modelling	350B	-	<20	-
NR067	Clean air	Characterisation	Mixed ^a	-	<20	-
NR068	Propene/NO _x	Modelling	BLB	-	<20	-
NR070	Propene/NO _x	Modelling	Mixed	-	<20	-
NR071	Propene/NO _x	Modelling	Mixed	-	<20	-
NR073	Propene/NO _x	Modelling	Mixed	-	<20	-
NR074	Propene/NO _x	Modelling	Mixed	-	<20	-
NR075	Propene/NO _x	Modelling	Mixed	-	<20	-
NR089	Propene/NO _x	Modelling	350B	-	<20	-
NR091	CO	Characterisation	350B	-	<20	-
NR092	CO	Characterisation	BLB	-	<20	-
NR093	CO/NO _x	Characterisation	350B	-	<20	-
NR094	CO/NO _x	Characterisation	BLB	-	<20	-
NR095	p-Xylene/NO _x	Modelling	Mixed ^a	180	4.9e4	10.0
NR096	p-Xylene/NO _x	Modelling	BLB	160	4.5e4	12.7
NR097	p-Xylene/NO _x	Modelling	350B	180	4.2e4	6.4
NR098	p-Xylene/NO _x	Modelling	Mixed ^a	195	3.6e4	4.6
NR099	p-Xylene/NO _x	Modelling	350B	220	3.4e4	3.7
NR100	p-Xylene/NO _x	Modelling	BLB	160	4.5e4	8.3
NR102	NO ₂ photo	Photolysis	Variable	-	<20	-
NR103	m-Xylene/NO _x	Aerosol wall loss	Mixed	40	9.0e4	65
NR152	o-Xylene/NO _x	Modelling	Mixed ^a	140	1.9e4	5.5
NR153	o-Xylene/NO _x	Modelling	350B	170	1.5e4	3.6
NR154	o-Xylene/NO _x	Modelling	BLB	120	2.3e4	7.1

Exp ID	Type	Purpose	Lights	Nucl.time (min)	Max PN (# cm ⁻³)	Max mass (μg m ⁻³)
NR155	NO ₂ photo	Photolysis	Variable	-	<20	-
NR169	p-Xylene/NOx	Modelling	Mixed	320	1.4e4	1.2
NR170	p-Xylene/NOx	Modelling	Mixed	130	4.0e4	4.4
NR171	o-Xylene/NOx	Product ID	Mixed	120	8.4e3	2.5
NR201	o-Xylene/NOx	Aerosol wall loss	Mixed	50	6.9e4	80
NR230	o-Xylene/NOx	Aerosol wall loss	Mixed	50	3.0e4	100
NR279	Hydrocarbons	Wall loss	-	-	<20	-

^a Experiments were performed at half light intensity

^b not measured

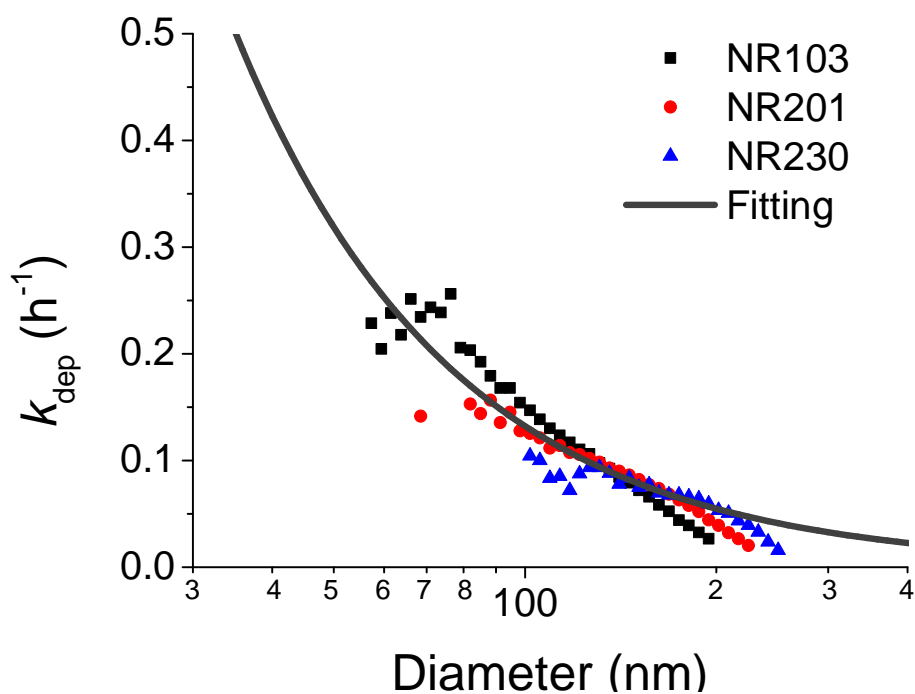


Fig. S1. Experimental and fitted results from aerosol wall loss test experiments (NR103, NR201, NR230). The fitted line was used to correct for chamber aerosol wall loss.

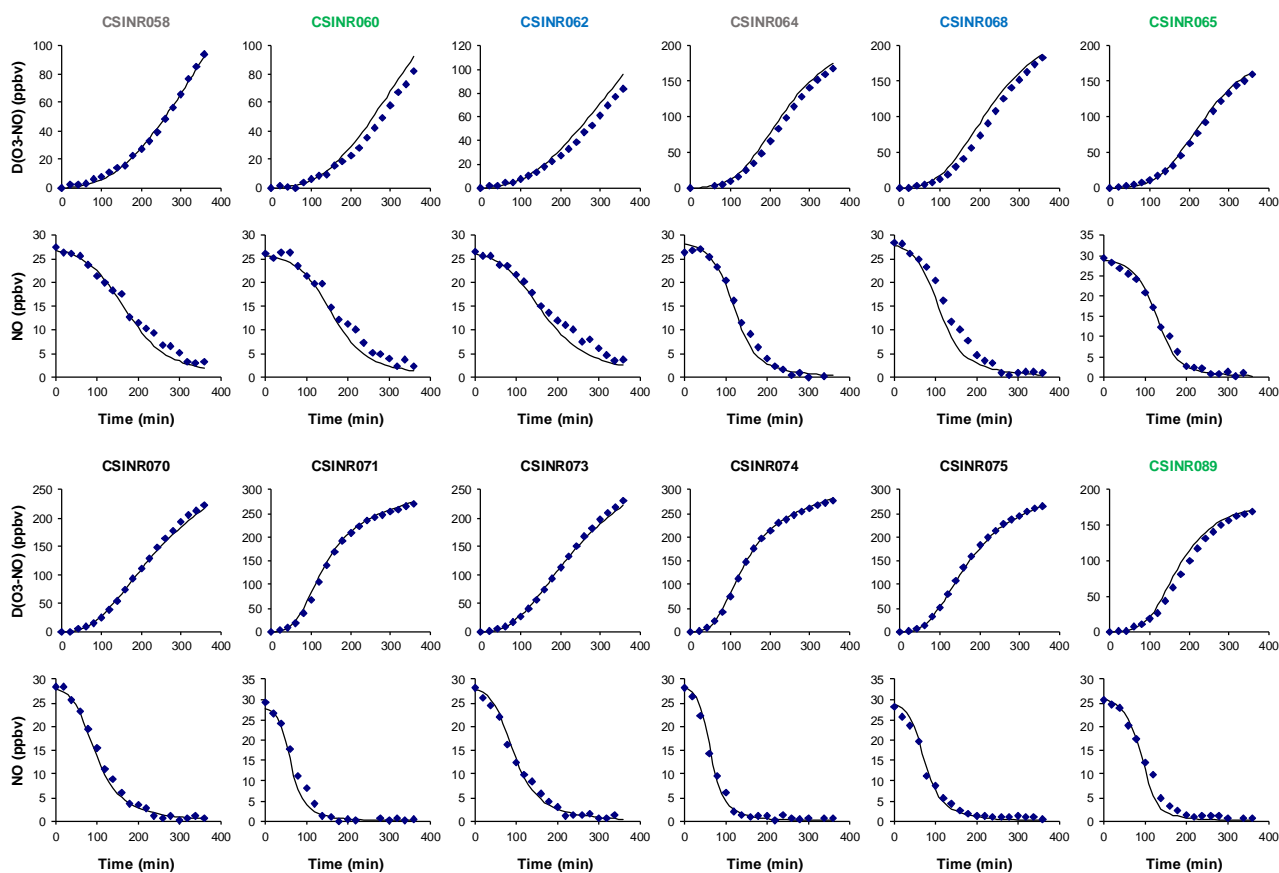


Fig. S2. $\Delta(\text{O}_3 - \text{NO})$ and NO predictions for SAPRC11 against propene experiments using blacklight (green; $J_{\text{NO}_2} = 0.18 \text{ min}^{-1}$), BLB (blue; $J_{\text{NO}_2} = 0.33 \text{ min}^{-1}$) and mixed blacklight+BLB experiments at full (black; $J_{\text{NO}_2} = 0.46 \text{ min}^{-1}$) and half (grey; $J_{\text{NO}_2} = 0.25 \text{ min}^{-1}$) light intensity.

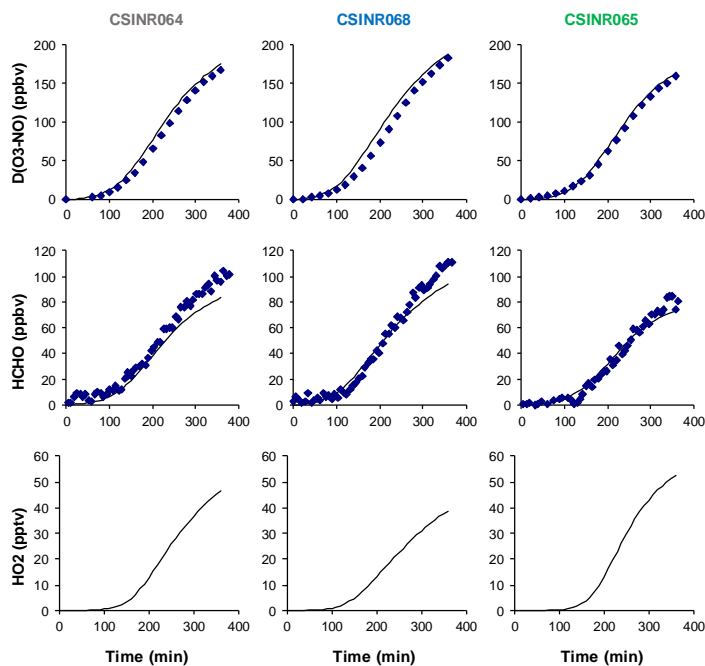


Fig. S3. Predictions of $\Delta(\text{O}_3 - \text{NO})$, HCHO and HO_2 for 3 propene- NO_x experiments with same initial concentrations but different light sources.

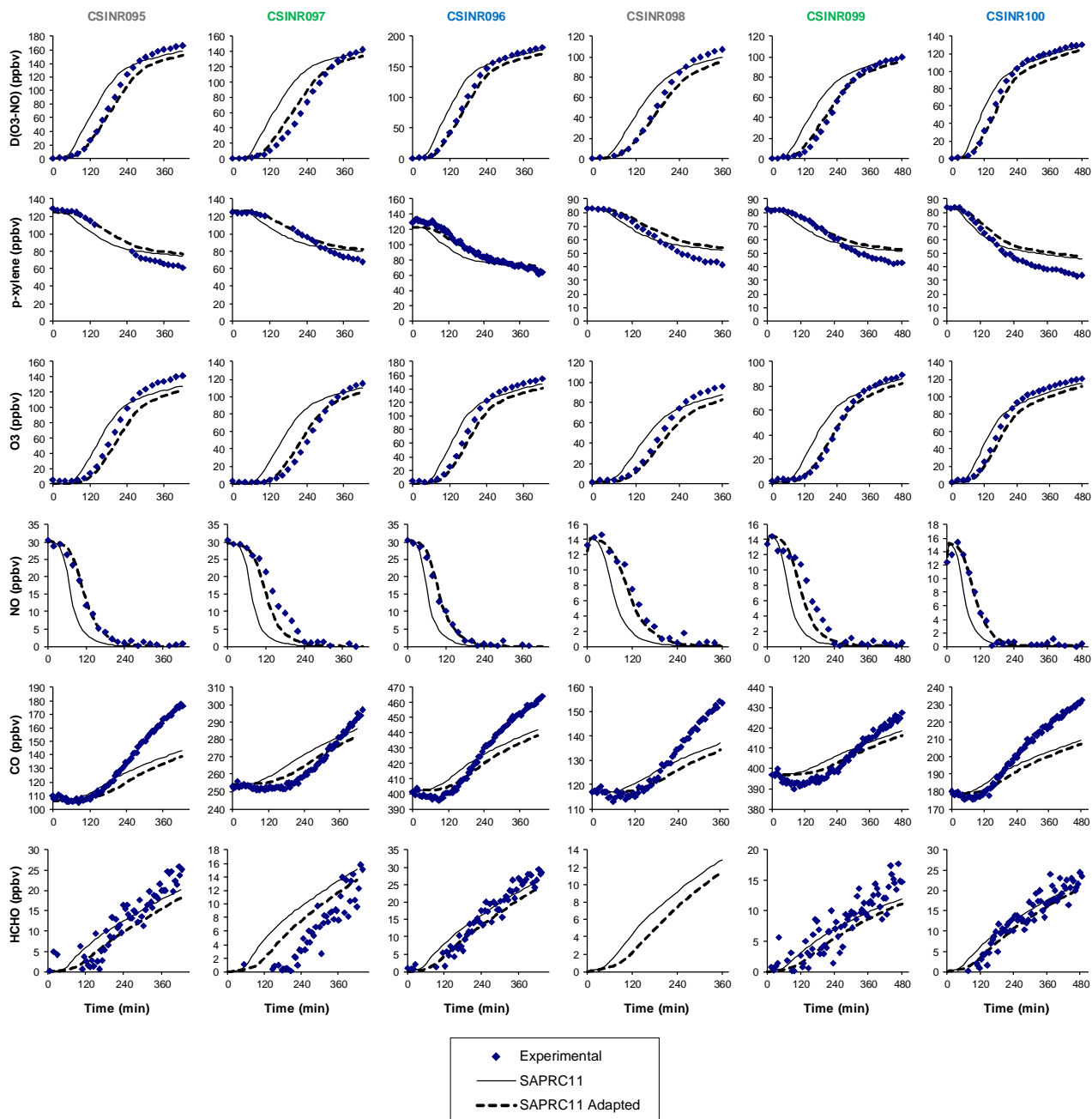


Fig. S4. Predictions of *p*-xylene and key products for 2 sets of 3 x *p*-xylene-NO_x experiments using similar initial concentrations (CSINR095-097; CSINR098-100) but different light sources.

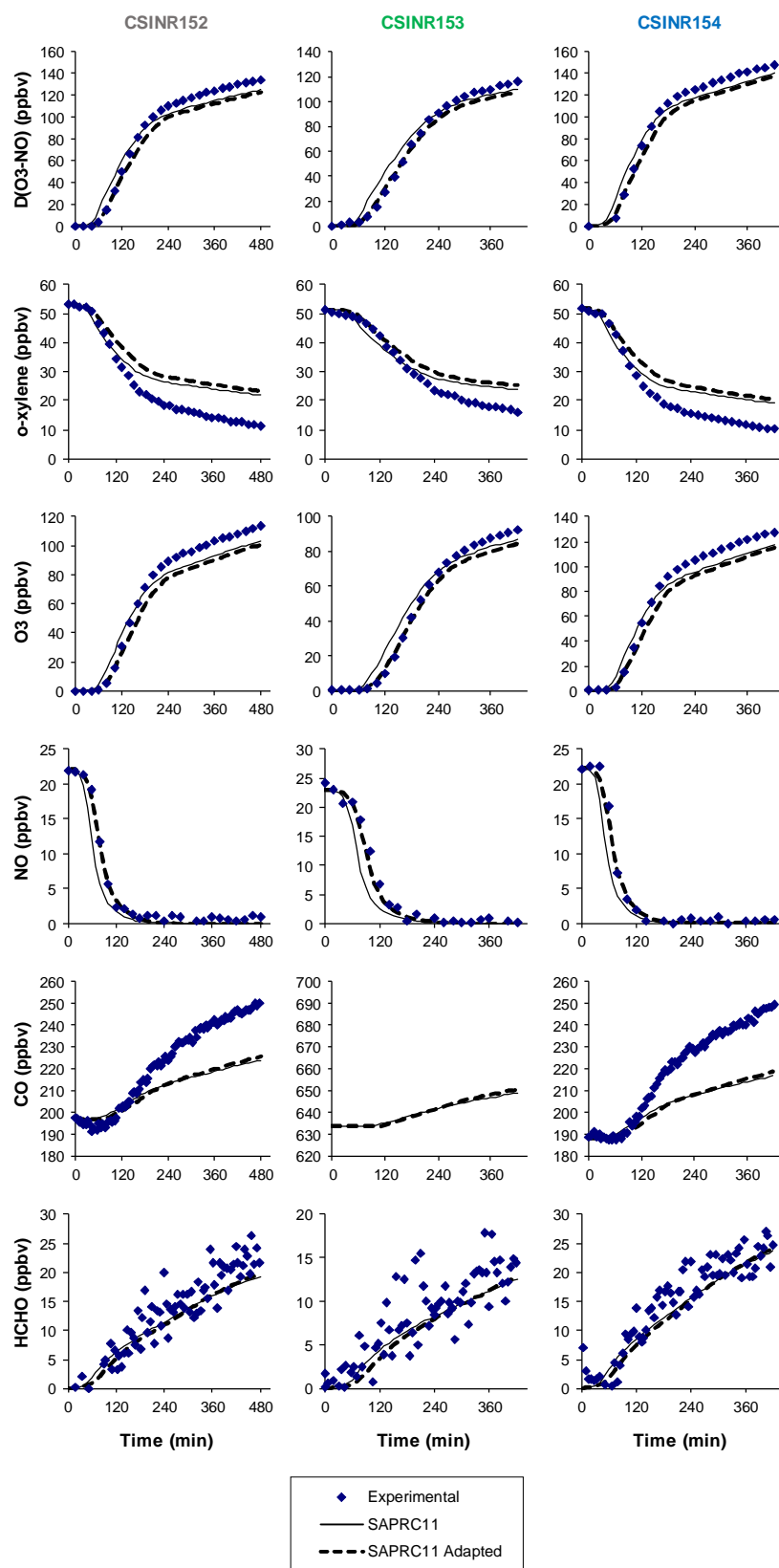


Fig. S5. Predictions of *o*-xylene and key products for 3 x *o*-xylene-NO_x experiments using initial concentrations but different light sources.

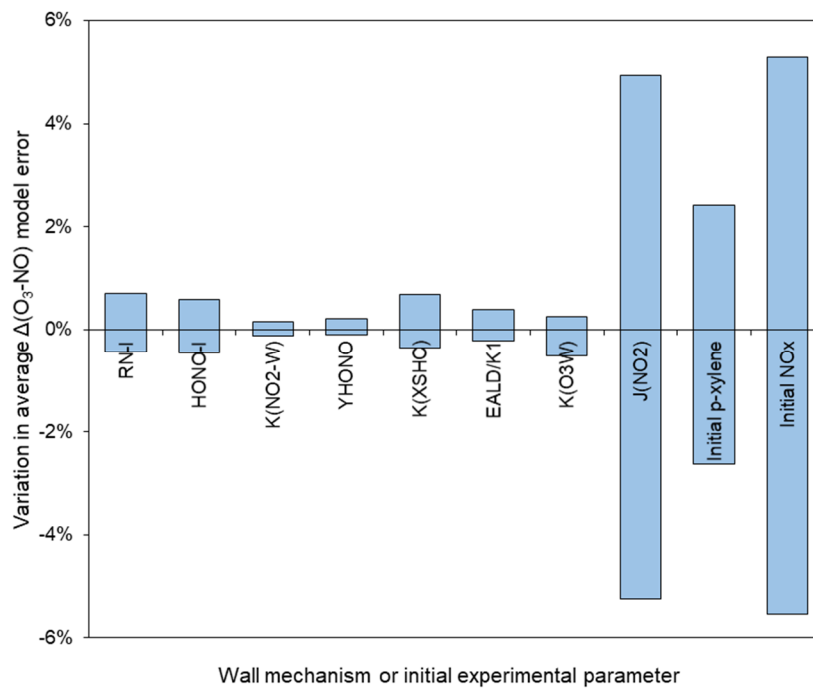


Fig. S6. Variation in mean six hour $\Delta(O_3 - NO)$ model error for the 8 p-xylene-NO_x experiments, with $\pm 50\%$ variation in wall parameters and $\pm 10\%$ variation in J_{NO_2} or initial concentrations.

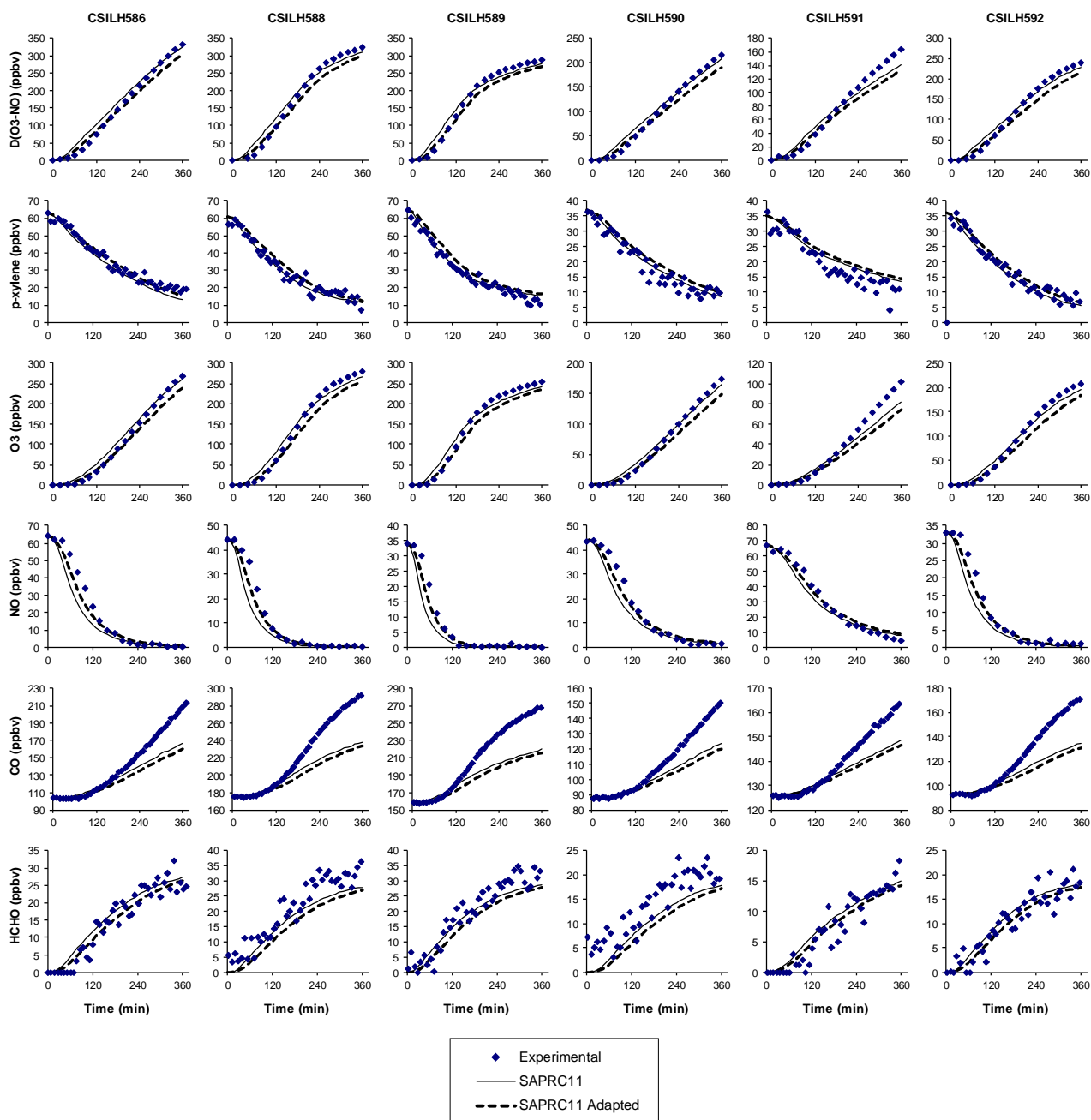


Fig. S7. Predictions of *p*-xylene and key products for $6 \times p$ -xylene-NO_x experiments from the previous CSIRO chamber (Lucas Heights (LH)).

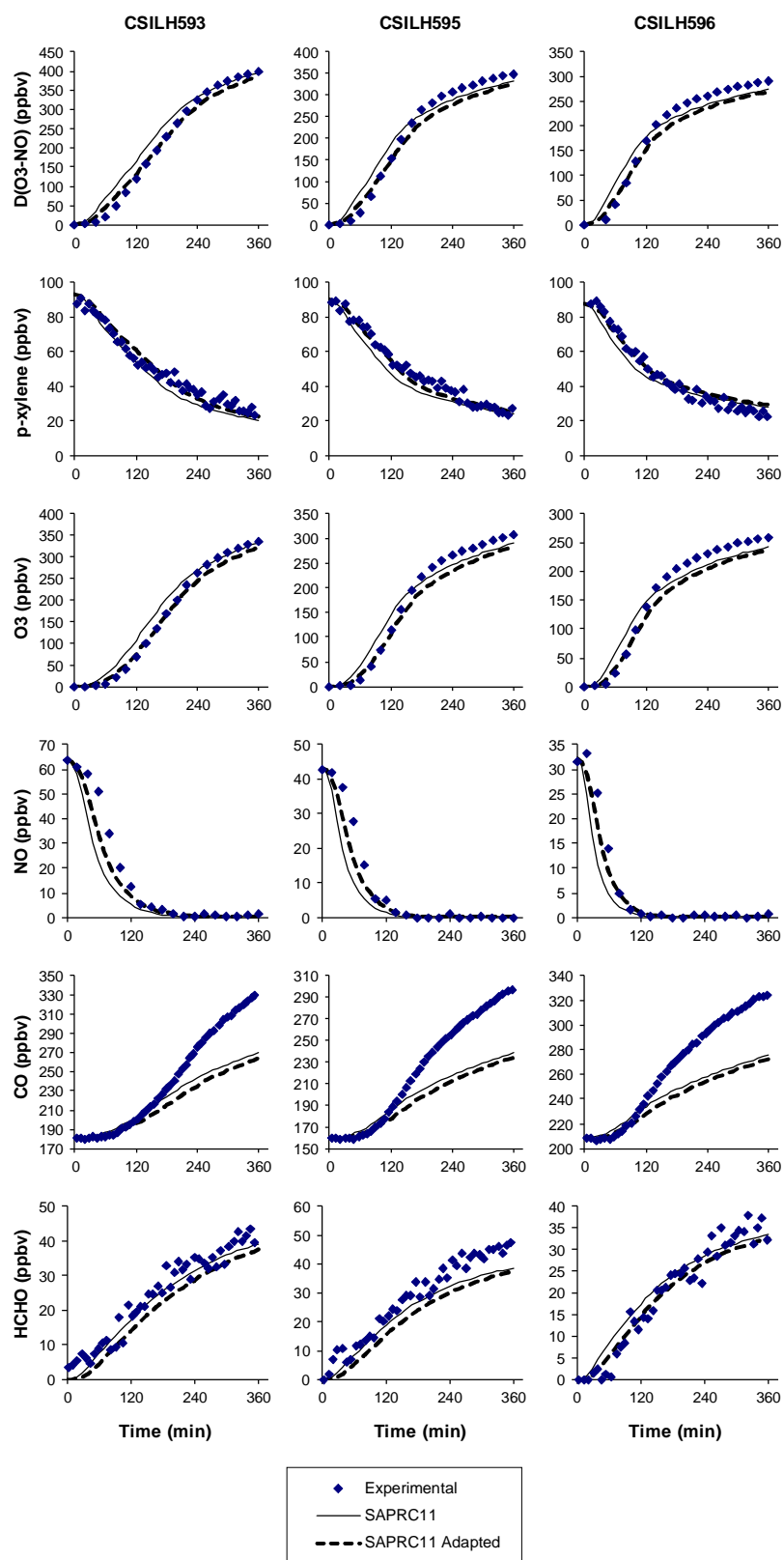


Fig. S8. Predictions of *p*-xylene and key products for 3 of the *p*-xylene-NO_x experiments from the previous CSIRO chamber (LH) with initial *p*-xylene of about 90 ppbv.

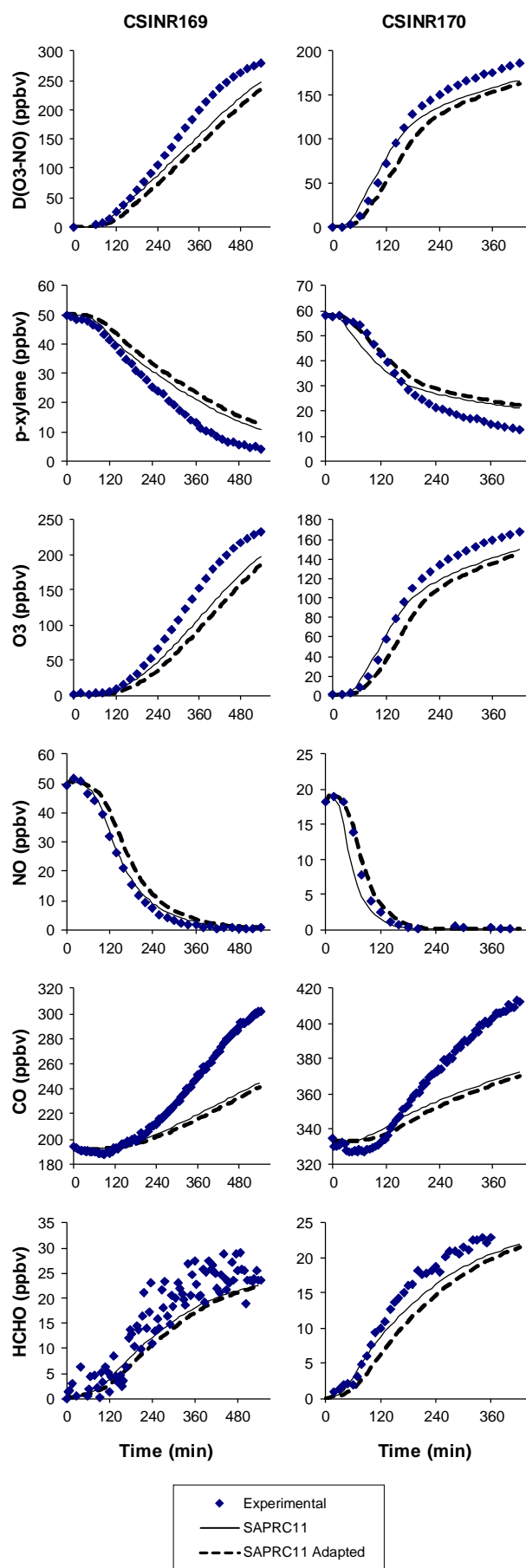
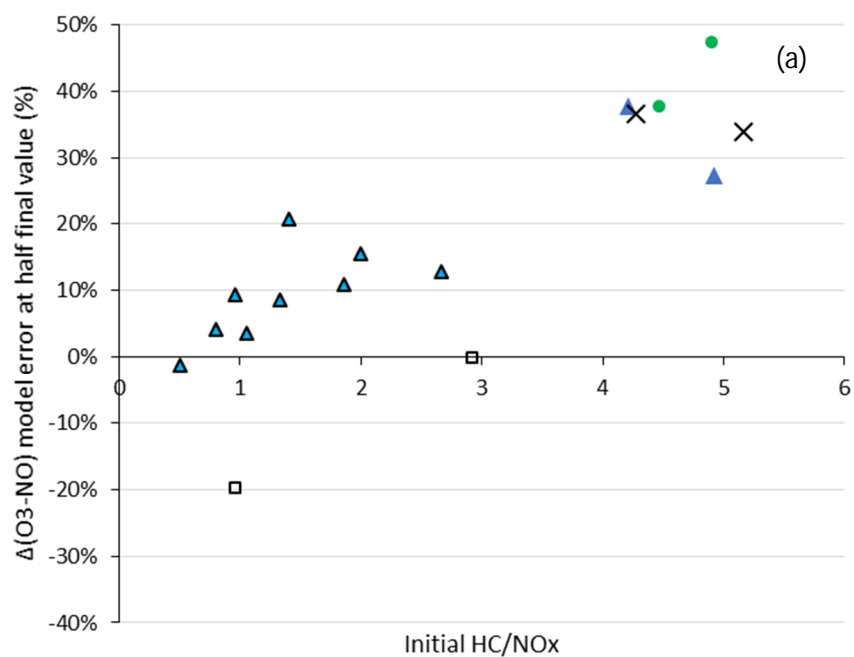
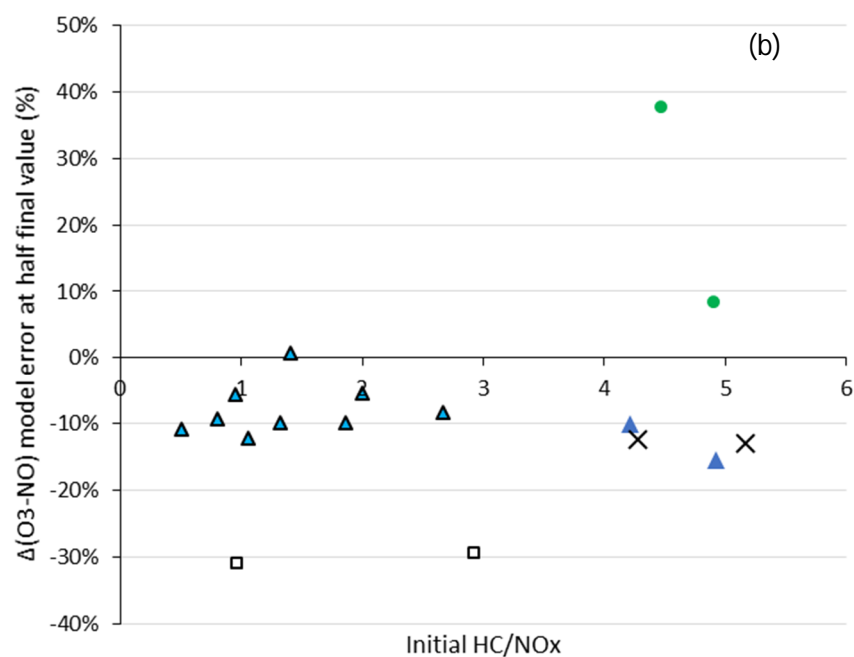


Fig. S9. Predictions of *p*-xylene and key products for 2 x *p*-xylene-NO_x experiments using full mixed light set (compared to Figure S.4).



▲ BLB LH (0.61) □ Full NR (0.44) ▲ BLB NR (0.33) × Half NR (0.24) ● BL NR (0.16)



▲ BLB LH (0.61) □ Full NR (0.44) ▲ BLB NR (0.33) × Half NR (0.24) ● BL NR (0.16)

Fig. S10. $\Delta(\text{O}_3 - \text{NO})$ model error for *p*-xylene experiments when experimental $\Delta(\text{O}_3 - \text{NO})$ is half of the amount at 6 hours for (a) SAPRC-11 mechanism and; (b) Adapted SAPRC-11 mechanism. Light sources: BLB (blue blacklight), BL (350 nm blacklight), Full/half (mixed at different intensities)

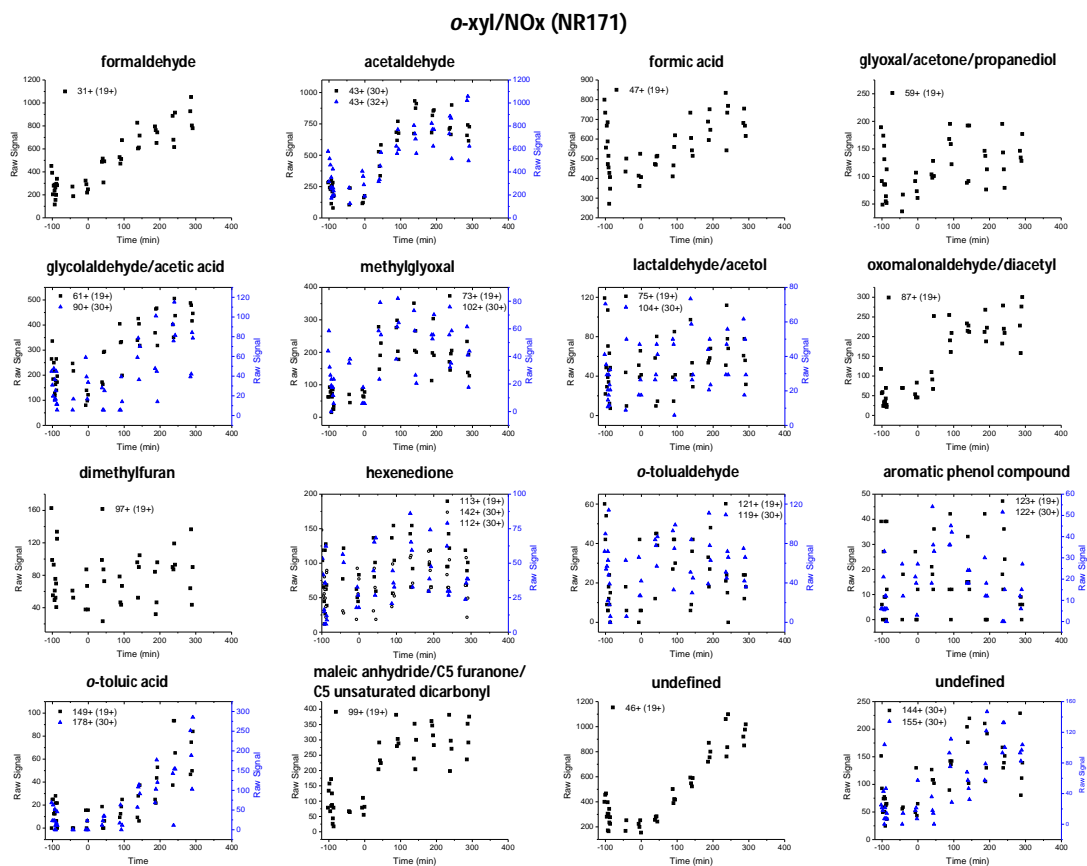
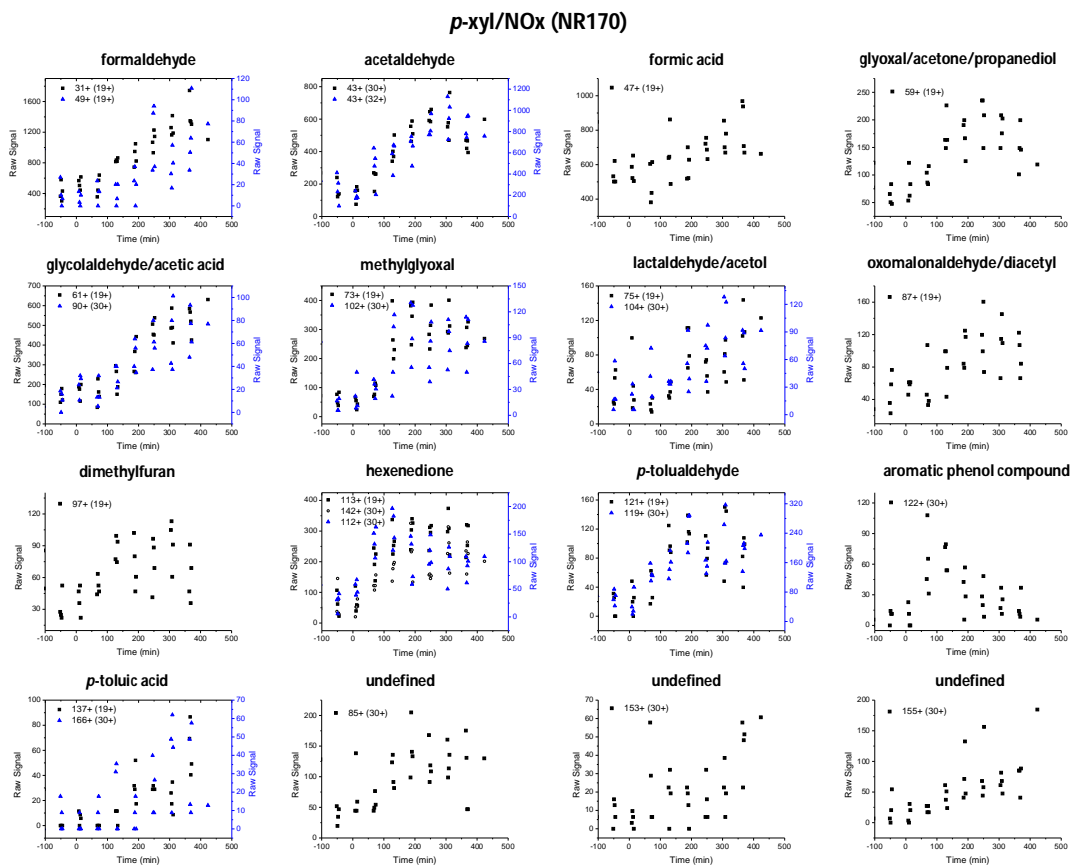


Fig. S11. SIFT-MS peak responses for identified products from periodic full-scan modes for two selected *p*-xylene and *o*-xylene experiments.

References

Azzi M, White S, Angove D, Jamie I, Kaduwela A (2010). Evaluation of the SAPRC-07 mechanism against CSIRO smog chamber data. *Atmospheric Environment* **44**, 1707-1713. doi:10.1016/J.ATMOENV.2010.02.013