

Iteration	Grid	Tested conditions	No. of combinations
Levogluconan			
1	Coarse	α : 0.1, 0.5, 1 C^* ($\mu\text{g m}^{-3}$) : 0.5, 2, 5, 10, 15, 20, 25 m_{wall} (mg m^{-3}) : 1.6, 3.2, 6.4, 12.8, 15, 25 $1/k_{\text{wall/g}}$ (min) : 5, 10, 15, 25, 35, 45, 55, 65, 75, 85, 95 k_{OH} ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) : 5×10^{-12} , 1×10^{-11} , 3×10^{-11} , 5×10^{-11} , 7×10^{-11} , 1×10^{-10}	8316
2	Fine	α : 0.1 C^* ($\mu\text{g m}^{-3}$) : 1, 2, 3, 4, 5, 6, 7, 8, 9, 10 m_{wall} (mg m^{-3}) : 1.6, 3.2, 6.4, 12.8, 15, 25 $1/k_{\text{wall/g}}$ (min) : 5, 10, 15, 20, 25, 30, 35, 40, 45 k_{OH} ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) : 5×10^{-12} , 1×10^{-11} , 3×10^{-11} , 5×10^{-11} , 7×10^{-11} , 1×10^{-10}	2880
3	Ultra-fine	α : 0.1 C^* ($\mu\text{g m}^{-3}$) : 3, 4, 5, 6, 7, 8, 9, 10 m_{wall} (mg m^{-3}) : 1.6, 3.2, 6.4 $1/k_{\text{wall/g}}$ (min) : 10, 15, 20 k_{OH} ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) : 5×10^{-12} , -1×10^{-10} by increments of 5×10^{-12}	1436
Other BBOA markers			
4	Fine	α : 0.1 C^* ($\mu\text{g m}^{-3}$) : 0.5, 2, 5, 10, 15, 20, 25 m_{wall} (mg m^{-3}) : 1.6, 3.2, 6.4, 12.8, 15, 25 $1/k_{\text{wall/g}}$ (min) : 10, 15, 20 k_{OH} ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) : 5×10^{-12} , 1×10^{-11} , 3×10^{-11} , 5×10^{-11} , 7×10^{-11} , 1×10^{-10}	756