Supporting Information for

Understanding the importance of atmospheric transformation in assessing the hazards of liquid crystal monomers

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Figure S1. Comparison between the reaction half-lives of atmospheric photo-oxidation (orange) and biodegradation in surface media (green) of EPPB and EFPT (dark colors) and their transformation products (light colors).



Figure S2. (A) The percentage of transformation products with their persistence, bioaccumulation potential and mobility higher (red), lower (green), and unchanged (grey) relative to the parent LCMs (EPPB and EFPT). Properties within $\pm 10\%$ of the parent LCMs are considered unchanged. (B) The octanol–air (log K_{OA}) and octanol–water (log K_{OW}) partition coefficients for LCMs and their transformation products at a pH of 7. Dark blue, and light blue represent EPPB and its transformation products, respectively. Dark purple and light purple represent EFPT and its transformation products, respectively.

Table S1. Structures of transformation products formed from atmospheric OH oxidation of twoLCMs (EPPB and EFPT).

Product ID	Chemical formula	Proposed chemical structure
E ₀	C ₂₃ H ₃₀	
E ₁	C ₂₃ H ₃₀ O ₂	ООН
E ₂	C ₂₃ H ₃₀ O	OH
E ₃	C ₂₃ H ₂₈ O	
E ₄	$C_{23}H_{28}O_2$	ОН
E ₅	$C_{23}H_{28}O_3$	ООН
E ₆	C ₂₃ H ₃₀ O ₄	ноо оон
E ₇	C ₂₃ H ₃₀ O ₃	HOO_OH
E ₈	C ₂₃ H ₂₈ O ₃	
E9	C ₂₃ H ₂₆ O ₂	

E ₁₀	C ₂₃ H ₂₆ O ₄	О О О О О О О О О О О О О О О О О О О
E ₁₁	C ₂₃ H ₂₆ O ₃	
E ₁₂	C ₂₃ H ₂₄ O ₃	
E ₁₃	$C_{23}H_{28}O_4$	ноо о
E ₁₄	$C_{23}H_{30}O_{6}$	ноо оон
E ₁₅	C ₂₃ H ₃₀ O ₅	ноо оон
E ₁₆	$C_{23}H_{28}O_5$	ноороон
E ₁₇	C ₂₃ H ₃₀ O	HO
E ₁₈	C ₂₃ H ₃₂ O ₃	HO, OOH
E ₁₉	C ₂₃ H ₃₂ O ₂	HO OH
E ₂₀	C ₂₃ H ₃₀ O ₂	HO O

E ₂₁	C ₂₃ H ₃₂ O ₅	HO HOO
E ₂₂	C ₂₃ H ₃₂ O ₄	HO HO HO
E ₂₃	C ₂₃ H ₃₀ O ₄	
E ₂₄	C ₁₉ H ₂₄ O ₂	
E ₂₅	$C_{19}H_{24}O_3$	но
E ₂₆	C ₁₉ H ₂₄ O ₄	
E ₂₇	C ₁₈ H ₂₄ O ₃	но
E ₂₈	$C_{21}H_{28}O_2$	
E ₂₉	$C_{21}H_{28}O_4$	ноо-о
E ₃₀	$C_{21}H_{28}O_3$	но

E ₃₁	C ₂₁ H ₂₆ O ₃	
E ₃₂	C ₂₁ H ₂₆ O ₄	
E ₃₃	C ₂₃ H ₃₄ O ₄	но он но он
E ₃₄	$C_{21}H_{26}O_2$	ООН
E ₃₅	C ₂₁ H ₂₆ O	ОН
E ₃₆	C ₂₁ H ₂₄ O	
E ₃₇	$C_{21}H_{24}O_2$	ОН
E ₃₈	$C_{16}H_{22}O_2$	HO HO
E ₃₉	$C_{16}H_{22}O_4$	о о о о о о о о о о о о о о о о о о о
E ₄₀	$C_{16}H_{20}O_{3}$	HO HO
F ₀	$C_{23}H_{23}F$	F
F ₁	C ₂₃ H ₂₃ FO ₂	F OOH

F ₂	C ₂₃ H ₂₃ FO	F OH
F ₃	C ₂₃ H ₂₁ FO	F C
F_4	$C_{23}H_{21}FO_2$	P O O H
F_5	C ₂₃ H ₂₁ FO ₃	Ф. OD H
F_6	C ₂₃ H ₂₃ FO ₄	F HOO OOH
F_7	C ₂₃ H ₂₃ FO ₃	F HOO OH
F ₈	C ₂₃ H ₂₁ FO ₃	F HOO O
F9	C ₂₃ H ₁₉ FO ₂	P
F ₁₀	C ₂₃ H ₁₉ FO ₃	P H H
F ₁₁	C ₂₃ H ₂₁ FO ₄	F HOO OH
F ₁₂	C ₂₃ H ₂₃ FO ₅	F HOO OOH OH
F ₁₃	C ₂₃ H ₂₁ FO ₅	F HOO OOH

F ₁₄	C ₂₃ H ₂₃ FO	F OH
F ₁₅	C ₂₃ H ₂₅ FO ₃	F HO OOH
F ₁₆	C ₂₃ H ₂₅ FO ₂	F HO OH
F ₁₇	C ₂₃ H ₂₅ FO ₅	HOO
F ₁₈	C ₂₃ H ₂₅ FO ₄	F HO O ^{r0} HO
F ₁₉	C ₂₃ H ₂₃ FO ₄	F HO O
F ₂₀	$C_{21}H_{21}FO_2$	F C
F ₂₁	C ₂₁ H ₂₁ FO ₄	С С С С С С С С С С С С С С С С С С С
F ₂₂	C ₂₁ H ₂₁ FO ₃	F C C C C C C C C C C C C C C C C C C C
F ₂₃	C ₂₁ H ₁₉ FO ₃	

F ₂₄	C ₂₁ H ₁₉ FO ₄	F C C C C C C C C C C C C C C C C C C C
F ₂₅	C ₁₅ H ₁₃ FO ₂	F OH
F ₂₆	C ₁₅ H ₁₁ FO ₃	O = C O H