

## Supplementary Information

### Biotransformation of 8:2 Fluorotelomer Alcohol by Recombinant Human Cytochrome P450s, Human Liver Microsomes and Human Liver Cytosol

Zhong-Min Li<sup>a</sup>, Liang-Hong Guo<sup>a,b\*</sup>, Xiao-Min Ren<sup>a</sup>

<sup>a</sup> State Key Laboratory of Environmental Chemistry and Ecotoxicology, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, P.O. Box 2871, 18 Shuangqing Road, Beijing 100085, China.

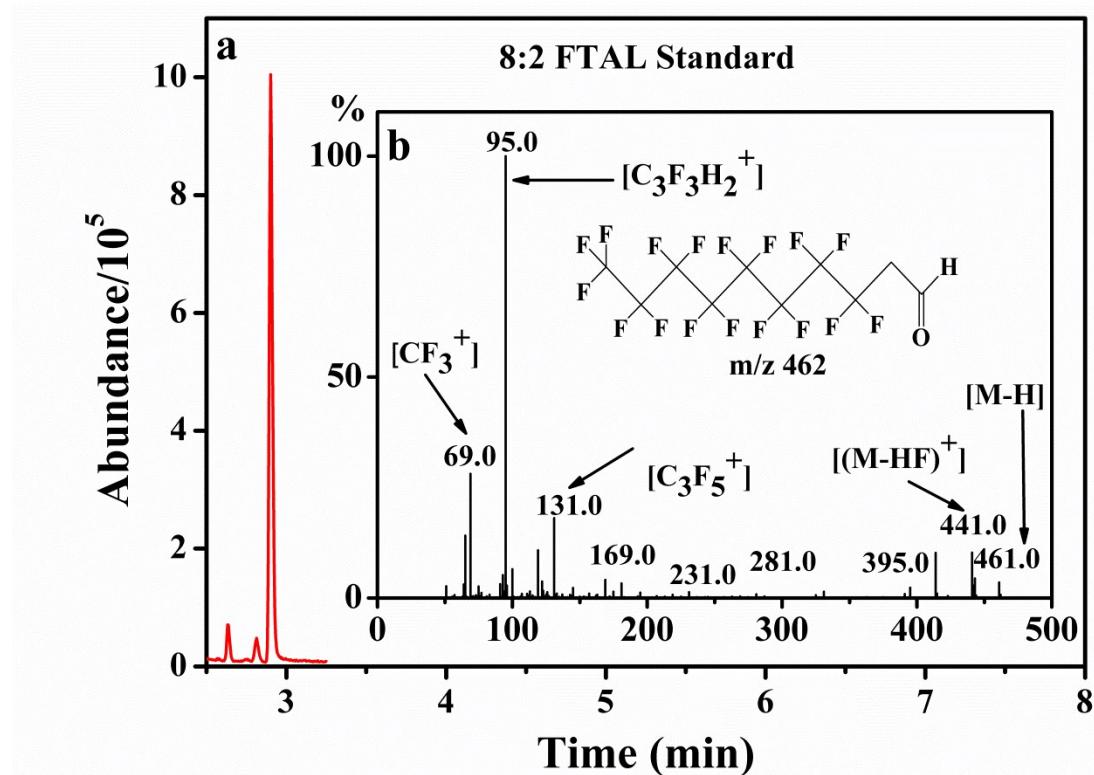
<sup>b</sup> Institute of Environment and Health, Jianghan University, Wuhan, Hubei 430056, China.

#### Corresponding Author

\* Research Center for Eco-environmental Sciences, Chinese Academy of Sciences, 18 Shuangqing Road, P.O. Box 2871, Beijing 100085, P.R. China. Phone & Fax: (86)10-62849685. E-mail: LHGuo@rcees.ac.cn

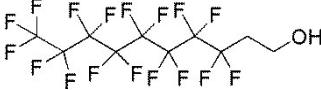
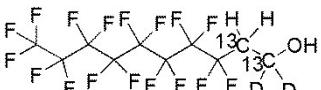
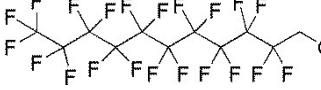
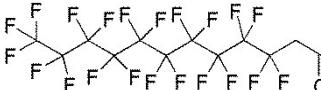
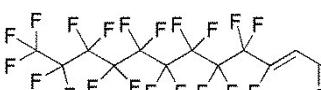
## **TABLE OF CONTENTS**

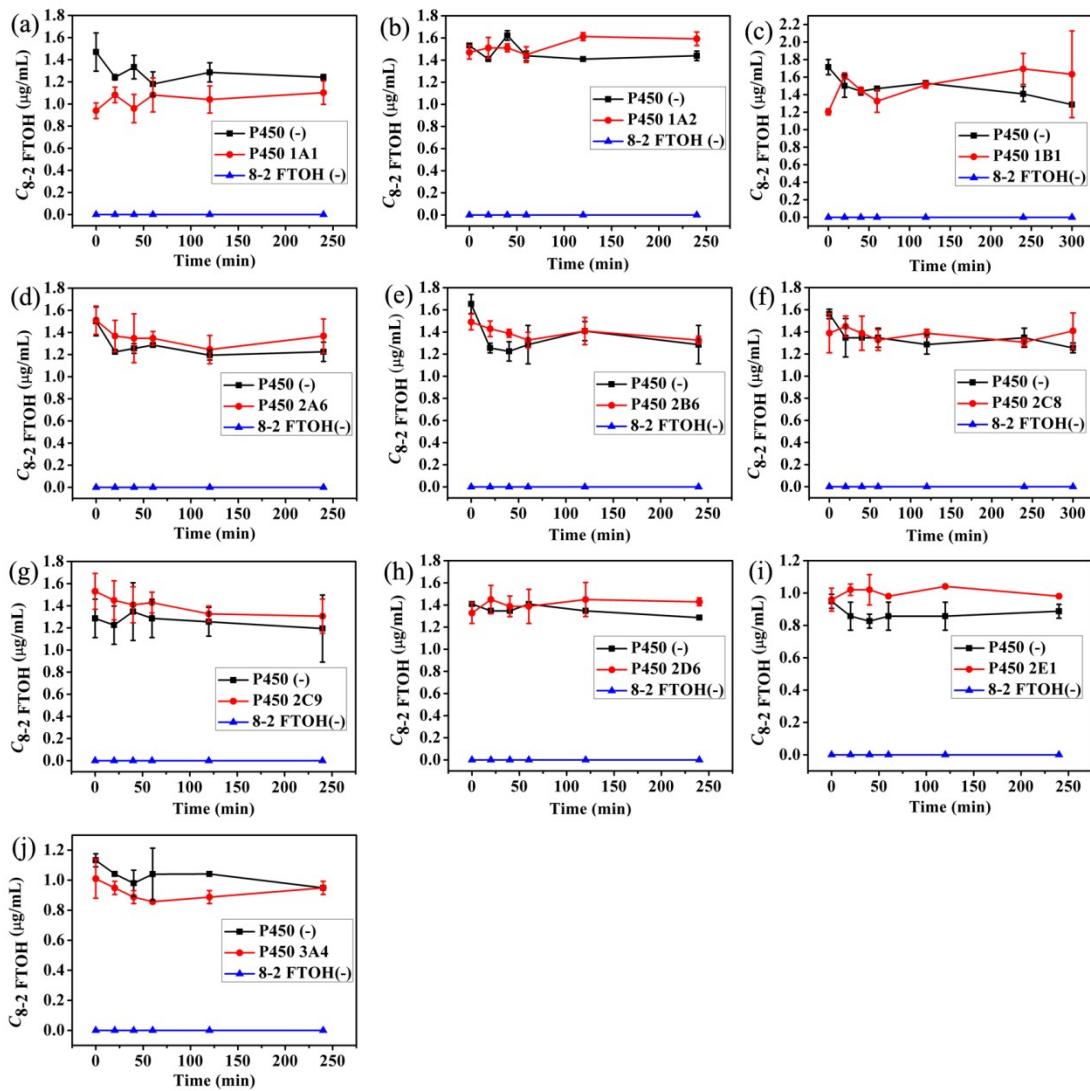
<b>Fig. S1</b> Gas chromatogram (a) and mass spectrum (b) of the synthesized 8:2 FTAL.....	3
<b>Table 1</b> Abbreviations, molecular structures, and molecular weight of 8:2 FTOH and the analogs.....	4
<b>Fig. S2</b> 8:2 FTOH metabolism by various recombinant human CYPs. 4 $\mu$ M 8:2 FTOH incubated with 21.4 pmol/mL (a) CYP1A1, (b) CYP1A2, (c) CYP1B1, (d) CYP2A6, (e) CYP2B6, (f) CYP2C8, (g) CYP2C9, (h) CYP2D6, (i) CYP2E1 and (j) CYP3A4 for up to 4 hr. Samples were prepared in triplicate。 .....	5
<b>Fig. S3</b> HPLC-MS/MS chromatogram of DNPH derivatized 8:2 FTAL standard.....	6
<b>References</b> .....	7



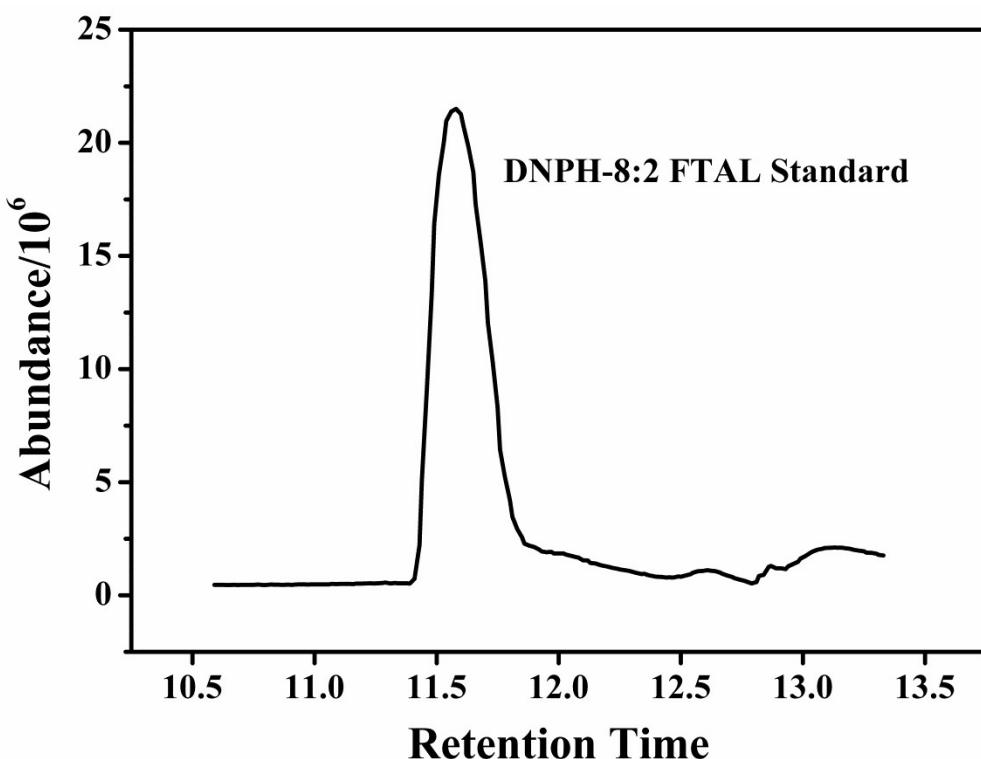
**Fig. S1** Gas chromatogram (a) and mass spectrum (b) of the synthesized 8:2 FTAL (Ions of  $m/z$ : 69 ( $CF_3^+$ ), 95 ( $C_3F_3H_2^+$ ), 131 ( $C_3F_5^+$ ), 441 ( $M-HF$ ) $^+$  and 461  $M^+$  were identified according to Szostek et al.<sup>1</sup>

**Table S1** Abbreviations, molecular structures, and molecular weight of 8:2 FTOH and the analogs.

FTOHs or FTOH analogs	Abbreviation	Molecular Structure	Molecular Weight
8:2 Fluorotelomer Alcohol	8:2 FTOH		464.12
Isotope labeled 8:2 Fluorotelomer Alcohol	m8:2 FTOH		468.12
8:1 Fluorotelomer Alcohol	8:1 FTOH		450.09
8:2 Fluorotelomer Aldehyde	8:2 FTAL		462.10
8:2 Fluorotelomer $\alpha, \beta$ - Unsaturated Aldehyde	8:2 FTUAL		442.10



**Fig. S2** 8:2 FTOH metabolism by various recombinant human CYPs. 4 µM 8:2 FTOH incubated with 21.4 pmol/mL (a) CYP1A1, (b) CYP1A2, (c) CYP1B1, (d) CYP2A6, (e) CYP2B6, (f) CYP2C8, (g) CYP2C9, (h) CYP2D6, (i) CYP2E1 and (j) CYP3A4 for up to 4 hr. Samples were prepared in triplicates.



**Fig. S3** HPLC-MS/MS chromatogram of DNPH derivatized 8:2 FTAL standard.

## **References**

1. B. Szostek and K. B. Prickett, *J. Chromatogr. B*, 2004, **813**, 313-321.