Supporting Information

Uptake, Translocation and Metabolism of 8:2 Fluorotelomer Alcohol in Soybean (*Glycine max* L. Merrill)

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22 This Supporting Information contains 25 pages, 11 tables and 5 figures.

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Enzyme Assays. ADH activity was measured according to the method described by Kimmerer et al.[1] The reaction solution contained 50 mM MES-NaOH, 5 mM $MgCl_2$, 1 mM dithiothreitol, 0.1 mM NADH (β-nicotinamide adenine dinucleotide, reduced form), 4% (v/v) acetaldehyde and 100 μL of the protein extract in a final volume of 2.0 mL. NADH oxidation was monitored at 340 nm at 25 °C for 5 min.

ALDH activity was measured followed the methodology of Liu et al.[2] Briefly, 100 μL of protein extract was added to a reaction mixture containing 1.5 mM NAD (β-nicotinamide adenine dinucleotide, oxidized form) and 0.1 M sodium pyrophosphate buffer (pH 8.5) in a final volume of 1.0 mL. After 30 s of prereaction, 17 mM acetaldehyde was added to the mixture, which was excited at 360 nm, and the emission fluorescence of NADH was recorded at 460 nm at 10 s intervals for up to 2 min.

GST activity was determined based on the method described by Habig et al.[3] The reaction mixture contained 1.0 mM 1-chloro-2,4-dinitrobenzne (CDNB), 5.0 mM glutathione (GSH), and 100 μL of protein extract in phosphate buffered saline (PBS, pH 6.5) in a final volume of 3.0 mL. The change in absorbance of CDNB-GSH conjugate was measured at 25 °C for 5 min at 340 nm. The enzyme activity was calculated using an extinction coefficient of 9.6 $mM^{-1} \cdot cm^{-1}$.

CYP450 activity was determined as following the Plant CYP450 ELISA Kit (Dongge Biotechnology Co. Ltd, Beijing, China). The color change was measured spectrophotometrically at a wavelength of 450 nm. All the enzyme activities are expressed as $U \cdot mg^{-1}$ protein.

Extraction and Cleanup of 8:2 FTOH and Its Degradation Products in Plant Tissues. The analyte extraction and cleanup procedures for the plant samples were as previously described[4] with some modifications. In brief, about 0.1-0.3 g of freeze-dried soybean samples were placed in 15 mL polypropylene (PP) centrifuge tubes, and a suite of isotope-labeled surrogate standards (M8:2 FTOH, M8:2 FTCA, M8:2 FTUCA, MPFBA, MPFHxA, MPFOA, MPFNA) was spiked into the samples prior to extraction. Six mL of methanol was added to the samples. After mixing and shaking for 8 h, the solvents were separated by centrifugation (4000 rpm, 20 min) and then transferred to a second PP tube. The samples were extracted twice with 2 × 6 mL methanol. All organic supernatants of the three extractions were combined and allowed to evaporate under nitrogen to 1.0 mL. Half of the extract (0.5 mL) was placed into a 2 mL disposable PP microcentrifuge tube, which contained 20 mg Envi-Carb graphitized carbon (Supelco, St. Louis, MO) that was treated with 40 μL of 0.1 M NaOH. The tube was capped and vortexed for 1 min, then centrifuged at 12,000 rpm for 30 min at 4 °C. The supernatant was gathered before UPLC-MS/MS analysis for FTOHs (8:2 FTOH and 7:2 sFTOH). The other 0.5 mL extract was diluted with Milli-Q water to a final volume of 15 mL and subjected to solid phase extraction (SPE) cleanup. Before SPE cleanup, the samples were filtered using a 0.45 μm nylon filter (Nylon 66, Tianjin Navigation Instrument Ltd, Tianjin, China) and then passed through Oasis® WAX SPE cartridges (3 cm^3, 60 mg, 30 μm, Waters, Milford, MA, USA) pre-conditioned sequentially with 4 mL of 0.1 % ammonium hydroxide in methanol, 4 mL of methanol, and 4 mL of Milli-Q water. The cartridges were then

washed with 25 mM sodium acetate buffer solution (pH 4) and dried completely under vacuum. The target compounds were eluted by 4 mL of 0.1% ammonium hydroxide in methanol. The elution was concentrated to 0.5 mL under a nitrogen stream. The final extraction was centrifuged (12,000 rpm, 4 °C, 30 min) before UPLC-MS/MS analysis for acid degradation products.

Extraction and Cleanup of 8:2 FTOH and Its Degradation Products in Solution Samples. FTOHs and acid degradation products in solution samples were extracted separately. For FTOHs, 25 mL solutions were transferred into 50 mL PP centrifuge tubes, and M8:2 FTOH was added as surrogate standard to the samples. The solutions were extracted three times with 6 mL of ethyl acetate for 8 h. The combined extracts were allowed to evaporate under a gentle stream of nitrogen to 0.5 mL. The concentrated extractions were diluted 1:2 with methanol and centrifuged (12,000 rpm, 30 min) before UPLC-MS/MS analysis. For acid degradation products, solution samples were extracted with SPE cartridges. Briefly, 40 mL solutions were transferred into 50 mL PP centrifuge tubes, and six isotope-labeled surrogate standards (M8:2 FTCA, M8:2 FTUCA, MPFBA, MPFHxA, MPFOA, MPFNA) were spiked into the samples. The solutions were filtered using a 0.45 μm nylon filter and then passed through Oasis® WAX SPE cartridges as described above. The eluate was concentrated to 0.5 mL and centrifuged (12,000 rpm, 30 min) before UPLC-MS/MS analysis.

Distribution of 8:2 FTOH in unplanted controls. Distribution of 8:2 FTOH in unplanted controls sampled at 144 h was determined. Extractions were carried out for the reactor and the rubber plug after decanting the culture solution. Thirty mL of methanol was added to each reactor after the reactor was rinsed two times with Milli-Q water, and re-sealed with a fresh rubber plug. The removed rubber plug was placed in a sealed container, and extracted with 40 mL of methanol. All reactors and containers were kept in a shaker at 50 ℃ for 48 h. Ten mL of each extract was transferred into a 15 mL PP centrifuge tube, concentrated to 1.0 mL and centrifuged (12,000 rpm, 4 ˚C, 30 min) before determination of 8:2 FTOH and its degradation products.

Effect of Freeze-drying on the Recoveries of 8:2 FTOH and Its Metabolites in Plant Tissues. Six subsamples of homogenized fresh blank soybean tissues (about 1.0 g each) were weighed in 15 mL PP tubes. Three of the subsamples were spiked with 50 μL of 8:2 FTOH and its metabolite mixture solutions (200 $ng \cdot mL^{-1}$ for each analyte in methanol), and aged for 24 h (stored at 4 ℃ to avoid possible degradation). No analytes were added to the other three subsamples. These subsamples were freeze-dried simultaneously for 48 h. Then 8:2 FTOH and its metabolites in all subsamples were extracted with methanol, cleaned up and determined by UPLC-MS/MS. The results are shown in Table S7. The recoveries of 8:2 FTOH and its metabolites in roots, stems and leaves ranged 78.2-95.5%, 77.2-92.8% and 75.9-94.3%, respectively, which did not differ significantly from those of the samples

spiked after freeze-drying (Table S6). No 8:2 FTOH or its metabolites were found in unspiked subsamples (data not shown). These results suggested that compound loss and cross contamination during freeze-drying was negligible.

REFERENCES

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131 **Table S1. Chemical names, acronyms and molecular structures of the poly- and perfluorinated substances described in this paper**

Acronym	Chemical name	Molecular structure
8:2 FTOH	8:2 Fluorotelomer alcohol	$F(CF_2)_8CH_2CH_2OH$
8:2 uFTOH	8:2 Fluorotelomer unsaturated alcohol	$F(CF_2)_7CF=CHCH_2OH$
7:2 sFTOH	7:2 Secondary polyfluorinated alcohol	$F(CF_2)_7CHOHCH_3$
8:2 FTAL	8:2 Fluorotelomer aldehyde	$F(CF_2)_8CH_2CHO$
8:2 FTUAL	8:2 Fluorotelomer unsaturated aldehyde	$F(CF_2)_7CF=CHCHO$
8:2 FTCA	8:2 fluorotelomer saturated carboxylic acid	$F(CF_2)_8CH_2COOH$
8:2 FTUCA	8:2 fluorotelomer unsaturated carboxylic acid	$F(CF_2)_7CF=CHCOOH$
7:3 FTCA	7:3 polyfluorinated acid	$F(CF_2)_7CH_2CH_2COOH$
7:3 FTUCA	7:3 polyfluorinated unsaturated acid	$F(CF_2)_7CH=CHCOOH$
PFBA	Perfluorobutyric acid	$F(CF_2)_3COOH$
PFPeA	Perfluoropentanoic acid	$F(CF_2)_4COOH$
PFHxA	Perfluorohexanoic acid	$F(CF_2)_5COOH$
PFHpA	Perfluoroheptanoic acid	$F(CF_2)_6COOH$
PFOA	Perfluorooctanoic acid	$F(CF_2)_7COOH$
PFNA	Perfluorononanoic acid	$F(CF_2)_8COOH$
Conjugates		
8:2 FTUAL-GSH	8:2 Fluorotelomer unsaturated aldehyde glutathione	$F(CF_2)_7C–[S–(C_{10}H_{16}N_3O_6)]=CHCHO$
8:2 uFTOH-GSH	8:2 Fluorotelomer unsaturated alcohol glutathione	$F(CF_2)_7C–[S–(C_{10}H_{16}N_3O_6)]=CHCH_2OH$
8:2 uFTOH-SCysGly	8:2 Fluorotelomer unsaturated alcohol cysteinylglycine	$F(CF_2)_7C–[S–(C_5H_9N_2O_3)]=CHCH_2OH$
8:2 uFTOH-SCys	8:2 Fluorotelomer unsaturated alcohol cysteine	$F(CF_2)_7C–[S–(C_3H_6NO_2)]=CHCH_2OH$
8:2 uFTOH-SCysNAcetyl	8:2 Fluorotelomer unsaturated alcohol N-acetylcysteine	$F(CF_2)_7C–[S–(C_5H_8NO_3)]=CHCH_2OH$
8:2 FTUCA-GSH	8:2 Fluorotelomer unsaturated acid glutathione	$F(CF_2)_7C–[S–(C_{10}H_{16}N_3O_6)]=CHCOOH$
8:2 FTUCA-SCysGly	8:2 Fluorotelomer unsaturated acid cysteinylglycine	$F(CF_2)_7C-[S–(C_5H_9N_2O_3)]=CHCOOH$
8:2 FTUCA-SCys	8:2 Fluorotelomer unsaturated acid cysteine	$F(CF_2)_7C–[S–(C_3H_6NO_2)]=CHCOOH$

Isotope-labeled standards		
M8:2 FTOH	[1,1-D_2,1,2-$^{13}C_2$] 8:2 FTOH	$F(CF_2)_8{}^{13}CH_2{}^{13}CD_2OH$
M8:2 FTCA	[1,2-$^{13}C_2$] 8:2 FTCA	$F(CF_2)_8{}^{13}CH_2{}^{13}COOH$
M8:2 FTUCA	[1,2-$^{13}C_2$] 8:2 FTUCA	$F(CF_2)_7CF={}^{13}CH{}^{13}COOH$
MPFBA	[1,2,3,4-$^{13}C_4$] PFBA	$F({}^{13}CF_2)_3{}^{13}COOH$
MPFHxA	[1,2-$^{13}C_2$] PFHxA	$F(CF_2)_4{}^{13}CF_2{}^{13}COOH$
MPFOA	[1,2,3,4-$^{13}C_4$] PFOA	$F(CF_2)_4({}^{13}CF_2)_3{}^{13}COOH$
MPFNA	[1,2,3,4,5-$^{13}C_5$]PFNA	$F(CF_2)_4({}^{13}CF_2)_4{}^{13}COOH$

Table S2. 1/4-strength Hoagland nutrient solution recipe used in the study (pH = 6.0, Eh = 280 mV) [a]

Component	Molecular weight	Conc. of stock solution (M)	Conc. of stock solution (g/L)	Volume of stock solution per liter of final solution (mL)	Element	Final conc. of element in nutrient solution (ppm)
Macronutrients						
KNO_3	101.10	0.5	50.6	2.5	K	58.7
$Ca(NO_3)_2 \cdot 4H_2O$	236.15	0.5	118	2.5	Ca	50
NH_4NO_3	80.04	0.1	8	2.5	N	59.5
KH_2PO_4	136.09	0.1	13.6	2.5	P	7.75
$MgSO_4 \cdot 7H_2O$	246.47	0.2	49.3	2.5	Mg	12
					S	16
Iron (Fe-EDTA)				0.25	Fe	0.28
$FeSO_4 \cdot 7H_2O$	278.05		5.57			
EDTA·2Na	372.24		7.45			
Micronutrients				0.25		
H_3BO_3	61.83		2.86		B	0.125
$MnCl_2 \cdot 4H_2O$	197.91		1.81		Mn	0.125
$ZnSO_4 \cdot 7H_2O$	287.56		0.22		Zn	0.0125
$CuSO_4$	159.61		0.051		Cu	0.005
$Na_2MoO_4 \cdot 2H_2O$	241.95		0.025		Mo	0.0025

[a] Eh = oxidation-reduction potential.

Table S3. Instrumental method for the analysis of 8:2 FTOH and 7:2 sFTOH by UPLC-MS/MS

Instrument	Waters ultra-performance liquid chromatography system coupled to a Xevo TQS tandem mass spectrometer with an electrospray ionization interface. The mass spectrometer was operated in the negative ion multiple reaction-monitoring mode.			
Analytical Column	Waters ACQUITY UPLC BEH Shield RP18 column (1.7 μm particles, 150 mm × 2.1 mm)			
Column Temperature	35 °C			
Mobile Phases	A: methanol B: 1 mM ethanolamine in water			
Gradient Profile	Time (min)	Percentage A (%)	Flow Rate (mL/min)	
	0.0	50	0.15	
	1.0	85	0.15	
	6.0	85	0.15	
	6.5	50	0.15	
	10.0	50	0.15	
Injection Volume	5 μL			
Monitored Ion Transitions for Analytes	Analytes	Ion Transitions	Cone Voltage (V)	Collision Energy (eV)
	8:2 FTOH	462.97 > 355.00	14	18
	7:2 sFTOH	393.00 >219.00	20	15
	M8:2 FTOH	467.03 > 356.02	12	22
MS Parameters	Capillary Voltage (kV) = 2.6	Desolvation Temperature (°C) = 350		
	Source Temperature (°C) = 120			
	Cone Gas Flow (L/Hr) = 50	Desolvation Gas Flow (L/Hr) = 600		

Table S4. Instrumental method for the analysis of acid degradation products by UPLC-MS/MS

Instrument	Waters ultra-performance liquid chromatography system coupled to a Xevo TQS tandem mass spectrometer with an electrospray ionization interface. The mass spectrometer was operated in the negative ion multiple reaction-monitoring mode.			
Analytical Column	Waters ACQUITY UPLC BEH C18 column (1.7 μm particles, 50 mm × 2.1 mm)			
Column Temperature	35 °C			
Mobile Phases	A: acetonitrile B: 0.15% acetic acid in water			
Gradient Profile	Time (min)	Percentage A (%)	Flow Rate (mL/min)	
	0.0	5	0.40	
	2.5	60	0.40	
	4.0	60	0.40	
	4.5	5	0.40	
	6.0	5	0.40	
Injection Volume	5 μL			
Monitored Ion Transitions for 8:2 FTOH Degradation	Analytes	Ion Transitions	Cone Voltage (V)	Collision Energy (eV)
	8:2 FTCA	476.97 > 393.05	14	22
	8:2 FTUCA	456.97 > 393.02	16	12
	7:3 FTCA	441.03 > 337.04	22	14
	PFBA	212.97 > 169.03	16	8
	PFPeA	262.97 > 219.03	14	6
	PFHxA	312.97 > 269.03	12	12
	PFHpA	362.97 > 319.04	14	12
	PFOA	412.97 > 368.97	16	8
	PFNA	462.97 > 419.04	14	8
	M8:2 FTCA	478.97 > 394.05	14	22
	M8:2 FTUCA	458.97 > 394.05	18	18
	MPFBA	216.97 > 172.05	14	8
	MPFHxA	314.97 > 270.05	14	8
	MPFOA	416.97 > 372.06	14	10
	MPFNA	467.97 > 423.00	16	6
MS Parameters	Capillary Voltage (kV) = 3.0		Desolvation Temperature (°C) = 350	
	Source Temperature (°C) = 150			
	Cone Gas Flow (L/Hr) = 50		Desolvation Gas Flow (L/Hr) = 600	

141 **Table S5. Instrumental method for the analysis of GSH-conjugated metabolites**
142 **by UPLC-MS/MS**

Instrument	Waters ultra-performance liquid chromatography system coupled to a Xevo TQS tandem mass spectrometer with an electrospray ionization interface. The mass spectrometer was operated in the negative ion MS/MS mode (daughter scan, parent scan, or multiple reaction monitoring).			
Analytical Column	Waters ACQUITY UPLC BEH Shield RP18 column (1.7 μm particles, 150 mm × 2.1 mm)			
Column Temperature	35 ˚C			
Mobile Phases	A: methanol B: 2 mM ammonium acetate			
Gradient Profile	Time (min)	Percentage A (%)	Flow Rate (mL/min)	
	0.0	50	0.15	
	1.5	85	0.15	
	5.0	85	0.15	
	5.5	50	0.15	
	8.0	50	0.15	
Injection Volume	5 μL			
Monitored Ion Transitions for Analytes in MRM mode	Analytes	Ion Transitions	Cone Voltage (V)	Collision Energy (eV)
	8:2 uFTOH-SCysNAcetyl	586 > 475	20	15
	8:2 FTUCA-SCys	558 > 471	20	15
MS Parameters	Capillary Voltage (kV) = 2.6	Desolvation Temperature (˚C) = 350		
	Source Temperature (˚C) = 120			
	Cone Gas Flow (L/Hr) = 50	Desolvation Gas Flow (L/Hr) = 600		

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144 **Table S6. Isotope-labeled compounds used for quantification of analytes**.

Isotope-labeled compound	Analyte quantified using specified isotope-labeled compound	Recovery (%)			
		Soybean tissues			Solution samples
		roots	stems	leaves	
M8:2 FTOH	8:2 FTOH, 7:2 sFTOH	83.8-101.6	86.5-105.4	79.7-107.8	73.9-94.0
M8:2 FTCA	8:2 FTCA, 7:3 FTCA	73.8-86.2	72.1-87.5	68.2-85.7	72.4-90.5
M8:2 FTUCA	8:2 FTUCA	85.4-106.1	79.5-104.3	88.9-102.2	86.2-111.6
MPFBA	PFBA	82.5-94.3	79.4-96.7	72.1-92.2	79.3-105.2
MPFHxA	PFPeA, PFHxA	72.9-91.5	77.2-93.0	78.4-93.6	71.7-96.7
MPFOA	PFHpA, PFOA	86.3-97.4	84.4-100.7	80.8-99.5	83.6-97.6
MPFNA	PFNA	82.1-98.3	80.5-94.4	76.1-92.0	80.3-93.1

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Table S7. Effect of freeze-drying on the recoveries of 8:2 FTOH and its metabolites in plant roots, stems and leaves (%)

Analyte	Spiked freeze-drying tissues		
	roots	stems	leaves
8:2 FTOH	91.6 ± 4.8 [a]	90.5 ± 4.9	87.3 ± 3.7
7:2 sFTOH	88.2 ± 7.2	89.4 ± 3.2	90.4 ± 5.1
8:2 FTCA	80.2 ± 1.7	77.2 ± 4.7	78.8 ± 3.5
8:2 FTUCA	95.1 ± 3.0	92.5 ± 7.6	94.3 ± 4.2
7:3 FTCA	78.2 ± 4.5	78.4 ± 5.1	75.9 ± 8.2
PFBA	87.1 ± 4.1	83.2 ± 4.0	83.1 ± 4.6
PFPeA	85.7 ± 3.8	86.6 ± 4.4	83.9 ± 4.9
PFHxA	84.3 ± 6.8	85.3 ± 5.4	86.8 ± 3.6
PFHpA	93.9 ± 6.2	92.8 ± 2.5	91.6 ± 4.7
PFOA	95.5 ± 4.6	91.1 ± 7.4	92.8 ± 6.8
PFNA	91.9 ± 3.3	85.3 ± 5.0	79.0 ± 7.1

[a] Standard deviation for triplicate measurements.

Table S8. Limits of detection (LODs) and quantification (LOQs) in soybean tissues and in nutrient solution. Values in ng/g dry weight and ng/L.

Analyte	Soybean tissues		Solution	
	LOD	LOQ	LOD	LOQ
8:2 FTOH	0.44	1.46	2.20	7.33
7:2 sFTOH	0.14	0.44	1.50	5.00
8:2 FTCA	0.22	0.70	1.02	3.40
8:2 FTUCA	0.06	0.20	0.35	1.17
7:3 FTCA	0.08	0.26	0.38	1.25
PFBA	0.24	0.80	0.75	2.50
PFPeA	0.12	0.40	0.65	2.17
PFHxA	0.08	0.26	0.50	1.67
PFHpA	0.08	0.26	0.50	1.67
PFOA	0.12	0.40	0.75	2.50
PFNA	0.18	0.58	0.88	2.93

153 **Table S9. Distribution of 8:2 FTOH in unplanted controls at 144 h**

sample type	concentration ($nmol \cdot L^{-1}$)	mol % of initial mass	Recovery (mol %)
Solution	38.5 ± 7.2 [a]	23.1 ± 4.3	
Adsorbed to the reactor	-	0.27 ± 0.10	38.0
Adsorbed to rubber plug	-	14.6 ± 2.7	

154 [a] Standard deviation for triplicate measurements.

Table S10. Mass composition of 8:2 FTOH and quantified metabolites in different samples during exposure time [a]

Samples	Sample type	8:2 FTOH (mol %)	8:2 FTCA (mol %)	8:2 FTUCA (mol %)	7:2 sFTOH (mol %)	7:3 FTCA (mol %)	PFOA (mol %)	PFHpA (mol %)	PFHxA (mol %)	Recovery (mol %)	
Whole soybean	solution	21.95 ± 2.12 [b]	11.21 ± 1.53	1.67 ± 0.23	1.52 ± 0.53	1.65 ± 0.001	0.277 ± 0.052	0.025 ± 0.007	< LOD	38.31	46.3
system (12 h)	root	3.41 ± 0.56	2.75 ± 0.66	0.334 ± 0.053	0.637 ± 0.354	0.621 ± 0.007	0.060 ± 0.037	< LOD	< LOD	7.81	
	stem A	0.085 ± 0.022	0.042 ± 0.014	0.009 ± 0.002	0.010 ± 0.003	0.015 ± 0.007	0.0028 ± 0.00006	< LOD	< LOD	0.164	
	stem B	0.007 ± 0.003	0.0010 ± 0.0003	0.0003 ± 0.00006	0.0015 ± 0.0005	0.0005 ± 0.0003	0.0008 ± 0.0003	< LOD	< LOD	0.011	
	leaf	0.020 ± 0.007	0.0008 ± 0.0003	0.0001 ± 0.00001	0.0037 ± 0.0012	0.0008 ± 0.0003	0.0019 ± 0.0012	< LOD	< LOD	0.027	
Whole soybean	solution	3.89 ± 0.40	18.84 ± 2.78	4.20 ± 0.56	2.73 ± 1.91	2.94 ± 0.54	0.789 ± 0.122	0.037 ± 0.007	0.022 ± 0.004	33.45	44.0
system (24 h)	root	4.41 ± 0.31	3.48 ± 0.28	0.404 ± 0.026	1.09 ± 0.14	0.714 ± 0.104	0.089 ± 0.022	< LOD	< LOD	10.19	
	stem A	0.170 ± 0.035	0.081 ± 0.028	0.012 ± 0.002	0.021 ± 0.003	0.017 ± 0.005	0.0084 ± 0.0004	< LOD	< LOD	0.310	
	stem B	0.009 ± 0.0004	0.0015 ± 0.0010	0.0001 ± 0.00005	0.0019 ± 0.0003	0.0010 ± 0.0001	0.0015 ± 0.0006	< LOD	< LOD	0.015	
	leaf	0.028 ± 0.007	0.0012 ± 0.0001	0.0003 ± 0.00005	0.0061 ± 0.0023	0.0009 ± 0.0005	0.0036 ± 0.0009	< LOD	< LOD	0.040	
Whole soybean	solution	1.25 ± 0.09	9.34 ± 2.64	2.50 ± 0.67	6.47 ± 1.35	4.74 ± 0.44	1.43 ± 0.21	0.231 ± 0.101	0.086 ± 0.005	26.05	32.2
system (48 h)	root	1.88 ± 0.13	0.999 ± 0.380	0.252 ± 0.012	1.80 ± 0.33	0.765 ± 0.039	0.133 ± 0.014	0.0054 ± 0.0021	< LOD	5.83	
	stem A	0.095 ± 0.017	0.027 ± 0.007	0.007 ± 0.001	0.021 ± 0.005	0.042 ± 0.007	0.013 ± 0.002	< LOD	< LOD	0.206	
	stem B	0.014 ± 0.001	0.0049 ± 0.0017	0.0009 ± 0.0001	0.0044 ± 0.0005	0.0051 ± 0.0008	0.005 ± 0.003	< LOD	< LOD	0.035	
	leaf	0.012 ± 0.002	0.0037 ± 0.0004	0.0008 ± 0.0001	0.0075 ± 0.0019	0.0026 ± 0.0006	0.017 ± 0.006	< LOD	< LOD	0.044	
Whole soybean	solution	0.734 ± 0.103	2.99 ± 0.77	2.63 ± 0.23	8.41 ± 1.59	7.23 ± 1.05	2.40 ± 0.05	0.412 ± 0.303	0.137 ± 0.080	24.94	29.3
system (72 h)	root	1.09 ± 0.25	0.262 ± 0.095	0.221 ± 0.011	1.39 ± 0.06	0.833 ± 0.017	0.221 ± 0.012	0.011 ± 0.001	0.0023 ± 0.0013	4.03	
	stem A	0.119 ± 0.018	0.020 ± 0.003	0.009 ± 0.003	0.029 ± 0.005	0.075 ± 0.019	0.020 ± 0.001	< LOD	< LOD	0.272	
	stem B	0.010 ± 0.001	0.0053 ± 0.0010	0.0015 ± 0.0008	0.0049 ± 0.0006	0.010 ± 0.003	0.0054 ± 0.0004	< LOD	< LOD	0.037	
	leaf	0.015 ± 0.005	0.0018 ± 0.0001	0.0005 ± 0.0003	0.0064 ± 0.0024	0.0033 ± 0.0008	0.041 ± 0.009	< LOD	< LOD	0.068	
Whole soybean	solution	0.412 ± 0.142	0.145 ± 0.037	0.662 ± 0.229	5.79 ± 1.92	5.82 ± 1.10	4.01 ± 0.93	0.583 ± 0.207	0.161 ± 0.011	17.58	22.4
system (96 h)	root	0.135 ± 0.003	0.036 ± 0.002	0.121 ± 0.048	1.74 ± 0.16	1.86 ± 0.12	0.500 ± 0.214	0.020 ± 0.006	0.0062 ± 0.0004	4.42	
	stem A	0.043 ± 0.002	0.0062 ± 0.0008	0.0032 ± 0.0003	0.025 ± 0.004	0.119 ± 0.022	0.025 ± 0.0001	< LOD	< LOD	0.221	

		stem B	0.007 ± 0.0003	0.0028 ± 0.0001	0.0012 ± 0.0001	0.0054 ± 0.0013	0.030 ± 0.002	0.0067 ± 0.0015	< LOD	< LOD	0.054	
		leaf	0.014 ± 0.002	0.0018 ± 0.0001	< LOD	0.0068 ± 0.0015	0.0059 ± 0.0008	0.094 ± 0.026	< LOD	< LOD	0.123	
Whole soybean		solution	0.064 ± 0.010	0.025 ± 0.008	0.038 ± 0.015	0.746 ± 0.154	3.32 ± 0.79	5.00 ± 1.12	0.656 ± 0.079	0.213 ± 0.051	10.06	15.0
system (144 h)		root	0.099 ± 0.040	0.013 ± 0.002	0.017 ± 0.002	1.37 ± 0.06	2.00 ± 0.59	0.808 ± 0.205	0.031 ± 0.012	0.011 ± 0.0004	4.35	
		stem A	0.032 ± 0.010	0.0031 ± 0.0006	0.0019 ± 0.0006	0.022 ± 0.007	0.185 ± 0.048	0.041 ± 0.010	< LOD	< LOD	0.284	
		stem B	0.008 ± 0.002	0.0008 ± 0.00004	0.0008 ± 0.0001	0.0073 ± 0.0009	0.058 ± 0.010	0.012 ± 0.002	< LOD	< LOD	0.086	
		leaf	0.013 ± 0.005	< LOD	< LOD	0.0058 ± 0.0010	0.0091 ± 0.0030	0.147 ± 0.020	< LOD	< LOD	0.175	
Ethanol-washed		solution	0.501 ± 0.024	0.980 ± 0.488	2.20 ± 0.28	3.05 ± 0.48	2.48 ± 0.18	3.41 ± 0.59	0.187 ± 0.050	0.047 ± 0.028	12.86	17.2
controls (144 h)		root	0.322 ± 0.014	0.224 ± 0.074	0.184 ± 0.030	0.924 ± 0.237	0.711 ± 0.157	0.412 ± 0.064	0.0081 ± 0.0022	0.0032 ± 0.0011	2.79	
		stem A	0.122 ± 0.001	0.069 ± 0.028	0.0089 ± 0.0041	0.022 ± 0.004	0.287 ± 0.011	0.142 ± 0.044	< LOD	< LOD	0.65	
		stem B	0.042 ± 0.006	0.062 ± 0.028	0.0091 ± 0.0042	0.022 ± 0.005	0.208 ± 0.006	0.036 ± 0.003	< LOD	< LOD	0.38	
		leaf	0.027 ± 0.007	0.009 ± 0.003	0.0009 ± 0.0004	0.0059 ± 0.0012	0.016 ± 0.009	0.434 ± 0.037	< LOD	< LOD	0.49	
Root	12 h	solution	49.57 ± 3.60	12.13 ± 3.71	2.51 ± 0.10	1.05 ± 0.11	1.91 ± 0.49	0.052 ± 0.004	0.086 ± 0.005	< LOD	67.3	
exudate	24 h	solution	26.52 ± 6.18	18.14 ± 2.17	6.82 ± 1.35	3.16 ± 0.77	4.87 ± 0.83	0.190 ± 0.058	0.431 ± 0.142	0.025 ± 0.007	60.2	
controls	48 h	solution	13.00 ± 3.64	22.87 ± 3.10	9.72 ± 1.97	5.01 ± 1.31	6.30 ± 1.43	0.489 ± 0.131	0.653 ± 0.008	0.104 ± 0.006	58.1	
	72 h	solution	8.06 ± 2.70	8.32 ± 0.97	13.55 ± 2.62	9.74 ± 1.97	9.66 ± 0.83	0.636 ± 0.034	1.28 ± 0.52	0.157 ± 0.043	51.4	
	96 h	solution	3.40 ± 1.16	2.30 ± 0.11	10.98 ± 0.71	12.24 ± 3.82	13.91 ± 1.90	0.733 ± 0.143	2.08 ± 0.65	0.180 ± 0.067	45.8	
	144 h	solution	0.707 ± 0.317	0.240 ± 0.054	8.86 ± 1.74	14.13 ± 1.50	14.37 ± 1.68	1.05 ± 0.27	2.54 ± 0.73	0.246 ± 0.012	42.1	

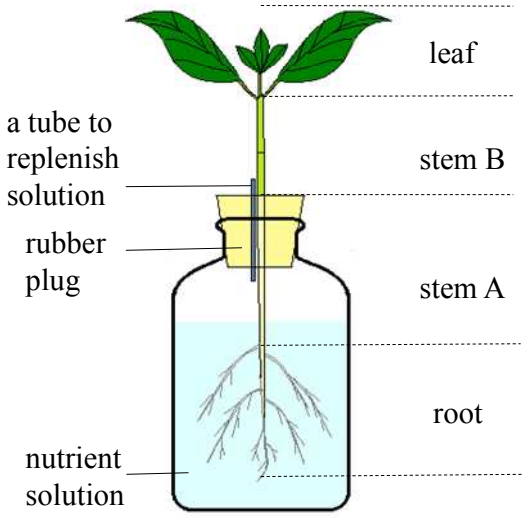
156 [a] The percentage of 8:2 FTOH and metabolites in the solution and soybean to the initial amount of 8:2 FTOH applied.

157 [b] Standard deviation for triplicate measurements.

158 **Table S11. Estimates of kinetic parameters for 8:2 FTOH decreases**

Sample type	k (h^{-1})	R^2	P value
Whole soybean systems	0.081 ± 0.012	0.978	0.0002
Root exudate controls	0.033 ± 0.002	0.987	0.0003

159



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161 **Figure S1.** Scheme of hydroponic exposure reactor and sampling.

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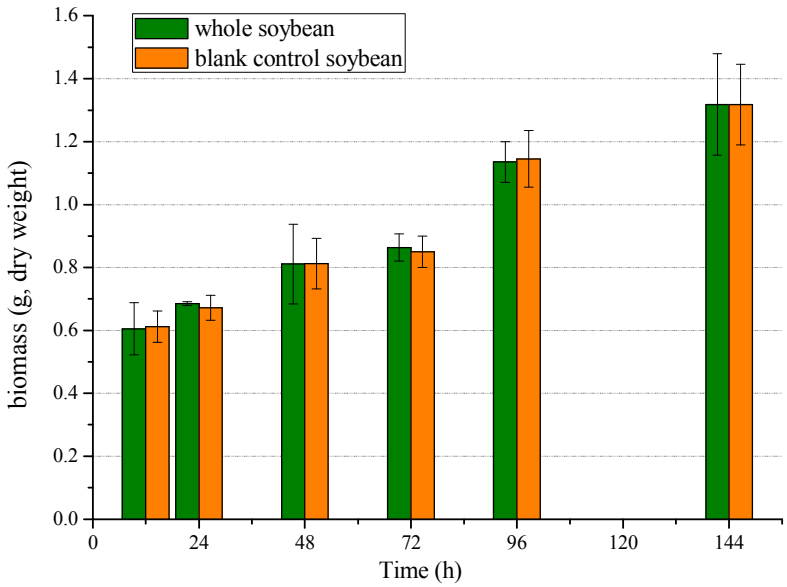
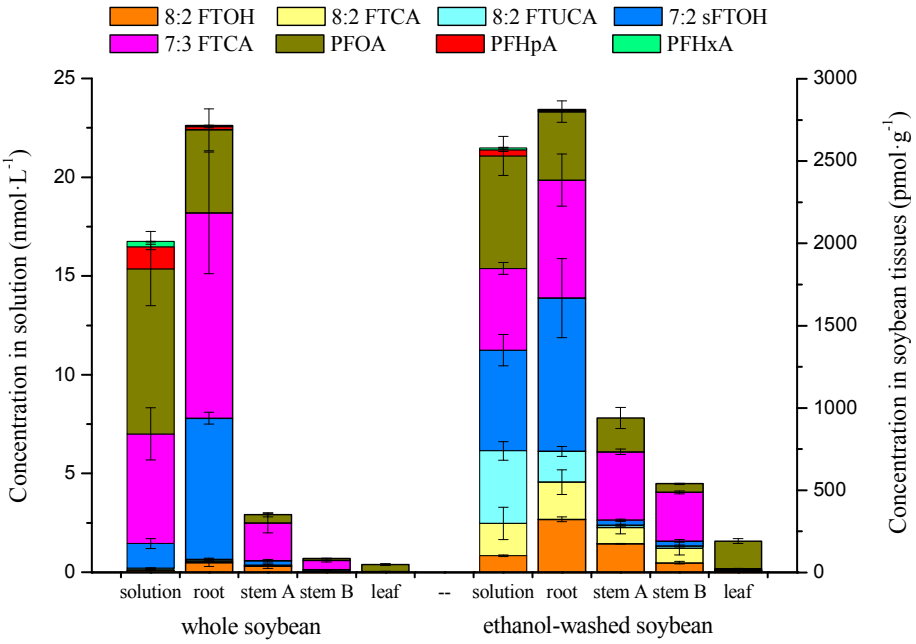


Figure S2. Soybean biomass on dry weight basis (g) per reactor in whole soybean systems and blank controls during exposure time.



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169 **Figure S3.** Comparison of 8:2 FTOH and metabolite concentrations in whole soybean

170 systems and ethanol-washed soybean controls at 144 h.

171

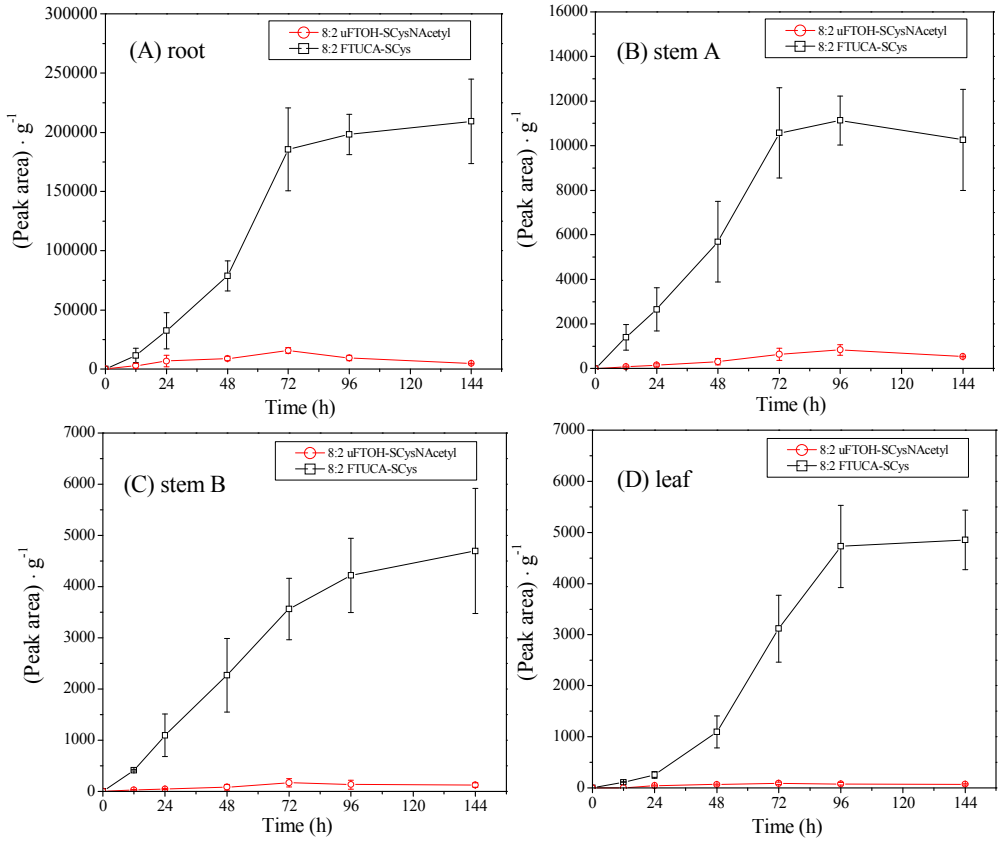

Figure S4. Time-dependent levels of 8:2 uFTOH-SCysNAcetyl and 8:2 FTUCA-SCys in different parts of whole soybean. The Y value was the peak area of 8:2 uFTOH-SCysNAcetyl (586 > 457) and 8:2 FTUCA-SCys (558 > 471) divided by the weight (g) of the extracted tissues.

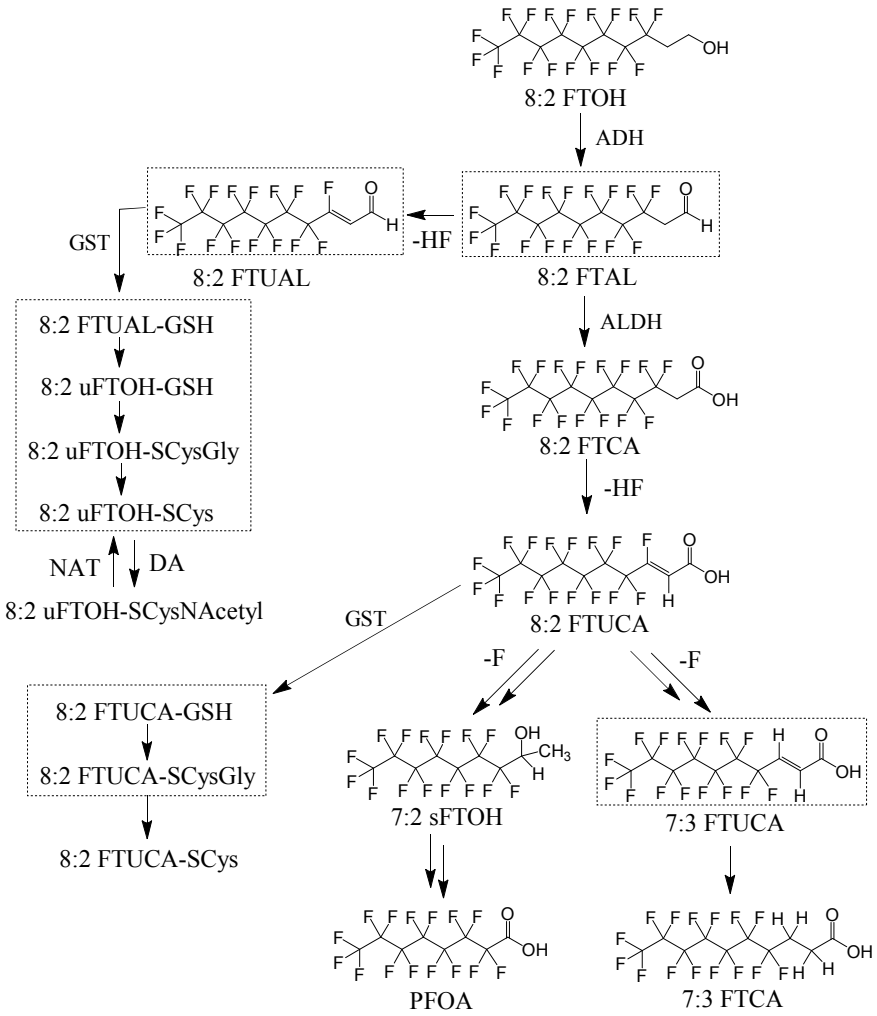

Figure S5. Proposed metabolic pathways of 8:2 FTOH in soybean tissues. Compounds inside dashed boxes are predicted and not monitored due to lack of standard materials or weak signals. The double arrows indicate multiple transformation steps. N-acetylase (NAT); deacetylase (DA).