Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts. This journal is © The Royal Society of Chemistry 2022

Table SI: The list of generalized reaction schemes for the PFAS conjugation reactions and structure of the parent PFAS on which the reaction schemes were based are taken from Table 3. Column 4 provides the structure of the predicted TP based on the transformation of the parent PFAS column by the reaction scheme. Column 5 states if the predicted TP is formed based on the parent PFAS and execution of the BioTransformer-Phase I transformer. Column 6 lists additional TPs that were observed from the parent PFAS and execution of the BioTransformer Phase I transformer reaction libraries executed through the CTS. Column 7 lists additional TPs formed from the parent PFAS based on execution of EnviPath. Cells shaded in grey represent transformations occurring in environmental systems and cells shaded in blue represent transformations occurring in biological systems.

Reaction Scheme	Generalized Reaction Scheme	Parent PFAS	Predicted TP based on the parent PFAS and execution of the reaction scheme	Is the predict- ed TP formed by BioTran s- former- Phase 1?	Other TPs predicted by BioTransformer -Phase 1	Is the predict ed TP formed by Envi- Path?	Other TPs predicted by EnviPath
22. Decarboxylati on: Alpha carboxy ether to ether	$2H \xrightarrow{11}{B} \xrightarrow{11}{F} \xrightarrow{10}{G} \xrightarrow{6}{F} \xrightarrow{10}{F} \xrightarrow{10}{F}$					NO	











33. Hydrolysis: Carboxylic acid ester to carboxylic acid	$[\mathbb{N}:\tilde{\mathfrak{G}}]^{-L} \xrightarrow{2}_{0} \overset{0}{\overset{0}{\overset{0}{\overset{0}{\overset{0}{\overset{0}{\overset{0}{\overset$		YES	-the alpha-beta epoxide -the alpha-keto carboxylic acid ester	NO	-the alpha- beta epoxide -the saturated carboxylic acid ester -the alpha- hydroxy carboxylic acid ester
34. Hydrolysis: Diphosphate ester to monophospha te ester	$\begin{bmatrix} 1 & & & & & & & & & & & \\ & & & & & & &$	$F \xrightarrow{F} F \xrightarrow{F} $			YES	-the alpha- hydroxy phosphat e ester

35. Hydrolysis: Epoxide to diol_PTP	$[H;C;F] = \begin{bmatrix} H;C;F \\ 0 \\ 1 \\ 2 \\ H;C;F \end{bmatrix} = \begin{bmatrix} H;C \\ H;C;F \end{bmatrix} = \begin{bmatrix} H;C \\ 0 \\ 1 \\ 1 \\ H;C;F \end{bmatrix} = \begin{bmatrix} H;C \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ $	$F \xrightarrow{F} F \xrightarrow{F} HO \xrightarrow{H} F \xrightarrow{F} OH$		YES	
36. Hydrolysis: Perfluorinated epoxide to beta keto carboxylic acid	$F_{5}^{[C:\overline{F}]}$		NO	NO	

37. Hydrolysis: Fluorotelomer aldehyde to fluorotelomer unsaturated aldehyde	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$\mathbf{r}_{\mathbf{r}_}}}}}}}}}}$	NO	-the 8:2 fluorotelomer alcohol -the 8:2 fluorotelomer carboxylic acid the 8:2 alpha hydroxy telomer alcohol		
38. Hydrolysis: Fluorotelomer acid to unsaturated telomer acid	$\begin{bmatrix} 10 \\ F \\ 2 \\ 10 \\ F \\ 10 \\ 10 \\ 10 \\ 10 \\ 10 \\ 10 $		NO	-the alpha- hydroxy carboxylic acid.	NO	-the alpha- hydroxy carboxylic acid -the alpha keto carboxylic acid



41. Hydrolysis: Hydrodefluori nation of PFC chain	$ \begin{array}{c} 29 \\ F \\ 10.91 \\ 31 \\ F \\ 27 \\ 59 \\ 61 \\ F \\ 61 \\$				NO	-the beta- hydroxyl carboxylic acid -the saturated carboxylic acid
42. Hydrolysis: Monophospha te ester to alcohol	$ \begin{array}{c} 12 & 11 & 8 \\ H & H & H \\ 2H & H_{1} & 7P & 0 \\ 2H & H_{1} & 12 \\ 11 & 12 \\ 11 & H & H \\ 2H & H_{1} & 6 \\ 2H & H_{1} & 12 \\ 11 &$		NO	-TP resulting from alpha hydroxylation -TP resulting from beta hydroxylation	NO	

43. Hydrolysis: Diperfluoro- phosphinate to monoperfluor o- phosphonate	$\begin{bmatrix} 2 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\$			NO		
44. Hydrolysis: Sulfonamide to sulfonate	$\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 $	$\begin{array}{c} F \\ F $		NO		
45. Hydrolysis: Sulfonyl fluoride to sulfonate	7F - S - S - S - S - S - S - S - S - S -	$F \xrightarrow{0}_{F} \stackrel{F}{\xrightarrow{0}_{F}} F$	HO $ S$ F		NO	-TP resulting from alpha hydroxylati on -TP resulting from beta hydroxylati on -TP resulting from loss of amide group

46. Hydroxylation : N-Alkyl sulfonamide to N-alkyl sulfonamide alcohol_PTP	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$				YES	
47. Hydroxylation : Unsaturated Fluorotelomer acid to alpha hydroxy fluorotelomer acid	$\begin{bmatrix} C; A \end{bmatrix}^{2} \\ H \\ C; A \end{bmatrix}^{2} \\ H \\ $		NO	-the beta-keto fluorotelomer carboxylic acid -the alpha-beta epoxide of the fluorotelomer carboxylic acid		

48. Hydroxylation : Unsaturated Fluorotelomer acid to beta hydroxy fluorotelomer acid	$\begin{array}{c} 3 \\ F \\ (C,H)^{L} \\ (C,$			NO	-the alpha-beta keto carboxylic acid -the alpha-beta epoxide of the carboxylic acid.	NO	-the alpha- hydroxy carboxylic acid -the 5:2 carboxylic acid telomer
49. N- Deacetylation: N-acetyl, N- alkyl sulfonamide to N-alkyl sulfonamide	$\begin{array}{c} 0 \\ P \\ F \\ H \\ H \\ F \\ H \\ H \\ H \\ H \\ H \\ H$	$r \xrightarrow{r} \qquad r \xrightarrow{r} \qquad r$	$r \xrightarrow{F} F \xrightarrow{F} F \xrightarrow{F} F \xrightarrow{F} F \xrightarrow{F} F \xrightarrow{F} 0$	NO	-the N-acetyl sulfonamide -the N-alpha- hydroxy acetyl sulfonamide		



52. N- Demethylatio n: fluorotelomer sulfonamide N-dimethyl-N- acetyl betaine to fluorotelomer sulfonamide N-methyl-N- acetyl betaine		$r \xrightarrow{s} r \xrightarrow{s} r \xrightarrow{r} r \xrightarrow{r} r \xrightarrow{r} r \xrightarrow{0} \frac{1}{0} \xrightarrow{s} r \xrightarrow{r} r$	NO		
53. N- Deacetylation: fluorotelomer sulfonamide N-methyl-N- acetyl-betaine to fluorotelomer sulfonamide N-methyl betaine	$ \begin{array}{c} \begin{array}{c} \begin{array}{c} \\ \\ \\ \end{array} \end{array} \\ \\ \end{array} \\ \\ \\ \end{array} \\ \\ \\ \\ \end{array} \\ \\ \\ \\ \\ \\ \\ \end{array} \\ \\ \\ \\ \\ \\ \\ \end{array} \\ \\ \\ \\ \\ \\ \\ \\ \end{array} \\ \\ \\ \\ \\ \\ \\ \\ \\ \end{array} \\$		YES	-N-Oxide of tertiary amine -Hydroxylation of terminal methyl group -Demethylation of tertiary amine -Hydroxylation of C alpha to tertiary amine	

54. N- Deacetylation: fluorotelomer sulfonamide N-dimethyl-N- acetyl-betaine to fluorotelomer sulfonamide N-dimethyl betaine	$\begin{array}{c} 1 \\ 1 \\ 1 \\ 2 \\ 1 \\ 2 \\ 1 \\ 2 \\ 1 \\ 2 \\ 1 \\ 2 \\ 1 \\ 2 \\ 1 \\ 2 \\ 2$	$\frac{1}{2}$	$ \int_{-\infty}^{\infty} \int_{-\infty}^{$	NO		
55. N- Demethylatio n: fluorotelomer sulfonamide N-methyl betaine to fluorotelomer sulfonamide betaine	$\begin{bmatrix} 2^{7} \\ - \\ - \\ - \\ - \\ - \\ - \\ - \\ - \\ - \\ $	[−] [−] →→ [−]	r = r + r + r + r + r + r + r + r + r +	YES	-Hydroxylation of terminal methyl group -N-Demethylati of secondary amine	

56. O- Demethylatio n: Alpha difluoro methyl ether to carboxylic acid	2_{F} F 8_{F} F F CH_{3}^{9} 1_{F} 1_{2} 1_{10} CH_{3}^{9} 6_{F} $1_{5,F}$ $1_{5,F}$ 0 1_{F} 1_{2} 1_{10} H^{14} 6_{F} $1_{5,F}$ 0 1_{10} H^{14}		YES	-the fluorinated propyl alcohol -the beta- hydroxy propyl alcohol.	
57. O- Demethylatio n: Fluoromethyl ether to secondary alcohol	2_{F} 1	$F \xrightarrow{OH}_{F} F$	YES	- the ditrifluoro ketone -the alpha hydroxy fluoromethyl ether	

58. Oxidation: Alcohol to ketone	$\begin{array}{c} 4 & 5 \\ H & 0 \\ & H \\ & & CH_{3}_{6} \\ & & & CH_{3}_{6} \\ & & & & & \\ & & & & \\ & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\$	$F \xrightarrow{F} F \xrightarrow{F} $			YES	-Methyl hydroxylati on
59. Oxidation: Alpha fluoro diol to acid fluoride and carboxylic acid with C-C bond cleavage_PTP	$\begin{bmatrix} 0.9\\ 1 \\ 1 \\ 1 \\ 5 \\ 5 \\ 5 \\ 5 \\ 5 \\ 5 \\ 5 $		F = F = 0 $F = F = F$ $F =$		NO	-the alpha hydroxy- alpha fluoro ketone -





64. Oxidation: Beta-keto aldehyde to beta-keto acid_PTP	$\begin{bmatrix} 0 + 3 \\ F \\$		YES	-the beta- hydroxy, alpha- keto aldehyde - the beta-keto alcohol -the beta-keto aldehyde		
65. Oxidation: Beta oxidation of beta keto fluorotelomer acid	$\begin{bmatrix} 0 & A^{L} \\ 0 & B^{L} $		NO	-the alpha- hydroxy -beta keto carboxylic acid the beta- hydroxy carboxylic acid	NO	

66. Oxidation: Fluorotelomer iodide to alpha beta unsaturated fluorotelomer iodide_PTP	$ \begin{array}{c} 7 & 4 \\ F & H \\ 6 & H \\ 9 & F \\ 9 & F \\ 9 & F \\ 9 & F \\ 8 & 2 \\ 7 \\ 7 \\ 7 \\ 8 & F \\ 9 & H \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$		$ \begin{array}{c} \mu \\ \mu $	NO	-the alpha- hydroxy fluorotelomer iodide -the beta- hydroxy fluorotelomer iodide	NO	
67. Oxidation: Fluorotelomer alcohol to fluorotelomer aldehyde	$\begin{array}{c} {}^{9}F \\ {}^{14} \\ {}^{15}F \\ {}^{10} \\ {}^{7}F \\ {}^{7}F \\ {}^{7}F \\ {}^{7}F \\ {}^{8}H \\ {}^{12} \\ {}^{13} \\ {}^{10} \\ {}^{10} \\ {}^{10} \\ {}^{7}F $	P F F F F F F F OH		NO	-the beta-keto fluorinated hexane -the alpha-beta diol fluorinated hexane	YES	-the alpha- beta diol fluorinated hexane



70. Oxidation: Fluorotelomer aldehyde to fluorotelomer carboxylic acid	$\begin{bmatrix} 0, \beta \end{bmatrix}^{L} \\ \begin{bmatrix} 0, \beta \end{bmatrix}^{L} \\ \end{bmatrix} \begin{bmatrix} F \\ F$		YES	-the beta- hydroxy fluorotelomer carboxylic acid.	NO	-the beta- hydroxy fluorotelo mer carboxylic acid.
71. Oxidation: Fluorotelomer carboxylic acid to 2,3- unsaturated fluorotelomer carboxylic acid	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 &$		NO	-the alpha- hydroxy caroboxylic acid -the beta- hydroxy carboxylic acid.	NO	-the alpha- hydroxy caroboxylic acid.

72. Oxidation: Fluorotelomer polyethoxylat e alcohol to fluorotelomer ethoxylate aldehyde		, , , , , , , , , , , , , , , , , , ,		NO	-Oxidative cleavage of the C-O bond beta to the hydroxyl group -the alpha- hydroxy carboxylic acid -the alpha hydroxylati on of the carbon alpha to the CF ₂ group
73. Oxidation: Fluorotelomer ethoxylate aldehyde to fluorotelomer ethoxylate carboxylic acid		$i \xrightarrow{k} \sum_{k=1}^{k} \sum_{i=1}^{k} \sum_{j=1}^{k} \sum_{i=1}^{$		YES	 hydroxylati on of the carbon alpha to the CF₂ group the aldehyde from cleavage of the C-O bond

74. Oxidation: Fluorotelomer thioether amido sulfonate to fluorotelomer sulfoxide amido sulfonate					NO	
75. Oxidation: Fluorotelomer sulfoxide amido sulfonate to fluorotelomer sulfone amido sulfonate	$\begin{array}{c} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 $	$\sum_{j=1}^{j}\sum_{j=1}^{j}\sum_{i=1}^{j}\sum_{j=1}^{j}\sum_{j=1}^{j}\sum_{j=1}^{j}\sum_{i=1}^{j}\sum_{j=1}^{j}\sum_{j=1}^{j}\sum_{j=1}^{j}\sum_{i=1}^{j}\sum_{j=1}^{$	$r \xrightarrow{r}_{r} \xrightarrow{r} \xrightarrow{r}_{r} \xrightarrow{r} \xrightarrow{r}_{r} \xrightarrow{r} \xrightarrow{r}_{r} \xrightarrow{r} \xrightarrow{r} \xrightarrow{r}_{r} \xrightarrow$		NO	

76. Oxidation: Fluorotelomer sulfoxide amido sulfone to fluorotelomer sulfonate	$ \begin{array}{c} \mathbf{r} \\ \mathbf$	$ \begin{array}{c} $		NO	
77. Oxidation: Hydrodefluori nation with alpha hydroxylation and alpha oxidation	$\begin{bmatrix} G_{3}\\ & & \\ &$			NO	-the alpha- hydroxy ketone



80. Reduction: 2,3- Unsaturated fluorotelomer carboxylic acid to fluorotelomer carboxylic acid	$ \begin{array}{c} & & & & & & & & & \\ & & & & & & & \\ & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & $		NO	- the alpha- beta epoxide carboxylic acid -the beta-keto carboxylic acid	YES	-the beta- hydroxy carboxylic acid
81. Reduction: Beta fluoro unsaturated telomer acid to beta H unsaturated telomer acid	$\begin{bmatrix} c_1 f_1 \\ c_2 f_1 \end{bmatrix} \begin{bmatrix} 1 \\ c_1 \\ c_2 \\ c_1 \\ $		NO	-the beta-keto carboxylic acid	NO	-the beta- hydroxy beta-fluoro caboxylic acid -the beta- fluoro 7:2 fluorotelo mer carboxylic acid







Table S2: The list of generalized reaction schemes for the PFAS conjugation reactions and structure of the parent PFAS on which the reaction schemes were based are taken from Table 3. Column 3 provides the structure of the predicted TP based on the transformation of the parent PFAS by the reaction scheme. Column 4 states if the predicted TP is formed based on the parent PFAS and execution of BioTransformer Phase II Transformer through the CTS. Additional TPs that were observed upon execution of the BioTransformer Phase II transformer are listed in column 5.

















21. Conjugation: Taurine-	$\begin{array}{c} & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & & \\ & & & \\ & & & \\ & & & & \\ & & & & \\ & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ &$	F F F F F F F F F F F F F F F F F F F	$F \xrightarrow{F} F \xrightarrow{F} F \xrightarrow{F} F \xrightarrow{F} F \xrightarrow{F} H \xrightarrow{H} H \xrightarrow{H} 0 \xrightarrow{H} $	NO	-Gluconerate conjugation of the carboxlyic acid
acid conjugate formation	$\begin{bmatrix} 0, 0 \end{bmatrix}^{H} \\ 4 \\ 4 \\ H \\ 4 \\ H \\ 4 \\ H \\ H_{5} \\ 10 \\ 10 \\ 10 \\ 10 \\ 10 \\ 10 \\ 10 \\ 1$	FFFFFHHU O			-Glycine conjugation of the carboxylic acid