Supporting information

A pilot study on extractable organofluorine and per- and polyfluoroalkyl substances (PFAS) in water from drinking water treatment plants around Taihu Lake, China: what is missed by target PFAS analysis?

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Figure S1 Suspect PFAS composition (based on intensity)
| Class | Abbreviation | Name                        | Quantification ion (m/z) | Qualification ion (m/z) | Internal standard |
|-------|--------------|-----------------------------|--------------------------|-------------------------|-------------------|
|       | TFA          | Trifluoroacetic acid        | 112.9/68.96              |                         | $^{13}$C$_2$-PFBA |
|       | PFPrA        | Perfluoropropanoic acid     | 162.97/118.9             |                         | $^{13}$C$_2$-PFBA |
|       | PFBA         | Perfluorobutanoic acid      | 212.97/169               |                         | $^{13}$C$_2$-PFBA |
|       | PFPeA        | Perfluoropentanoic acid     | 262.97/219               |                         | $^{13}$C$_2$-PFPeA |
|       | PFHxA        | Perfluorohexanoic acid      | 312.97/269               | 312.97/118.95           | $^{13}$C$_2$-PFHxA |
|       | PFHpA        | Perfluoroheptanoic acid     | 362.97/319               | 362.97/168.97           | $^{13}$C$_2$-PFHpA |
|       | PFOA         | Perfluorooctanoic acid      | 412.97/369               | 412.97/168.97           | $^{13}$C$_2$-PFOA |
| PFCAs | PFNA         | Perfluorononanoic acid      | 462.99/419               | 462.99/219              | $^{13}$C$_2$-PFNA |
|       | PFDA         | Perfluorodecanoic acid      | 512.97/469               | 512.97/219              | $^{13}$C$_2$-PFDA |
|       | PFUnDA       | Perfluoroundecanoic acid    | 562.97/519               | 562.97/268.99           | $^{13}$C$_2$-PFUnDA |
|       | PFDoDA       | Perfluorododecanoic acid    | 612.97/569               | 612.97/168.96           | $^{13}$C$_2$-PFDoDA |
|       | PFTrDA       | Perfluorotridecanoic acid   | 662.9/619                 | 662.9/168.96            | $^{13}$C$_2$-PFTrDA |
|       | PFTDA        | Perfluorotetradecanoic acid | 712.9/669                 | 712.9/168.97            | $^{13}$C$_2$-PFTDA |
|       | PFHxDA       | Perfluorohexadecanoic acid  | 812.9/769                 | 812.9/168.96            | $^{13}$C$_2$-PFHxDA |
|       | PFOcDA       | Perfluoroocadecanoic acid   | 912.9/869                 | 912.9/168.96            | $^{13}$C$_2$-PFOcDA |
|       | TFMS         | Trifluoromethane sulfonic acid | 149.12/79.91          | 149.12/98.95            | $^{13}$C$_2$-PFBS |
|       | PFEtS        | Perfluoroethane sulfonic acid | 198.8/79.8                | 198.8/98.9              | $^{13}$C$_2$-PFBS |
|       | PFPs         | Perfluoropropene sulfonic acid | 248.9/79.9                | 248.9/98.9              | $^{13}$C$_2$-PFBS |
| PFSAs | PFBS         | Perfluorobutane sulfonic acid | 298.9/98.9               | 298.9/79.96             | $^{13}$C$_2$-PFBS |
|       | PFPs         | Perfluoropentane sulfonic acid | 348.9/98.96               | 348.9/79.96             | $^{18}$O$_2$-PFHxDA |
|       | PFHxS        | Perfluoroheptane sulfonic acid | 398.9/98.9               | 398.9/79.96             | $^{18}$O$_2$-PFHxDA |
|       | PFHpS        | Perfluorooctadecanoic acid  | 448.97/98.9              | 448.97/79.96            | $^{13}$C$_2$-PFOS |
| PFOS  | Perfluorooctane sulfonic acid | 498.97/98.9 | 498.97/79.96 | $^{13}$C$_2$-PFOS |
|-------|-------------------------------|-------------|-------------|------------------|
| PFNS  | Perfluorononane sulfonic acid | 548.9/98.96 | 548.9/79.96 | $^{13}$C$_4$-PFOS |
| PFDS  | Perfluorodecane sulfonic acid | 598.97/98.9 | 598.97/79.96 | $^{13}$C$_4$-PFOS |
| PFDoDS| Perfluorododecane sulfonic acid | 698.9/98.9 | 698.9/79.96 | $^{13}$C$_4$-PFOS |
| 4:2 FTSA | 4:2 fluorotelomer sulfonic acid | 327/307 | 327/81 | $^{13}$C$_2$-6:2 FTSA |
| 6:2 FTSA | 6:2 fluorotelomer sulfonic acid | 427/407 | 427/81 | $^{13}$C$_2$-6:2 FTSA |
| 8:2 FTSA | 8:2 fluorotelomer sulfonic acid | 527/507 | 527/81 | $^{13}$C$_2$-8:2 FTSA |
| 5:3 FTCA | 5:3 fluorotelomer carboxylic acid | 340.9/236.97 | 340.9/216.93 | $^{13}$C$_2$-6:2 FTUCA |
| 7:3 FTCA | 7:3 fluorotelomer carboxylic acid | 440.9/316.93 | 440.9/336.89 | $^{13}$C$_2$-8:2 FTUCA |
| ADONA | 3H-perfluoro-3-[(3-methoxy-propoxy)propanoic acid] | 376.97/316.93 | 376.97/336.89 | $^{13}$C$_2$-8:2 FTUCA |
| HFPO-DA | hexafluoropropylene oxide dimer acid | 284.92/168.72 | 328.95/284.86 | $^{13}$C$_2$-HFPO-DA |
| Novel PFAS | 8:2 Cl-PFESA | 630.904/450.98 | 630.904/83.027 | $^{13}$C$_4$-PFOS |
| 6:2 Cl-PFESA | 6:2 chlorinated polyfluorinated ether sulfonate | 530.904/350.98 | 530.904/83.027 | $^{13}$C$_4$-PFOS |
| PFCHS | Perfluoro-4-ethylcyclohexane sulfonate | 460.84/380.9 | 460.84/98.88 | $^{13}$C$_4$-PFOA |
Table S2 Parameters for QTOF analysis

The following parameters were set for initial filtering: (1) S/N > 3; (2) LC peak width less than 30 s; and (3) intensity > 5 times the intensity in the procedural blank. Suspect screening was conducted with the PFAS suspect list followed previous studies\textsuperscript{1, 2}, and the screening processes were performed by R scripts (R v3.6.2, R Foundation for Statistical Computing, Vienna, Austria).

| UPLC conditions | ESI- parameters |
|-----------------|-----------------|
| Analytical column: Acquity UPLC-BEH C18 (100 mm x 2.1 mm x 1.7 µm) | Ionization: ESI- |
| Mobile phase: (A) 2 mM NH\textsubscript{4}Ac + H\textsubscript{2}O / MeOH (70/30); (B) 2 mM NH\textsubscript{4}Ac + MeOH | Acquisition time: 0.5 to 15 min |
| Column temperature: 50 °C | Acquisition function: MS\textsuperscript{6} |
| Injection volume: 10 µL | Mass range: m/z 50-1200 |
| Rinse solvent: H\textsubscript{2}O:MeOH:ACN:IPA 1:1:1:1 | Analyzer mode: Sensitivity |
| Sample temperature: 10 °C | Capillary voltage: 0.5 kV |
| Flow rate: 0.3 mL/min | Sample cone: 10 V |
| Source temperature: 100 °C | Cone gas flow: 100 L/h |
| Mobile phase gradient: | Desolvation gas flow: 1000 L/h |
| Time | Composition A | Composition B | Desolvation temperature: 350°C |
| 0 min | 99% | 1% | Scan rate: 5 Hz |
| 0.5 min | 99% | 1% | Low energy: 4 eV |
| 13 min | 0% | 100% | High energy ramp: 20-70 |
| 14 min | 0% | 100% | Lockspray: Leucine Enkephalin m/z 554.2620 |
| 14.2 min | 99% | 1% | Scan time 0.25 s |
| 16 min | 99% | 1% | Interval: 10s |

Table S3 Spike recovery test results using Milli-Q water (n=3, 2 ng)

| Compounds | Mean recovery (%) | RSD | Compounds | Mean recovery (%) | RSD |
|-----------|-------------------|-----|-----------|-------------------|-----|
| PFBA      | 101               | 9%  | PFTrDA    | 74                | 5%  |
| PFPeA     | 96                | 5%  | PFBS      | 86                | 4%  |
| PFHxA     | 96                | 5%  | PFHxS     | 96                | 4%  |
| PFHpA     | 96                | 3%  | PFOS      | 89                | 8%  |
| PFOA      | 96                | 5%  | 6:2 FTSA  | 102               | 6%  |
| PFNA      | 90                | 14% | HFPO-DA   | 76                | 17% |
| PFDA      | 96                | 6%  | ADONA     | 83                | 18% |
| PFUnDA    | 96                | 6%  | F-53B     | 80                | 3%  |
| PFDaDA    | 95                | 6%  |           |                   |     |
| Compounds     | Mean recovery (%) | RSD  | Compounds     | Mean recovery (%) | RSD  |
|--------------|-------------------|------|--------------|-------------------|------|
| $^{13}$C$_3$-PFBA | 56                | 24%  | $^{13}$C$_2$-PFTDA | 48                | 34%  |
| $^{13}$C$_3$-PFPeA | 82                | 6%   | $^{13}$C$_2$-PFHxDA | 32                | 50%  |
| $^{13}$C$_2$-PFHxA | 82                | 6%   | $^{13}$C$_3$-PFBS | 90                | 12%  |
| $^{13}$C$_4$-PFHpA | 90                | 10%  | $^{18}$O$_2$-PFHxDA | 92                | 6%   |
| $^{13}$C$_3$-PFBS | 74                | 28%  | $^{13}$C$_2$-6:2 FTSA | 181              | 35%  |
| $^{13}$C$_2$-PFDoDA | 81                | 9%   | $^{13}$C$_2$-8:2 FTSA | 59                | 33%  |
| $^{13}$C$_2$-PFUnDA | 75                | 10%  | $^{13}$C$_2$-8:2 FTSA | 63                | 16%  |
| $^{13}$C$_2$-PFeDA | 67                | 16%  |              |                   |      |

Table S4 Internal standard recovery in raw and treated water samples (n=16, 2 ng)

| Individual compounds | Batch1   | Batch2   | Batch3   | Batch4   |
|----------------------|----------|----------|----------|----------|
|                      | MDL      | MQL      | MDL      | MQL      | MDL      | MQL      | MDL      | MQL      |
| PFBA                 | 0.0660   | 0.0720   | 0.0770   | 0.142    | 0.102    | 0.148    | 0.167    | 0.389    |
| PFPeA                | /        | 0.0200   | /        | 0.0200   | /        | 0.0200   | /        | 0.0200   |
| PFHxXa               | 0.0190   | 0.0250   | 0.0300   | 0.063    | 0.0350   | 0.0590   | 0.0350   | 0.0460   |
| PFHxA                | /        | 0.0200   | /        | 0.0200   | 0.0160   | 0.0250   | 0.111    | 0.293    |
| PFHPa                | 0.0470   | 0.0810   | 0.0540   | 0.103    | 0.0380   | 0.0380   | 0.0450   | 0.0560   |
| PFNA                 | /        | 0.0200   | /        | 0.0200   | 0.0360   | 0.0810   | 0.0260   | 0.0350   |
| PFBA                 | 0.0270   | 0.0560   | 0.0280   | 0.0400   | 0.0230   | 0.0400   | 0.0210   | 0.0220   |
| PFUnDA               | 0.0120   | 0.0130   | 0.0160   | 0.0220   | 0.0340   | 0.0750   | 0.0170   | 0.0170   |
| PFDoDA               | /        | 0.0200   | /        | 0.0200   | 0.00900  | 0.0160   | /        | 0.0200   |
| PFTrDA               | /        | 0.0200   | /        | 0.0200   | 0.00900  | 0.0180   | /        | 0.0200   |
| PFBS                 | 0.0200   | 0.0230   | 0.0310   | 0.0530   | 0.0420   | 0.0860   | 0.0320   | 0.0430   |
| PFPeS                | /        | 0.0200   | /        | 0.0200   | /        | 0.0200   | /        | 0.0200   |
| PFHxDA               | 0.0260   | 0.0570   | 0.0180   | 0.0330   | 0.0200   | 0.0280   | 0.0210   | 0.0270   |
| PFOS                 | 0.0410   | 0.100    | 0.0690   | 0.181    | 0.0280   | 0.0540   | 0.0340   | 0.0560   |
| 6:2 FTSA             | /        | 0.0200   | /        | 0.0200   | 0.0670   | 0.119    | 0.0460   | 0.0480   |
| HFPO-DA              | /        | 0.0500   | /        | 0.0500   | /        | 0.0500   | /        | 0.0500   |
| ADONA                | /        | 0.0500   | /        | 0.0500   | /        | 0.0500   | /        | 0.0500   |
| F-53B                | /        | 0.0500   | /        | 0.0500   | /        | 0.0500   | /        | 0.0500   |
| TFA                  | /        | 0.0200   | 0.0270   | 0.0280   | 0.224    | 0.448    | 0.449    | 1.05     |
| PFPrA                | /        | 0.0200   | 7.35     | 12.6     | 1.48     | 2.85     | 1.76     | 4.08     |
| TFMS                 | /        | 0.0200   | 0.0170   | 0.0370   | 0.100    | 0.266    | 0.0810   | 0.208    |
| PFETs                | /        | 0.0200   | /        | 0.0200   | 0.00700  | 0.0190   | /        | 0.0200   |
| PFPrS                | /        | 0.0200   | /        | 0.0200   | /        | 0.020   | /        | 0.0200   |

Table S5 MDL and MQL of the target PFAS (ng/L)
Table S6 Changes of EOF and different classes of PFAS after treatment processes

|            | D3          | D4          | D5          | D8          |
|------------|-------------|-------------|-------------|-------------|
| EOF        | 2.1%        | -9.9%       | -33.3%      | 59.4%       |
| Short-chain PFCAs | -7.1%        | 2.0%        | -15.2%      | 10.1%       |
| Short-chain PFSAs | -2.8%        | 9.2%        | 25.8%       | 91.9%       |
| Long-chain PFCAs | -1.1%        | 12.8%       | -10.3%      | -47.6%      |
| Long-chain PFSAs | -2.3%        | 7.4%        | 17.6%       | -31.6%      |
| Novel PFAS  | 25.8%       | 8.4%        | -0.7%       | 8.8%        |
| Ultra-short PFAS | -53.7%    | 35.2%       | 36.8%       | 99.4%       |

Table S7 Concentrations of PFAS in raw and treated water from 8 DWTPs in China (ng/L)

| PFAS | Raw water | Treated water | Raw water | Treated water | Raw water | Treated water | Raw water | Treated water | Raw water | Treated water | Raw water | Treated water | Raw water | Treated water | Raw water | Treated water | Raw water | Treated water |
|------|-----------|---------------|-----------|---------------|-----------|---------------|-----------|---------------|-----------|---------------|-----------|---------------|-----------|---------------|-----------|---------------|-----------|---------------|
| PFBA | 8.34      | 8.35          | 10.4      | 10.4          | 10.8      | 9.83          | 12.7      | 11.0          | 10.1      | 8.39          | 1.90      | 1.82          | 0.457     | 0.678         | 4.44      | 4.80          |
|         | 0.162 | 61.3 | 13.5 | 0.345 | 0.0290 | 0.381 | 0.0410 | 1.66 | 0.175 | 3.20 | 1.61 | 2.46 | 3.87 | 2.64 | 8.72 | 1.09 | 0.345 | 0.162 |
|---------|-------|------|------|-------|--------|-------|--------|------|-------|------|------|------|------|------|------|------|-------|-------|
| PFPeA   | 3.04  | 3.10 | 3.98 | 3.73  | 3.97   | 3.55  | 4.41   | 4.56 | 3.81  | 3.31 | 0.640 | 0.632 | 0.138 | 0.153 | 0.444 | 0.561 |
| PFHxA   | 8.42  | 9.37 | 8.83 | 9.11  | 9.44   | 8.86  | 11.6   | 13.2 | 5.96  | 5.12 | 1.63  | 1.69  | 0.188 | 0.212 | 0.606 | 0.770 |
| PFHpA   | 3.61  | 4.24 | 4.45 | 4.50  | 4.45   | 5.08  | 5.67   | 4.49 | 3.88  | 0.768 | 0.941 | <MQL | <MQL | 0.650 | 0.636 |
| PFOA    | 24.6  | 29.4 | 30.1 | 29.5  | 32.9   | 32.6  | 42.5   | 49.0 | 34.5  | 31.5 | 5.41  | 6.47  | 1.37  | 1.36  | 7.85  | 4.12  |
| PFNA    | 3.87  | 4.22 | 4.12 | 3.00  | 3.49   | 3.56  | 3.57   | 3.52 | 3.52  | 3.11 | 0.672 | 0.748 | 0.225 | 0.197 | 0.348 | 0.173 |
| PFDA    | 1.66  | 1.58 | 1.59 | 1.85  | 2.87   | 1.92  | 1.92   | 1.57 | 2.54  | 1.86 | 0.474 | 0.277 | 0.121 | 0.0680| 0.0970| 0.0520|
| PFUnDA  | 0.472 | 0.205| 0.416| 0.602 | 0.757  | 0.475 | 0.523  | 0.396| 1.85  | 0.509 | 0.293 | 0.0460| 0.105 | 0.0250| <MQL |
| PFDoDA  | 0.0650| <MQL | 0.0690| 0.103 | 0.112  | 0.0340| 0.0840 | 0.0220| 0.395 | 0.0290| 0.0620| <MQL |
| PFTrDA  | 0.0410| <MQL | 0.0440| 0.0780| 0.0930 | <MQL | 0.0590 | <MQL | 0.113 | <MQL | 0.0560| <MQL |
| PFBS    | 3.01  | 3.37 | 4.92 | 4.96  | 5.19   | 5.11  | 6.90   | 7.51 | 1.61  | 1.99  | 0.631 | 0.737 | 0.100 | 0.141 | 1.35  | 2.66  |
| PFPeS   | 0.381 | 0.391| 0.401| 0.380 | 0.479  | 0.401 | 0.515  | 0.592 | 0.0240| 0.0610| 0.0570| <MQL  | <MQL | 0.0660| 0.0570|       |
| PFHxs   | 44.0  | 48.7 | 50.1 | 45.9  | 57.4   | 57.2  | 54.2   | 61.4 | 2.57  | 3.47  | 7.43  | 13.4  | 0.0340| 0.187 | 1.55  | 1.23  |
| PFOS    | 5.13  | 6.234| 11.0 | 12.3  | 15.4   | 13.9  | 13.2   | 11.0 | 2.97  | 3.05  | 1.50  | 1.34  | 0.194 | 0.193 | 0.674 | 0.292 |
| 6:2 FTSA| 0.0290| <MQL | <MQL | 0.249 | 0.0360 | 0.0830| 0.108  | 0.195| <MQL | <MQL | 0.240 | 0.280 | 0.0490| 0.0530| 0.0480| 0.0970|
| HFPO-DA | 0.345 | 0.393| 0.615| 0.490 | 0.785  | 0.799 | 1.06   | 1.12  | 1.32  | 1.54  | 0.165 | 0.182 | <MQL  | <MQL | <MQL | 0.101 |
| F-53B   | 1.58  | 2.46 | 4.4 | 4.37 | 4.68   | 5.37  | 4.27   | 4.57 | 3.19  | 2.95  | 0.453 | 0.541 | 0.0890| 0.0770| 0.133 | <MQL |
| TFA     | 3.61  | 1.61 | 2.31 | 2.44  | 3.03   | <MQL  | <MQL   | <MQL | 0.567 | 4.14  | 8.96  | 7.94  | <MQL  | <MQL  | <MQL  |       |
| PFPrA   | 13.5  | 3.20 | 19.7 | 12.45 | 11.8   | <MQL  | 4.87   | 8.33 | 7.19  | 8.62  | 14.2  | 36.1  | 17.9  | 14.3  | <MQL  | 4.18  |
| TFMS    | 61.3  | 5.07 | 9.01 | 11.1  | 4.31   | 8.72  | 4.59   | 4.544| 8.49  | 12.3  | 1.08  | 0.580 | <MQL  | <MQL  | <MQL  | 7.48  |
| PFEnS   | 0.0830| 0.0480| 0.0580| 0.0650| 0.0540 | 0.0490| 0.0440 | 0.0400| 0.0390| 0.0320| 0.0320| <MQL  | <MQL  | 0.0220| 0.0330| 0.0590|
| PFPrS   | 0.162 | 0.0610| 0.0600| 0.0580| 0.0650 | 0.147 | 0.126  | 0.108| <MQL  | <MQL  | 0.0680| 0.0690| 0.0280| 0.0200| 0.0770|
Table S8 PFASs identified in samples by suspect screening with a confidence level of 2 or 3 (target PFAS not included)

| Class     | Name     | Theoretical m/z | Observed m/z | Mass error (ppm) | Molecular formula | RT (min) | Product ions formula | Confidence level | Semi-quantification reference PFAS | Concentrations (ng/L) |
|-----------|----------|-----------------|--------------|------------------|-------------------|----------|----------------------|------------------|------------------------------------|-----------------------|
| H-PFPeA   |          | 244.9854        | 244.9851     | -1.34            | C5H2F8O2          | 3.38     | C4F7-                | 2                | PFPeA                             | 0.161-0.975            |
| H-PFOA    |          | 394.9759        | 394.9752     | -1.65            | C8H2F14O2         | 7.32     | C3F7-C7F13-          | 3                | PFOA                              | 0.0120-0.0180          |
| H-PFNA    |          | 444.9727        | 444.9712     | -3.26            | C9H2F16O2         | 8.28     | C8F15-               | 3                | PFNA                              | 0.0190                |
| H-PFBS    |          | 280.9524        | 280.9523     | -0.43            | C4H2F8O3S         | 3.57     | FSO3-C3F5-C7F13-C5F9-| 3                | PFBS                              | 0.00500-0.0150         |
| H-PFOS    |          | 480.9396        | 480.9396     | -0.08            | C8H2F16O3S        | 8.21     | SO3-                 | 3                | PFOS                              | 0.00100-0.00200        |
| Cl-PFESA  | 5:2 Cl-  | 480.8988        | 480.8985     | -0.58            | C7HF14O4SCl       | 9.5      | C5OF10Cl-           | 2                | PFOS                              | 0.00100-0.00300        |
| Cl-PFESA  | 2:2 Cl-  | 296.9473        | 296.9473     | -0.10            | C4H2F8O4S         | 4.39     | FSO2-C2OF3-C2HOF4-C3F5-| 2                | PFBS                              | 0.00700-0.0320         |
| Cl-PFESA  | 4:2 Cl-  | 396.9409        | 396.9404     | -1.36            | C6H2F12O4S        | 7.43     | C4OF7-C4HOF8-FSO3-FSO2-C5F9-| 2                | PFHxS                             | 0.00200-0.0130         |
| Cl-PFESA  | 6:2 Cl-  | 496.9346        | 496.9346     | 0.08             | C8H2F16O4S        | 8.83     | C5F9-C6OF11-C6HOF12-| 2                | PFOS                              | 0.00800-0.439          |
| OBS | OBS | 602.9564 | 602.9560 | -0.71 | C15H5F17O4S | 10.75 | C6H4O2- | 2 | PFOS | 0.00100-0.0372 |
|-----|-----|----------|----------|-------|-------------|-------|----------|---|------|----------------|
|     |     |          |          |       | C6H4O4S-    |       | C11H4O3F7S- |   |      |                |
|     |     |          |          |       | C13H4O4F11S-|      |           |   |      |                |
|     |     |          |          |       |             |      |           |   |      |                |
Figure S1 Composition of identified PFAS suspects based on intensity

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