

**Electronic Supplementary Information**

**Adsorption and Advanced Oxidation of Diverse Pharmaceuticals and  
Personal Care Products (PPCPs) from Water Using Highly Efficient  
rGO-nZVI Nanohybrids**

Arvid Masud,<sup>1</sup> Nita G. Chavez Soria,<sup>2</sup> Diana S. Aga,<sup>2</sup> and Nirupam Aich<sup>1,\*</sup>

<sup>1</sup>Department of Civil, Structural and Environmental Engineering, University at Buffalo, The State

University of New York, Buffalo, NY 14260

<sup>2</sup>Department of Chemistry, University at Buffalo, The State University of New York, Buffalo, NY 14260

**Submitted to**

**Environmental Science: Water Research & Technology**

**06/22/2020**

\* Corresponding Author: Nirupam Aich, Phone: 716-645-0977, Email: nirupama@buffalo.edu

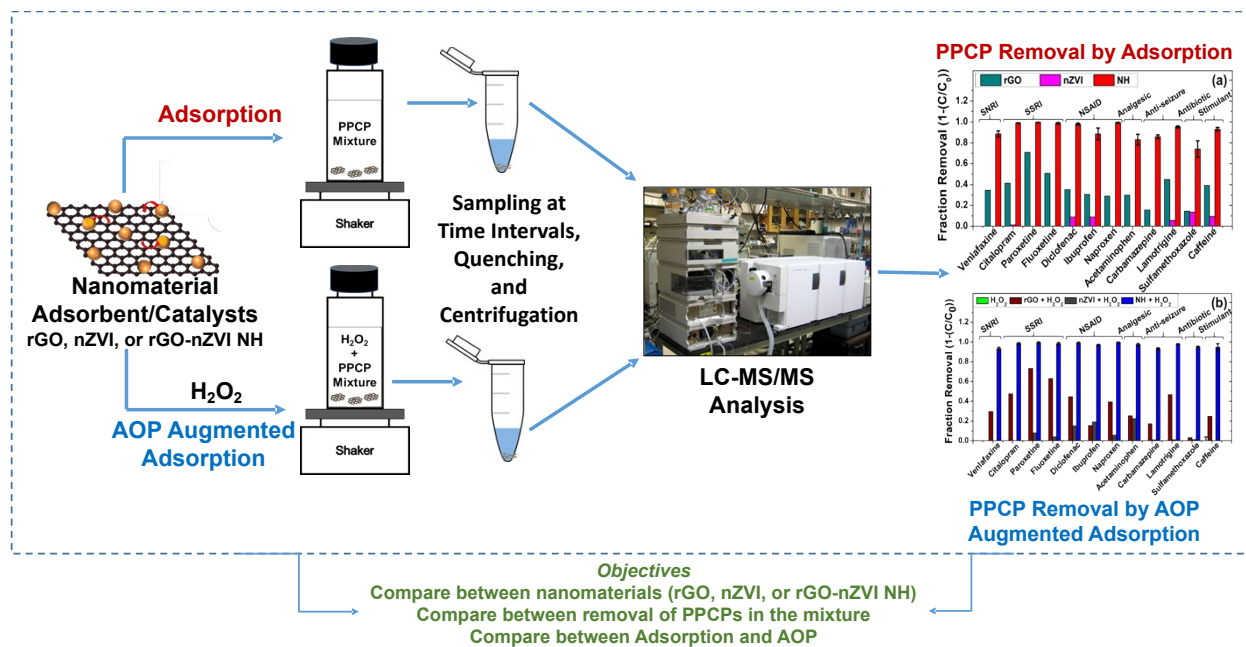


Figure S1. Experimental steps for evaluating the performance of nanomaterial catalyst/oxidant system in removing PPCPs in the mixture.

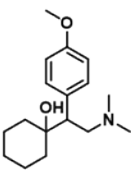
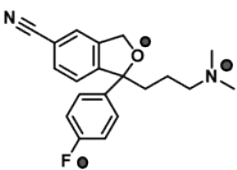
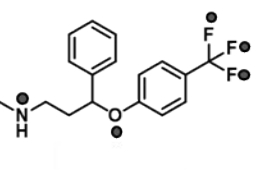
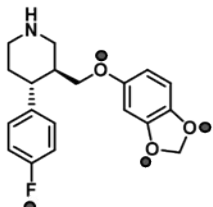
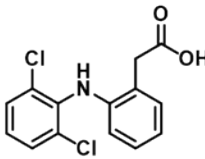
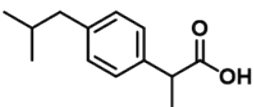
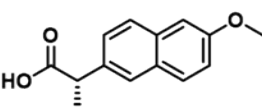
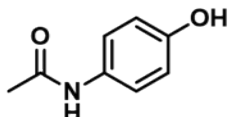
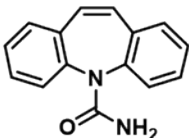
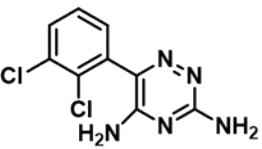
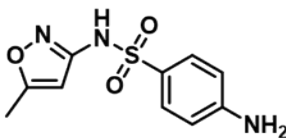
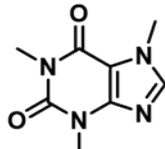
|                                                                                                                                                                                                                                                                                                                                                    |                                                                                                                                             |                                                                                                                                     |                                                                                                                                         |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------|
| <p><b>SNRI</b></p>  <p><b>Venlafaxine</b></p>                                                                                                                                                                                                                     | <p><b>SSRI</b></p>  <p><b>Citalopram</b></p>               | <p><b>SSRI</b></p>  <p><b>Fluoxetine</b></p>      |  <p><b>Paroxetine</b></p>                            |
| <p><b>NSAID</b></p>  <p><b>Diclofenac</b></p>  <p><b>Ibuprofen</b></p>  <p><b>Naproxen</b></p> |                                                                                                                                             |                                                                                                                                     | <p><b>Analgesic</b></p>  <p><b>Acetaminophen</b></p> |
| <p><b>Anti-seizure</b></p>  <p><b>Carbamazepine</b></p>  <p><b>Lamotrigine</b></p>                                                                                            | <p><b>Antibiotic</b></p>  <p><b>Sulfamethoxazole</b></p> | <p><b>Stimulant</b></p>  <p><b>Caffeine</b></p> |                                                                                                                                         |

Figure S2: Chemical structures of 12 PPCPs investigated in this study.

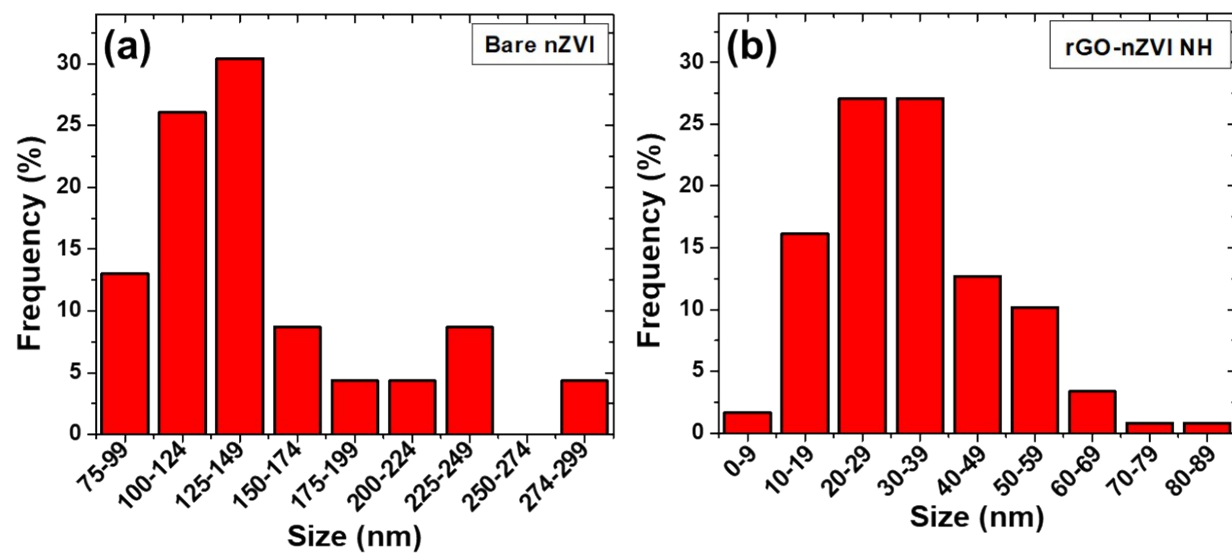


Figure S3: nZVI particle size distribution in bare (a) nZVI and (b) rGO-nZVI NH.

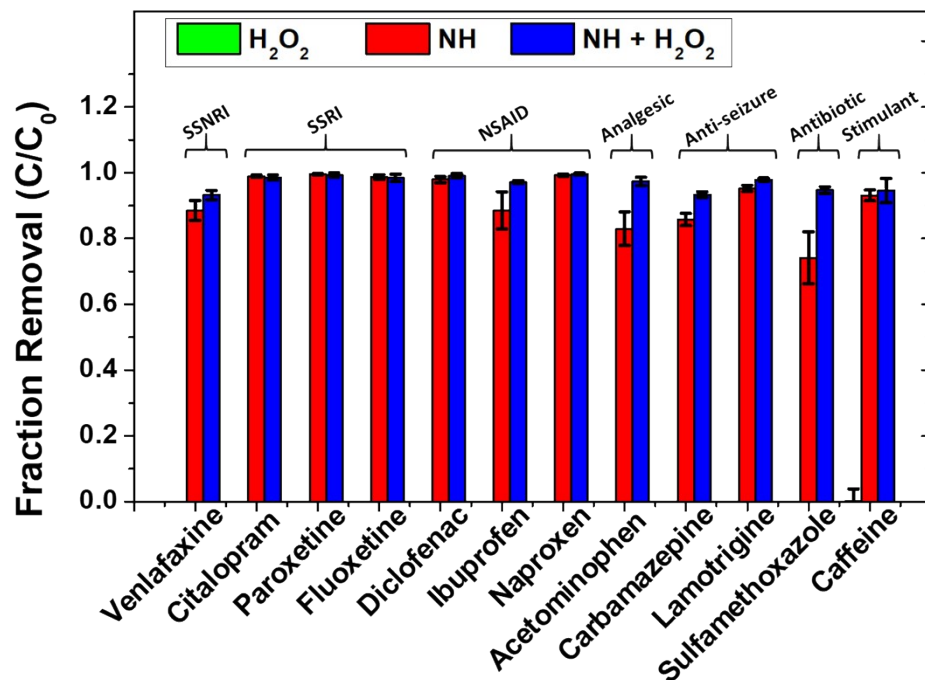


Figure S4: Comparison of adsorptive and AOP augmented adsorptive removal of first set of PPCPs by rGO-nZVI NH.

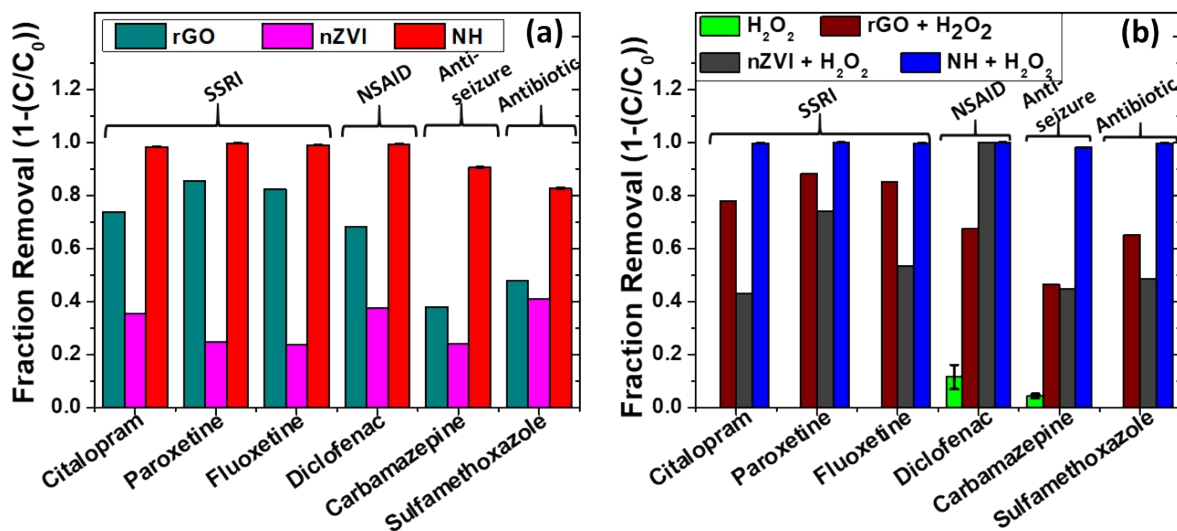


Figure S5: Adsorptive (a) and advanced oxidation augmented adsorptive (b) removal of second set of PPCPs by rGO-nZVI NH and parent nanomaterials after 30 minutes.

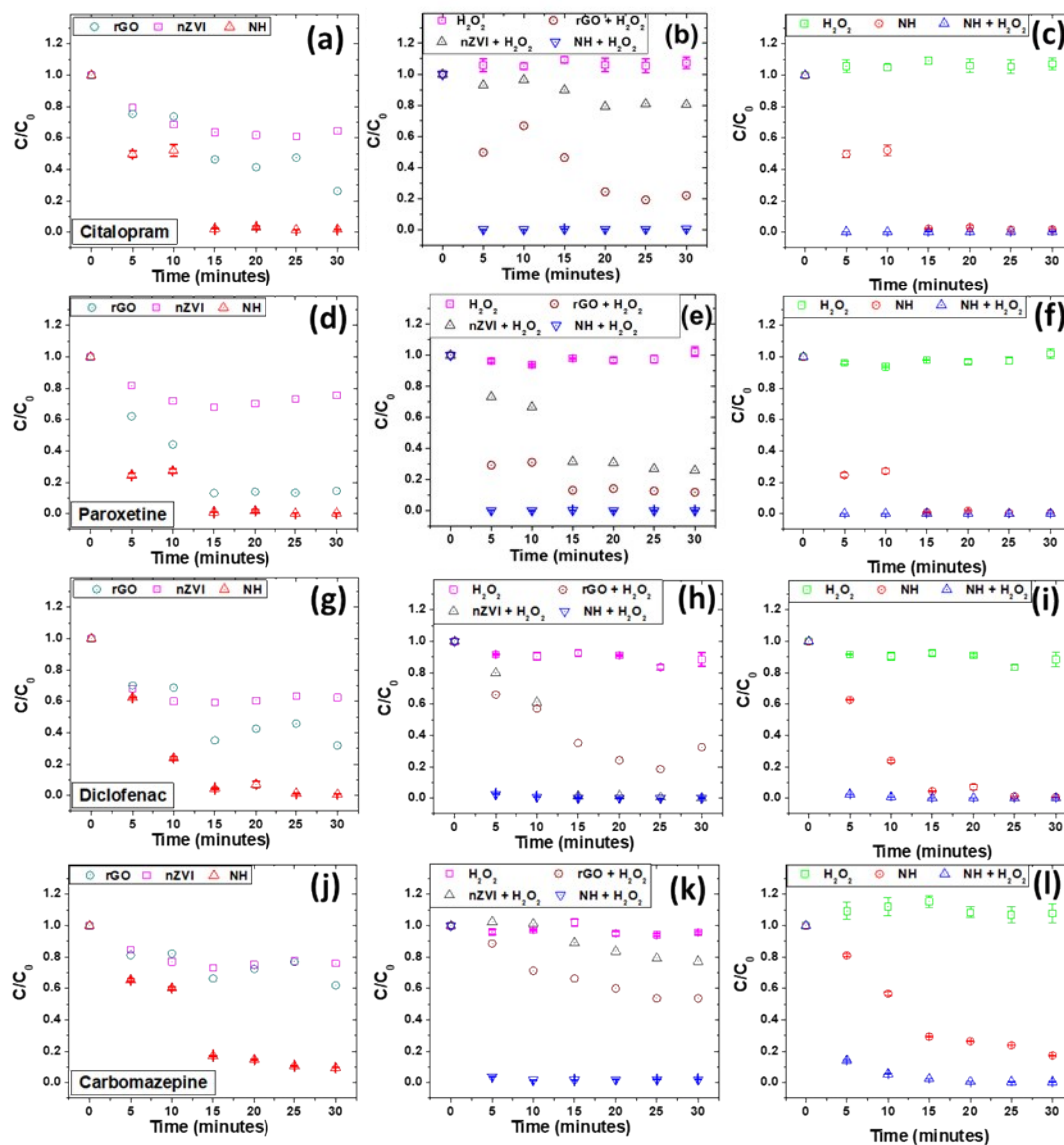


Figure S6: Kinetics of (a, d, g, j) adsorptive and (b, e, h, k) combined adsorption and AOP based removal by rGO-nZVI NH and parent nanomaterials rGO and nZVI, (c, f, i, l) comparative adsorptive and combined adsorption and AOP based removal for rGO-nZVI NH for citalopram, paroxetine, diclofenac, and carbamazepine respectively.

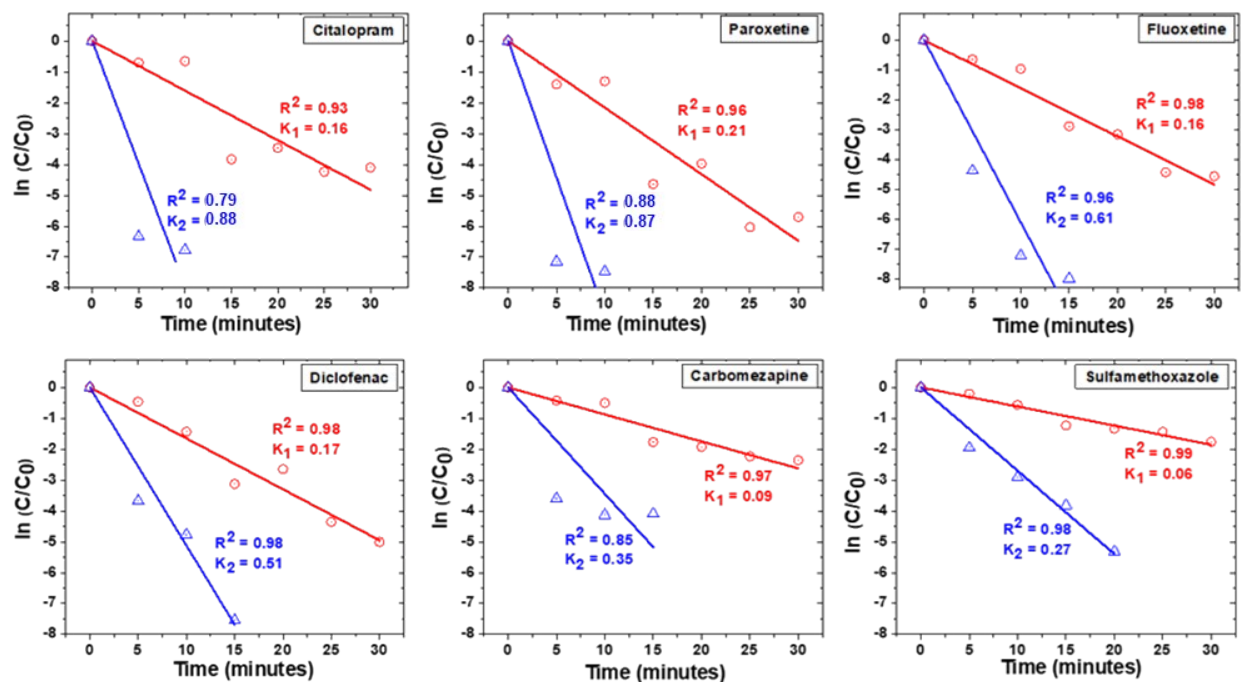


Figure S7: Reaction rate constants for adsorptive (red) and AOP augmented adsorptive (blue) removal of PPCPs by rGO-nZVI NH.

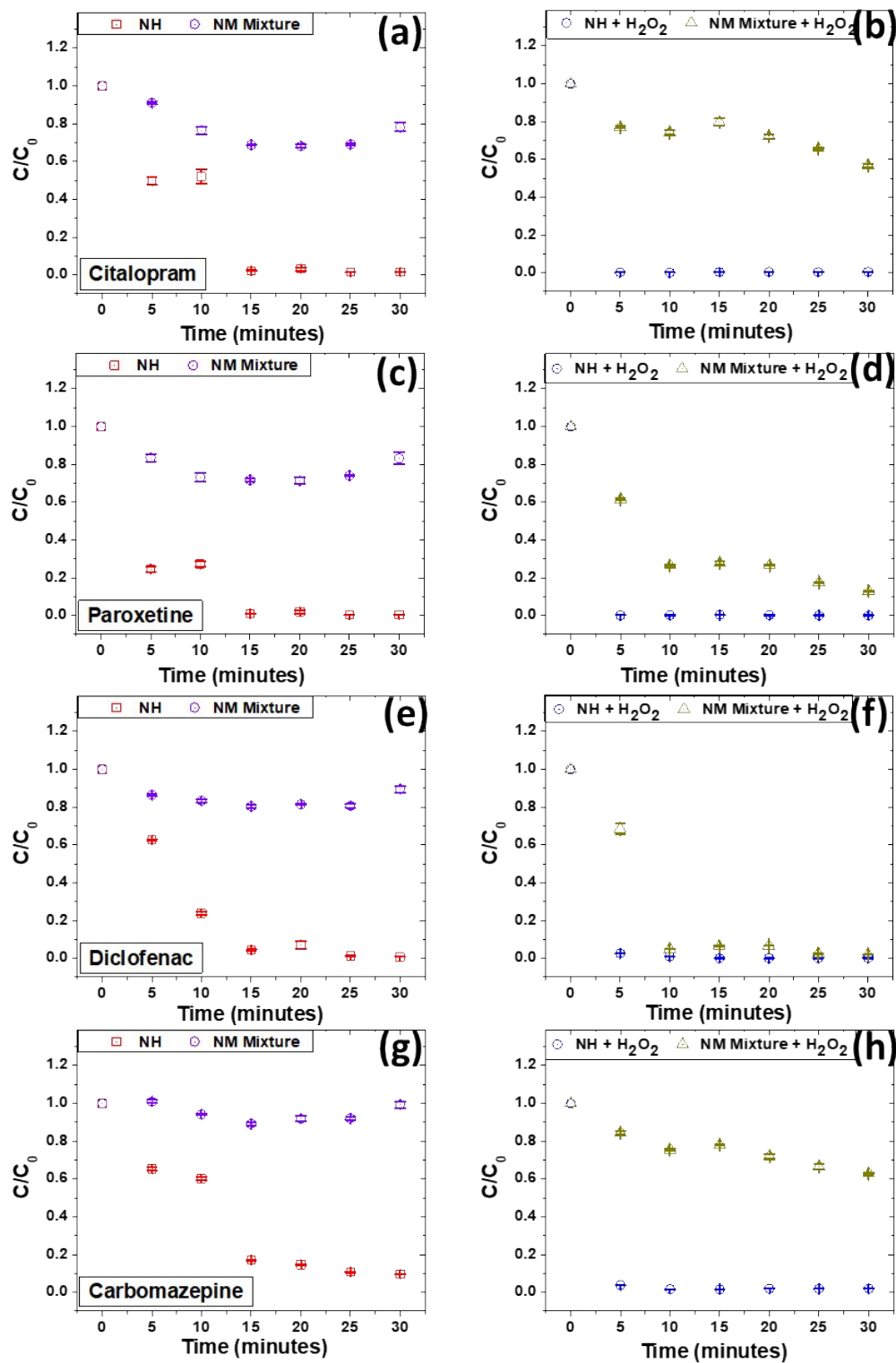


Figure S8: Comparative kinetics of (a, c, e, g) adsorptive, and (b, d, f, h) combined adsorptive and AOP based removal by NH and mixture of parent nanomaterial for citalopram, paroxetine, diclofenac, and carbamazepine respectively.

Table S1: Removal efficiency (%) of different PPCPs by parent nanomaterials and NH

| PPCP             | rGO   | nZVI  | NH    | H <sub>2</sub> O <sub>2</sub> | rGO + H <sub>2</sub> O <sub>2</sub> | nZVI + H <sub>2</sub> O <sub>2</sub> | NH + H <sub>2</sub> O <sub>2</sub> |
|------------------|-------|-------|-------|-------------------------------|-------------------------------------|--------------------------------------|------------------------------------|
| Venlafaxine      | 34.60 | 0.00  | 88.50 | 0.00                          | 29.47                               | 0.00                                 | 93.20                              |
| Citalopram       | 41.23 | 1.41  | 98.92 | 0.00                          | 47.60                               | 0.00                                 | 98.51                              |
| Paroxetine       | 71.07 | 0.00  | 99.58 | 0.00                          | 73.27                               | 7.86                                 | 99.34                              |
| Fluoxetine       | 50.87 | 0.00  | 98.71 | 0.00                          | 62.84                               | 3.99                                 | 98.43                              |
| Diclofenac       | 35.07 | 9.00  | 97.92 | 0.00                          | 44.46                               | 14.86                                | 99.06                              |
| Ibuprofen        | 30.68 | 8.94  | 88.55 | 0.00                          | 15.35                               | 18.93                                | 97.15                              |
| Naproxen         | 29.04 | 0.00  | 99.25 | 0.00                          | 39.30                               | 5.55                                 | 99.56                              |
| Acetaminophen    | 30.14 | 0.00  | 82.97 | 0.00                          | 25.30                               | 22.38                                | 97.37                              |
| Carbamazepine    | 15.67 | 0.00  | 85.75 | 0.00                          | 17.19                               | 0.70                                 | 93.33                              |
| Lamotrigine      | 45.10 | 5.83  | 95.23 | 0.00                          | 46.72                               | 0.92                                 | 97.90                              |
| Sulfamethoxazole | 14.51 | 13.46 | 74.13 | 0.00                          | 3.08                                | 1.09                                 | 94.77                              |
| Caffeine         | 39.24 | 9.47  | 93.12 | 0.05                          | 24.56                               | 0.00                                 | 94.60                              |

Table S2. Removal efficiency (%) of different PPCPs by parent nanomaterials and NH at 10 minute

| PPCP             | rGO   | nZVI  | NH    | H <sub>2</sub> O <sub>2</sub> | rGO + H <sub>2</sub> O <sub>2</sub> | nZVI + H <sub>2</sub> O <sub>2</sub> | NH + H <sub>2</sub> O <sub>2</sub> |
|------------------|-------|-------|-------|-------------------------------|-------------------------------------|--------------------------------------|------------------------------------|
| Citalopram       | 26.30 | 31.41 | 47.90 | 0.00                          | 33.16                               | 3.64                                 | 99.89                              |
| Paroxetine       | 55.88 | 28.01 | 72.81 | 6.18                          | 68.92                               | 33.36                                | 99.94                              |
| Sulfamethoxazole | 33.15 | 23.99 | 61.99 | 3.21                          | 42.79                               | 41.50                                | 99.93                              |
| Diclofenac       | 31.19 | 39.90 | 76.23 | 9.49                          | 42.80                               | 38.88                                | 99.15                              |
| Carbamazepine    | 17.72 | 22.97 | 39.80 | 2.62                          | 28.66                               | 0.00                                 | 98.40                              |
| Sulfamethoxazole | 21.54 | 31.85 | 43.21 | 0.00                          | 41.25                               | 1.74                                 | 94.56                              |