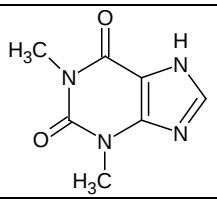
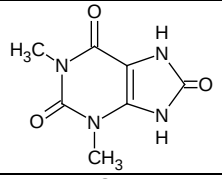
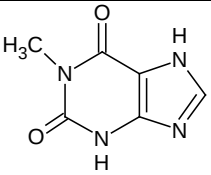
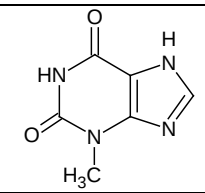
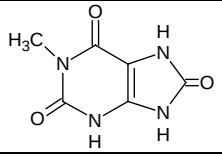
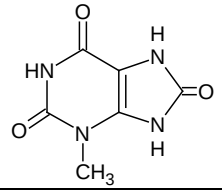
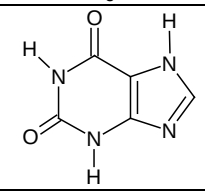
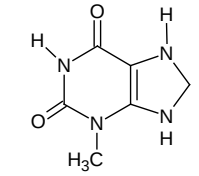
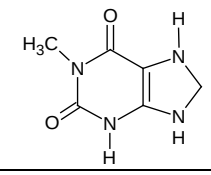
Electronic Supplementary Material (ESI) for Environmental Science: Nano.


**Table S1 –** Main products identified by LC-HR-ESI/MS during the photocatalytic degradation of theophylline

| Sl.no. | Product | Mol.wt. | Elemental composition | m/z | |
|---|---|---|---|---|---|
| --- | Theophylline | 180.16 | $C_7H_8N_4O_2$ | 181.0727 |  |
| I | 1,3-Dimethyluric acid | 196.16 | $C_7H_8N_4O_3$ | 197.0675 |  |
| II | 1-Methylxanthine | 166.14 | $C_6H_6N_4O_2$ | 167.0565 |  |
| III | 3-Methylxanthine | 166.14 | $C_6H_6N_4O_2$ | 167.0565 |  |
| IV | 1-Methyluric acid | 182.14 | $C_6H_6N_4O_3$ | 183.0518 |  |
| V | 3-Methyluric acid | 182.14 | $C_6H_6N_4O_3$ | 183.0518 |  |
| VI | Xanthine | 152.11 | $C_5H_4N_4O_2$ | 153.0410 |  |
| VII | 1/3-Methyltetrahydro-1*H*-purine-2,6-dione | 168.15 | $C_6H_8N_4O_2$ | 169.0720 |   |

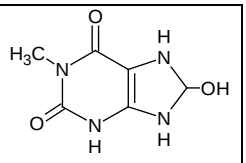
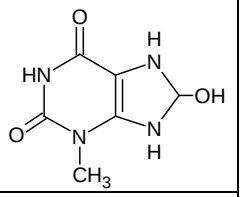
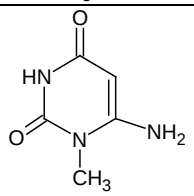
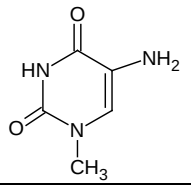
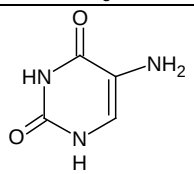
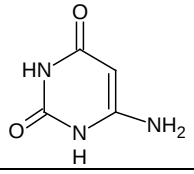
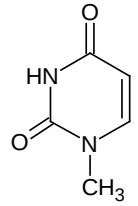
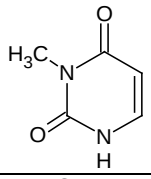
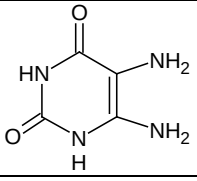
| | | | | | |
|---|---|---|---|---|---|
| VIII | 8-Hydroxy-1/3-methyl-3,7,8,9-tetrahydro-1*H*-purine-2,6-dione | 184.15 | $C_6H_8N_4O_3$ | 185.0669 |   |
| IX | 5/6-Amino derivative of 1/3-methylpyrimidine-2,4(1*H*,3*H*)-dione | 141.13 | $C_5H_7N_3O_2$ | 142.0611 |   |
| X | 5/6-Aminopyrimidine-2,4(1*H*,3*H*)-dione | 127.10 | $C_4H_5N_3O_2$ | 128.0454 |   |
| XI | 1/3-Methylpyrimidine-2,4(1*H*,3*H*)-dione | 126.11 | $C_5H_6N_2O_2$ | 127.0502 |   |
| XII | 5,6-Diaminopyrimidine-2,4(1*H*,3*H*)-dione | 142.12 | $C_4H_6N_4O_2$ | 143.0563 |  |

**Table S2 –** Main products identified by LC-HR-ESI/MS for the photodegradation of caffeine

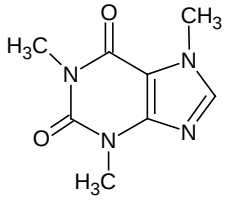
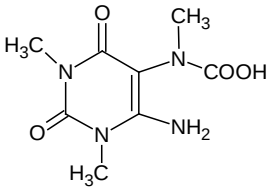
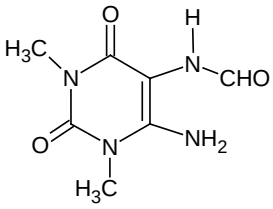
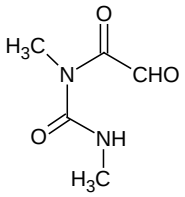
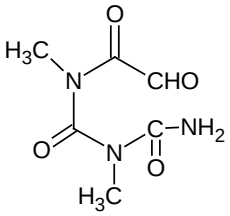
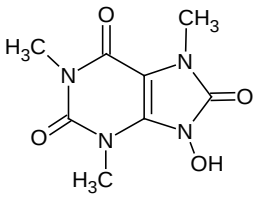
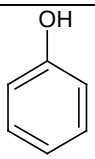
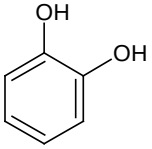
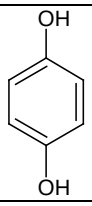
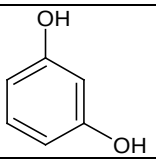
| Compound | Formula | Experimental mass (m/z) | Mol.wt. | structure |
|---|---|---|---|---|
| **Caffeine** | $C_8H_{11}N_4O_2$ | 195.0876 | 194 |  |
| **1** | $C_8H_{12}N_4O_4Na$ | 251.0751 | 228 |  |
| **2** | $C_7H_{11}N_4O_3$ | 199.0824 | 198 |  |
| **3** | $C_5H_8N_2O_3Na$ | 167.0426 | 144 |  |
| **4** | $C_6H_9N_3O_4Na$ | 210.0485 | 187 |  |
| **5** | $C_8H_{11}N_4O_4$ | 227.0774 | 226 |  |
| **6** | $C_8H_{10}N_4O_5Na$ | 265.0547 | --- | --- |
| **7** | $C_8H_9N_4O_4$ | 225.0620 | --- | --- |
| **8** | $C_7H_{10}N_3O_3$ | 184.0713 | --- | --- |
| **9** | $C_5H_7N_2O_2$ | 127.0499 | --- | --- |
| **10** | $C_5H_8N_3O_2$ | 142.0609 | --- | --- |
| **11** | $C_6H_8N_3O_3$ | 170.0560 | --- | --- |

**Table S3 –** Main products identified by GC-MS for the phenol photocatalytic degradation process

| **Product** | **Mol.wt.** | **Elemental composition** | |
|---|---|---|---|
| Phenol | 94 | $C_6H_6O$ |  |
| Catechol | 110 | $C_6H_6O_2$ |  |
| Hydroquinone | 110 | $C_6H_6O_2$ |  |
| Resorcinol | 110 | $C_6H_6O_2$ |  |

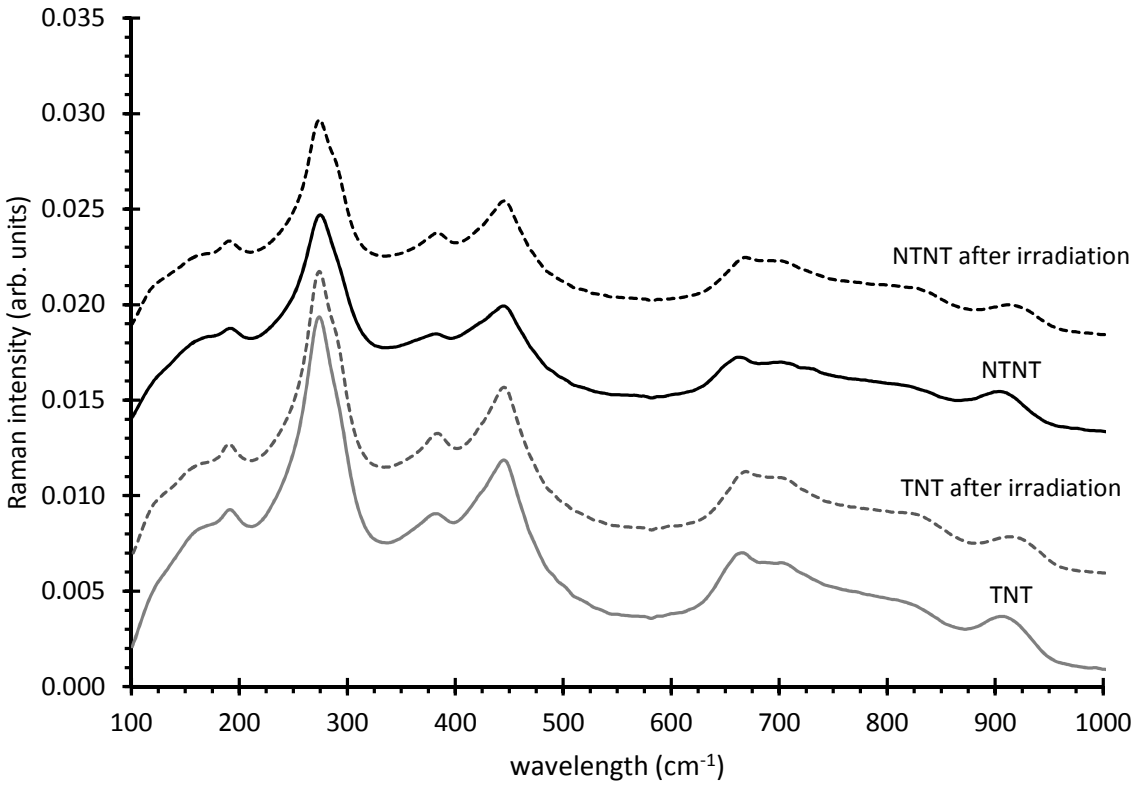



**Figure S1** – Raman spectra of the TNT and NTNT samples before and after being submitted to UV-vis radiation.