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# Mitigating Environmental Risks: Efficient Removal of Metronidazole from Pharmaceutical Wastewater Using Functionalized Graphene Membrane

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## INTRODUCTION


**Fig 2.** Metronidazole different form of its administration

- Metronidazole is commonly used antibiotic
- It belonging to the nitroimidazole class of antibiotics
- It can be administered as injectable or capsules
- It is used for treating gastrointestinal infections
- And it is also treated parasitic infections like trichomoniasis and giardiasis, and amebiasis

- It adverse reactions, which include brain toxicities[1].
- It long term use of drugs like metronidazole or ornidazole can cause toxicities like infertility[2].
- It is difficult to treat its abuse[2,3].

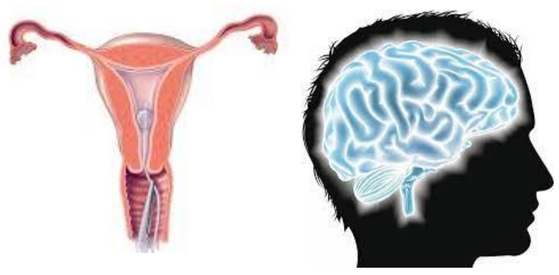

**Fig 2.** Human Part affected for when the drug is abused

## AIM

This study explores the potential of functionalized graphene membranes for the removal of metronidazole from industrial and pharmaceutical wastewater. Employing molecular simulations and the AM1 semi-empirical calculation method, we designed and simulated functionalized membranes to enhance metronidazole removal efficiency.

## METHOD

- Molecular modeling using AM1 semi-empirical method
- With evaluation of vacuum and aqueous system
- Adsorption strength calculation: **Eads = Eax – Ea – Ex**
- In the study, different material functionalization method like alcohol, acid, and others were explored.

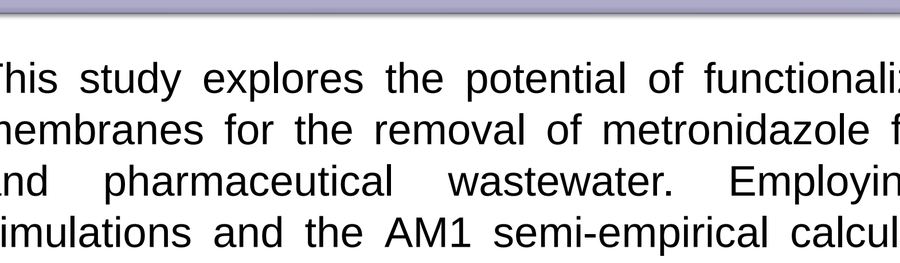


**Fig 3.** Surface Selectivity

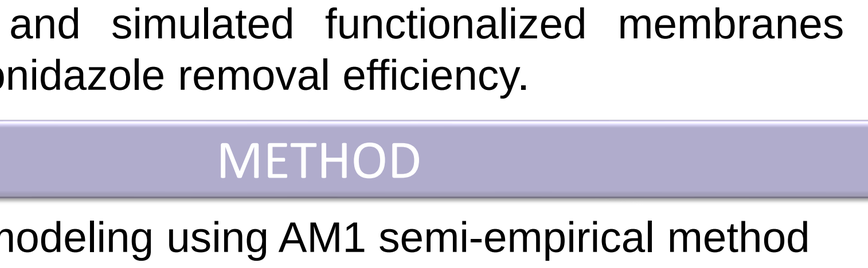


**Fig 4.** Surface adsorption across systems

## RESULTS & DISCUSSION

**Table 1:** The effect of water presence in metronidazole adsorption on the surfaces (all energies are in eV).

| Functionalization | $E_{ads}^{met,va}$ | $E_{ads}^{met,aq}$ | $E_{ads}^{met,va-aq}$ | $E_{ads}^{met,va-aq}$ % |
|---|---|---|---|---|
| **Normal (g-H)** | -0.06 | 0.06 | 0.12 | 200.00 |
| **Alcohol (g-OH)** | -0.36 | -0.06 | 0.3 | 83.33 |
| **Aldehyde (g-CHO)** | -0.21 | -0.13 | 0.08 | 38.10 |
| **Acid (g-COOH)** | -0.46 | -0.23 | 0.23 | 50.00 |
| **3rd Amine (g-CN)** | -0.15 | -0.07 | 0.08 | 53.33 |
| **2nd Amine (g-CHNH)** | -0.32 | -0.22 | 0.1 | 31.25 |
| **1st Amine (g-$CH_2NH_2$)** | -0.19 | 0.02 | 0.21 | 110.53 |

**Table 2:** The selectivity of the surface for metronidazole over water across the surfaces (all energies are in eV).

| Functionalization | $E_{ads}^{met}$ | $E_{ads}^{wat}$ | $E_{ads}^{met} > E_{ads}^{wat}$ | $E_{ads}^{met} - E_{ads}^{wat}$ |
|---|---|---|---|---|
| **Normal (g-H)** | 0.06 | -0.02 | FALSE | 0.08 |
| **Alcohol (g-OH)** | **-0.06** | **-0.05** | **TRUE** | **-0.01** |
| **Aldehyde (g-CHO)** | **-0.13** | **-0.03** | **TRUE** | **-0.10** |
| **Acid (g-COOH)** | -0.23 | -0.29 | FALSE | 0.06 |
| **3rd Amine (g-CN)** | **-0.07** | **-0.03** | **TRUE** | **-0.04** |
| **2nd Amine (g-CHNH)** | **-0.22** | **-0.17** | **TRUE** | **-0.05** |
| **1st Amine (g-$CH_2NH_2$)** | **0.02** | **0.07** | **TRUE** | **-0.05** |

**Note:** Met = Drug, Wat = Water, va = Vacuum system, aq = Aqueous system

## CONCLUSION

- Functionalized membranes show selective adsorption for metronidazole, promising efficient wastewater treatment.
- Adsorptive properties significantly drop for most membranes, except aldehyde (-CHO) and secondary amine (-CHNH) functionalized ones.
- Aldehyde-functionalized graphene membranes exhibit superior selective adsorption of metronidazole over water.
- Functionalized graphene membranes have strong potential for mitigating pharmaceutical effluent risks.
- Improved understanding of adsorption processes can lead to better wastewater treatment technologies.

## REFERENCES

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WAVEFUNCTION

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