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Enhanching Radiotherapy with High-Z doped Nitroimidazoles

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A way to induce local damage to cancerous tissue is by using radiotherapy-amplifying bioagents doped with high-Z elements. This enables deep core-level ionisation during radiotherapy with X-rays above the K-edge threshold, significantly increasing radiation absorption. Core electron ejection from high-Z elements also triggers a cascade of secondary particles, amplifying damage.
We studied the iodine- and bromine-doped nitroimidazole molecule, an oxygen mimetic that accumulates in oxygen-deficient tumours. We analysed fragmentation mechanisms and radiotherapy-relevant fragments in the gas phase using synchrotron light tuned to K- and L-edges. Additionally, DFT-based molecular dynamics simulations explored bond strengths and fragmentation pathways. To approximate biological conditions, we also examined monosolvated nitroimidazole.
High-Z ionisation produces large quantities of single-atom ions, while C, N, or O 1s-ionization yields heavier fragments like NO2, which can inhibit DNA repair. The addition of a single water molecule affects the local chemical environment and is thus reshaping the dissociation landscape, possibly through hydrogen bonding and charge redistribution—suggested to protect biomolecules from radiation damage.

Scholarship elegibility

no

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