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A promotional banner for the 240th ECS Meeting. The banner features a colorful striped border at the top. On the left, the ECS logo is displayed in a green circle. To the right of the logo, the text reads: "240th ECS Meeting", "Digital Meeting, Oct 10-14, 2021", "We are going fully digital!", "Attendees register for free!", and "REGISTER NOW" in bold orange letters. On the right side of the banner, there is a photograph of a diverse group of people in a professional setting, with a man in a white shirt and tie clapping and smiling.

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Influence of ionizing radiation on molecular recognition in the gas phase: VUV and X-ray photoabsorption of antibiotic-receptor non-covalent complexes

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Synopsis The intrinsic effects of ionizing radiation on molecular recognition between an antibiotic and its receptor have been probed by coupling a synchrotron beamline to a tandem mass spectrometer. Protonated vancomycin-receptor non-covalent complexes in the gas phase undergo inter- as well as intramolecular bond cleavage due to internal energy transfer after photoabsorption in the VUV-X energy range. The deprotonated complex undergoes electron detachment, but the native interactions underlying molecular recognition are not systematically lost.

The structure of biological molecules plays an important role in their activity, especially in the molecular recognition between drugs and their receptors. This is illustrated in figure 1 for the glycopeptide antibiotic vancomycin bound to its peptidic receptor Ac₂-Lys-DAla-DAla in condensed phase, where the two structures tightly fit each other. When isolated in the gas phase, this native structure is lost for gas-phase protonated but retained for deprotonated complexes.[1,2] Moreover, in the case of a chemio-radiotherapy to cure cancer, drugs can interact with ionizing radiation. Therefore, it is crucial to know if molecular recognition is affected by irradiation. We have thus studied photoionization of isolated protonated as well as deprotonated vancomycin/receptor complexes by means of a synchrotron beamline coupled to a tandem mass spectrometer, which allowed identifying the irradiation products. After absorption of one VUV photon by doubly-protonated Vancomycin, we observe non-dissociative ionization (NDI), but also peptide backbone fragmentation as well as sugar bond cleavages due to electronic to vibrational energy transfer. The latter rises with photon energy, making NDI to vanish at X-ray energies. For the doubly protonated vancomycin-receptor complex, NDI is not observed following photoabsorption, probably because of the low binding energy of this non-covalent complex. Interestingly, when deprotonated, the intact complex is observed after electron detachment, together with fewer fragmen-

tation channels, the main ones being loss of receptor and CO₂. The latter comes only from vancomycin, not from the receptor, which can be explained by the retained native structure of the deprotonated complex, where the receptor's CO₂ group is strongly bound to Vancomycin, even after electron detachment. Our results indicate that the geometrical structure of a drug-receptor complex has a large effect on the processes induced by photon irradiation in the VUV-X energy range. Furthermore, molecular recognition is not systematically lost after photoabsorption.

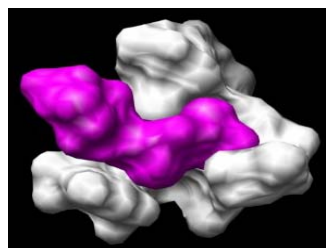


Figure 1. molecular surfaces of the native structure of vancomycin (white) and its receptor (purple) in a crystal (Protein Data Bank 1FVM).

References

- [1] Pouilly J C *et al* 2010 *International Journal of Mass Spectrometry* **297** 28–35
- [2] Pouilly J C *et al* 2010 *Phys. Chem. Chem. Phys.* **12** 3606

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