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Crystal structures of the selenoprotein glutathione peroxidase 4 in its apo form and in complex with the covalently bound inhibitor ML162

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The selenoprotein GPX4 is a potential cancer drug target. Inhibitors covalently target the active site selenocysteine. Co-crystallization with covalent inhibitors initially failed, most likely due to heterogenous covalent modification. A mass spec-based approach to monitor cysteine modification, together with a surface cysteine mutation, enabled the structure determination of GPX4 with the covalent inhibitor ML162 and opens the path to further inhibitor co-complex structures of this drug target.

Primary author: HILLIG, Roman

Presenter: HILLIG, Roman

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