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A structural biology approach for the discovery of aldehyde dehydrogenases 1A isozymes specific inhibitors

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The more than a century years old NAD(P)H still triggers a wealth of investigations that mainly focus on its role in signalling and aim to develop novel drugs that interfere with specific aspects of such a process in different pathological conditions. However, the cofactor plays a key, essential and long studied role as a redox molecule in central metabolism, a source of robust drug targets for the treatment of several pathologies, ranging from infective diseases to cancer. In this context, NAD(P)H dependent dehydrogenases are amongst the most studied and exploited enzymatic drug targets. Independently on the specific disease, a major issue in targeting NAD(P)H dependent dehydrogenases is represented by the selectivity of drug action. Within this context, we show that potent hit/lead compounds selectively targeting different isozymes of the human aldehyde dehydrogenases 1A sub-family can be identified for the development of novel therapeutic interventions to fight cancer.

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