This week in techniques

Approach	Summary	Licensing status	Publication and contact information
Computational models			
Rational design platform to generate dual-acting kinase and bromodomain inhibitors	<i>In vitro</i> studies suggest dual-acting kinase and bromodomain inhibitors can be rationally designed to treat cancer and inflammatory disease. <i>In vitro</i> , 9 of 628 structurally diverse kinase inhibitors potently inhibited bromodomain containing 4 (BRD4). In cultured multiple myeloma (MM) cells, two dual-acting kinase inhibitors suppressed expression of <i>c-Myc</i> (<i>MYC</i>)—a marker of BRD4 inhibition—whereas compounds that blocked the same kinase targets without inhibiting BRD4 did not. Structural studies suggested pharmacophores for the kinase and bromodomain inhibitory activities overlapped but had distinct features, so the activities could be independently optimized. Next steps include synthesizing inhibitors with potency optimized for both target classes.	Platform unpatented; licensing status not applicable	Ciceri, P. <i>et al. Nat. Chem. Biol.</i> ; published online March 2, 2014; doi:10.1038/nchembio.1471 Contact: Stefan Knapp, University of Oxford, Oxford, U.K. e-mail: stefan.knapp@sgc.ox.ac.uk Contact: Daniel K. Treiber, DiscoveRx Corp., San Diego, Calif. e-mail: dtreiber@discoverx.com
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