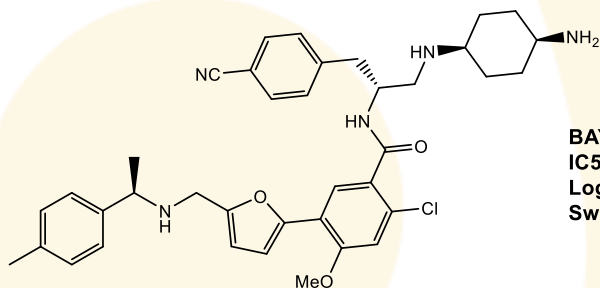


BAY-850, discovery of an ATAD2 chemical probe with unprecedented mode of action

On behalf of Bayer HealthCare, a chemistry Hit-to-Lead optimization program was conducted by Edelis against ATAD2.

The epigenetic regulator ATAD2 has been proposed to play a key role in cancer control, however, further validation of the role of ATAD2 in different cancer indications was limited by the absence of selective, potent and cell active ATAD2 inhibitors. We conducted the medicinal chemistry optimization of several chemical series of ATAD2 bromodomain binders initially identified from DNA-encoded compound libraries.



BAY-850
IC₅₀ = 22 nM
LogD(7.5) = 2.9
Sw (6.5) > 500mg/L

After rounds of potency and properties optimization, our efforts resulted in the identification of BAY-850, a potent and cell active isoform-selective ATAD2 chemical probe showing unprecedented chemical structure and mode of action.

Isoform-Selective ATAD2 Chemical Probe with Novel Chemical Structure and Unusual Mode of Action. [DOI: 10.1021/acscchembio.7b00708](https://doi.org/10.1021/acscchembio.7b00708)