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Structural optimization of pyridine-type DAPY derivatives to exploit the tolerant regions of the NNRTI binding pocket

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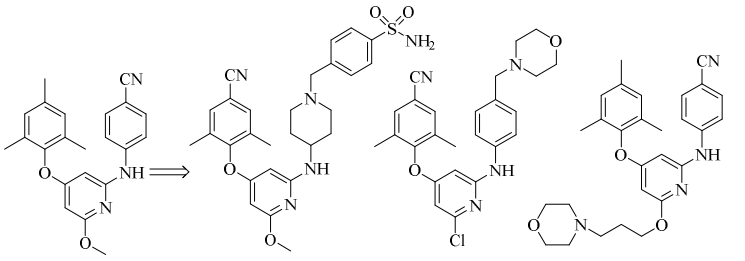
Pyridine-type DAPY derivatives were modified using the piperidyl or morpholinyl group to exploit the tolerant regions of RT NNRTI binding pocket.



6c
$EC_{50\ (IIIB)}$=0.84 μM;
$EC_{50\ (Y181+K103)}$> 29 μM

I-8c3
$EC_{50\ (IIIB)}$= 0.0078 μM;
$EC_{50\ (Y181+K103)}$ = 6.8 μM

II-4b
$EC_{50\ (IIIB)}$= 0.93 μM;
$EC_{50\ (Y181+K103)}$> 6.9 μM

II-6a
$EC_{50\ (IIIB)}$= 1.1 μM;
$EC_{50\ (Y181+K103)}$> 18.8 μM