PIPAc: towards flow chemistry and artificial intelligence powered API production

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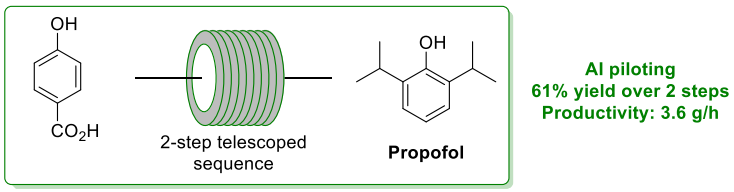
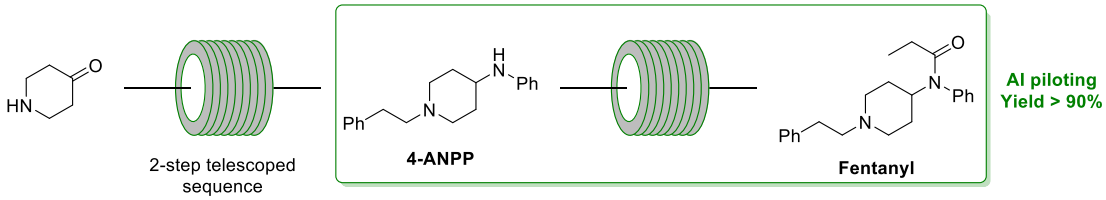
The use of flow chemistry [1] and artificial intelligence[2] in the production of API has witnessed significant interest both from academia and industry over the last years. Propofol[3] and fentanyl[4] are standing as privileged target because they experience shortage during COVID-19 crisis and are on the WHO's list of essential medicine. The PIPAc project aim is to bring the first AI-powered autonomous industrial demonstrator for APIs manufacturing through the combination of continuous flow chemistry, artificial intelligence, and additive manufacturing. In this frame, we successfully:

1) developed a two-step sequence towards propofol including intermediate in-line work-up and implemented an AI-agent to pilot the process:



2) translated fentanyl synthesis under flow conditions. A 2-step sequence allows the synthesis of penultimate fentanyl intermediate 4-ANPP while the final stage is piloted by AI using in-line ^{1}H NMR:



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