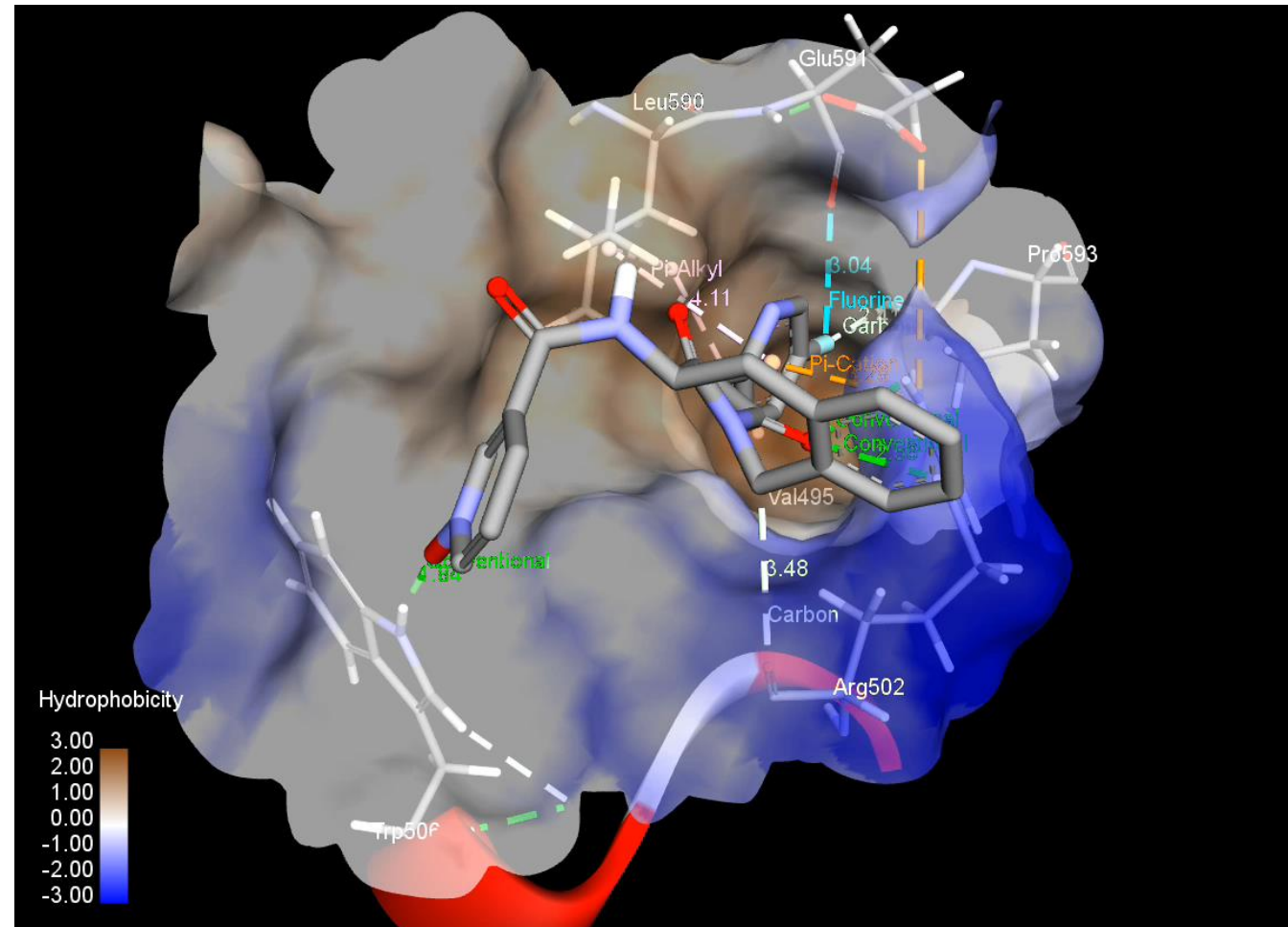
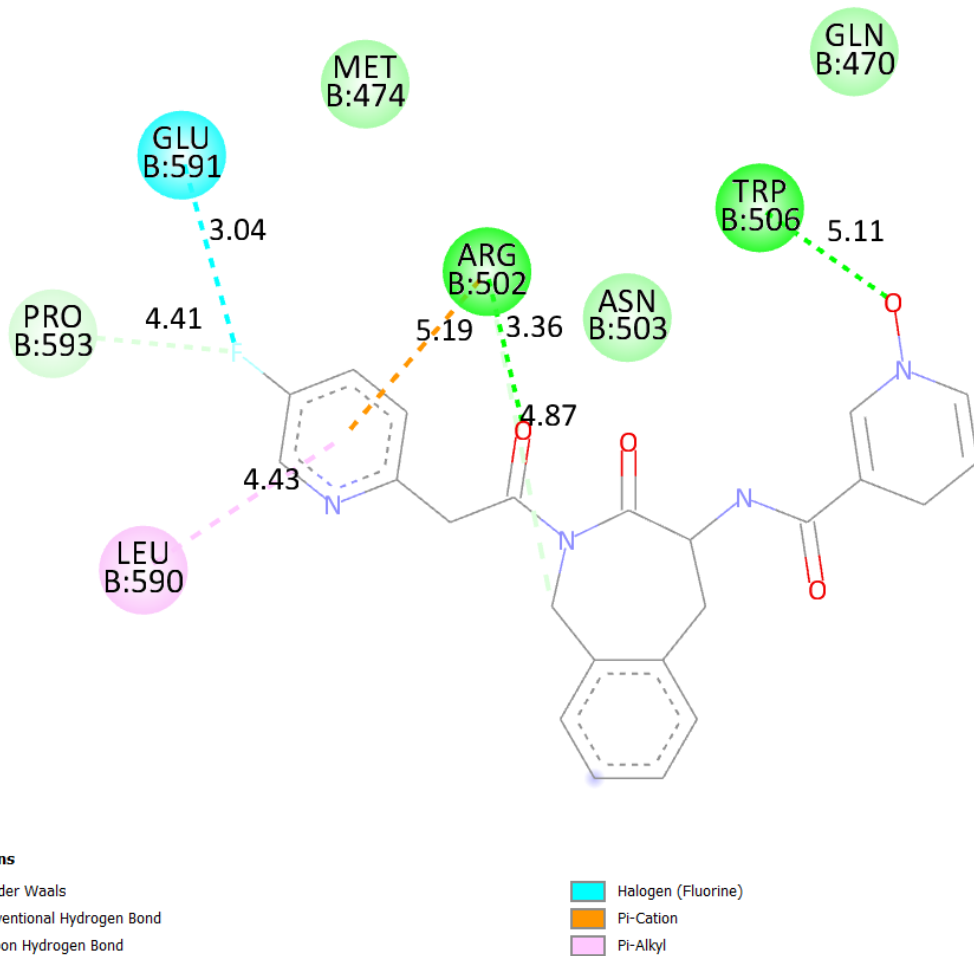
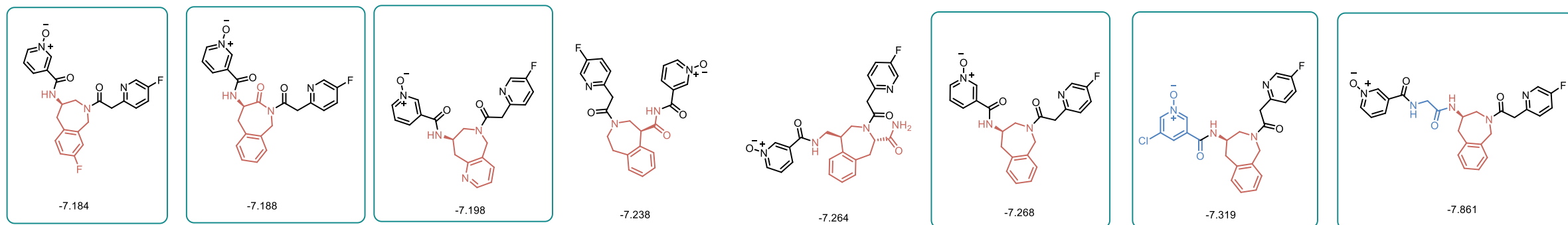


De-Novo Generated Top 100 Scoring Compounds: Benzoazepine series

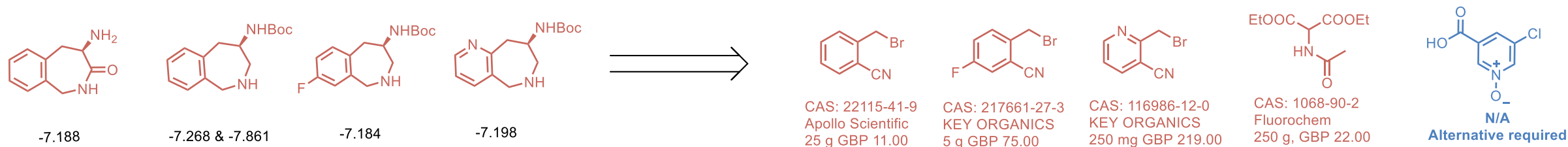


De-Novo Generated Top 100 Scoring Compounds:

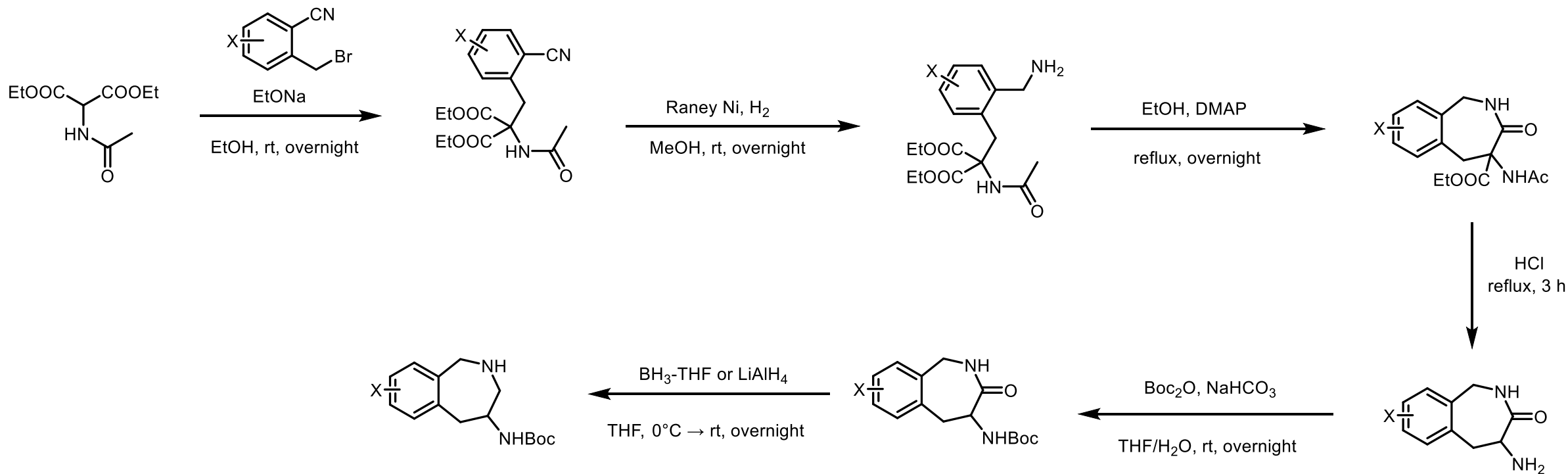
- **Benzoazepine series; 8 compounds total, currently targeting six using a general approach.**



- **Six non-commercial building blocks; four commercial starting materials.**



Benzoazepine route



Benzoazepine synthesis:

Romero, Donna L.; et al World Intellectual Property Organization, WO2021050992 A1 2021-03-18, [00453], pg 187 onwards.

Amide reduction:

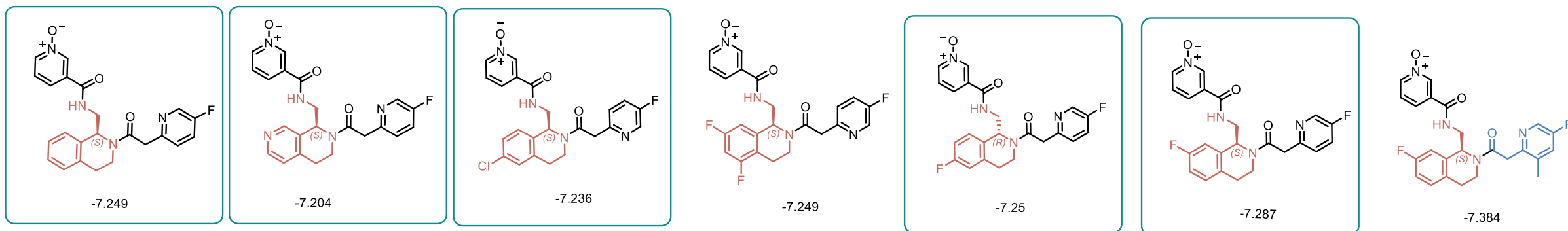
Zawodny, Wojciech; et al. Journal of the American Chemical Society (2018), 140(51), 17872-17877.

Shonberg, Jeremy; et al. Journal of Medicinal Chemistry (2015), 58(13), 5287-5307.

WO 2020/197991, pg 271 or 187, Compound 80a.

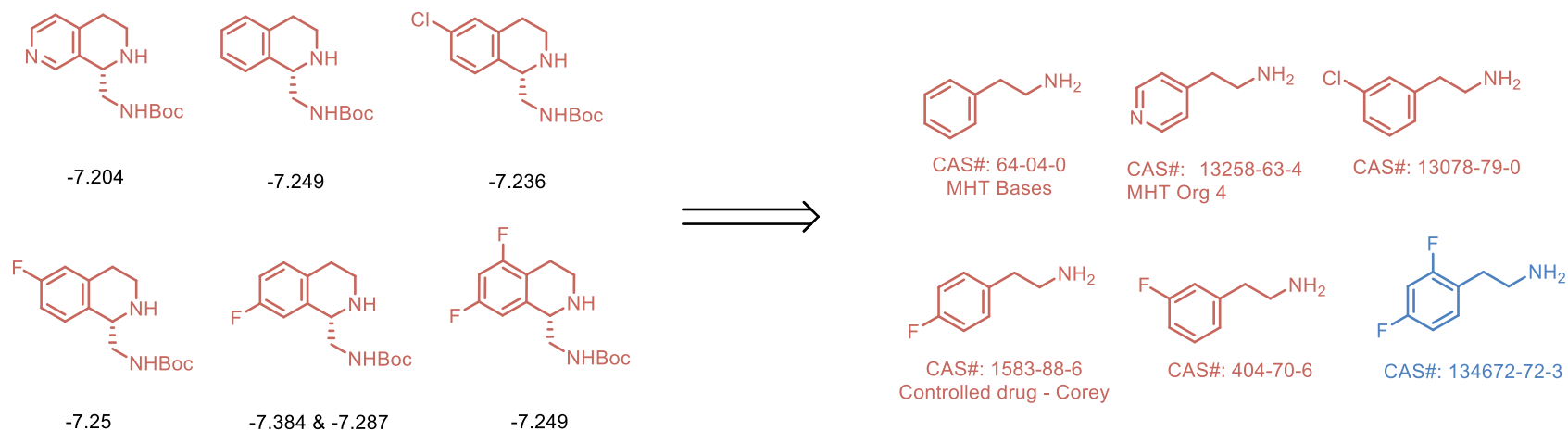
De-Novo Generated Top 100 Scoring Compounds:

- 1,2,3,4-tetrahydroisoquinolin-1-yl methanamine series; seven compounds.



Maestro GLIDE Score

- Six non-commercial building blocks; four commercial starting materials.



(1,2,3,4-tetrahydroisoquinolin-1-yl)methanamine series: E-rich and E-poor routes

Electron-rich Aryl route: Chen, Sheng-Ren; et al *European Journal of Medicinal Chemistry* (2017), 126, 202-217

