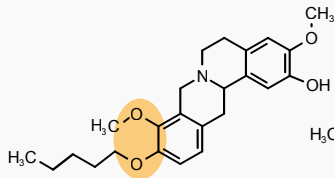
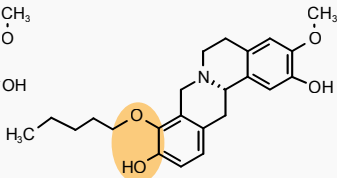
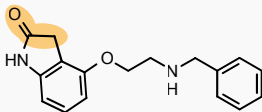
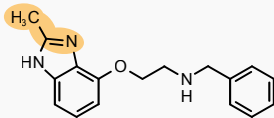


a

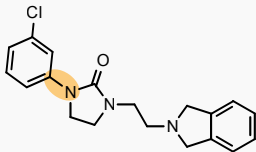
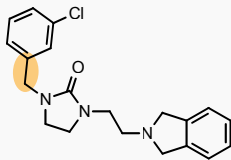
Substructure similarity

 $K_i = 101 \text{ nM}$  $K_i = 3213 \text{ nM}$ **b**

Scaffold similarity

 $K_i = 3 \text{ nM}$  $K_i = 95 \text{ nM}$ **c**

SMILES similarity

 $K_i = 3 \text{ nM}$  $K_i = 126 \text{ nM}$