Operation 1: Six-membered ring/ five membered ring exchange [#6,#7:1][C:2]c1ccc([C:3][#6,#7:4])cc1>>[#6,#7:1][C:2]c1sc([C:3][#6,#7:4])cc1 [#6,#7:1][C:2]c1ccc([C:3][#6,#7:4])cc1>>[#6,#7:1][C:2]c1scc([C:3][#6,#7:4])c1



Operation 2: Ring linkage



[cH:1][c:2][C:3][NH3+:4]>>[c:1]2ccc([C:3][NH3+:4])c[c:2]2

## Operation 3: Ring fusion [cH:1][c:2][C:3][NH3+:4]>>[c:1]2sc([C:3][NH3+:4])c[c:2]2





Operation 4: Primary amine/secondary amine exchange [c:1][C][NH3+]>>[nH+:1]



Operation 5: Linker length increase [#6:1][CH2:2][NH3+:3]>>[#6:1][CH2:2][CH2][NH3+:3]



Operation 6: Linker length decrease

Operation 7: Linker position change [cH:1][c:2][C:3]>>[cH:2][c:1][C:3]