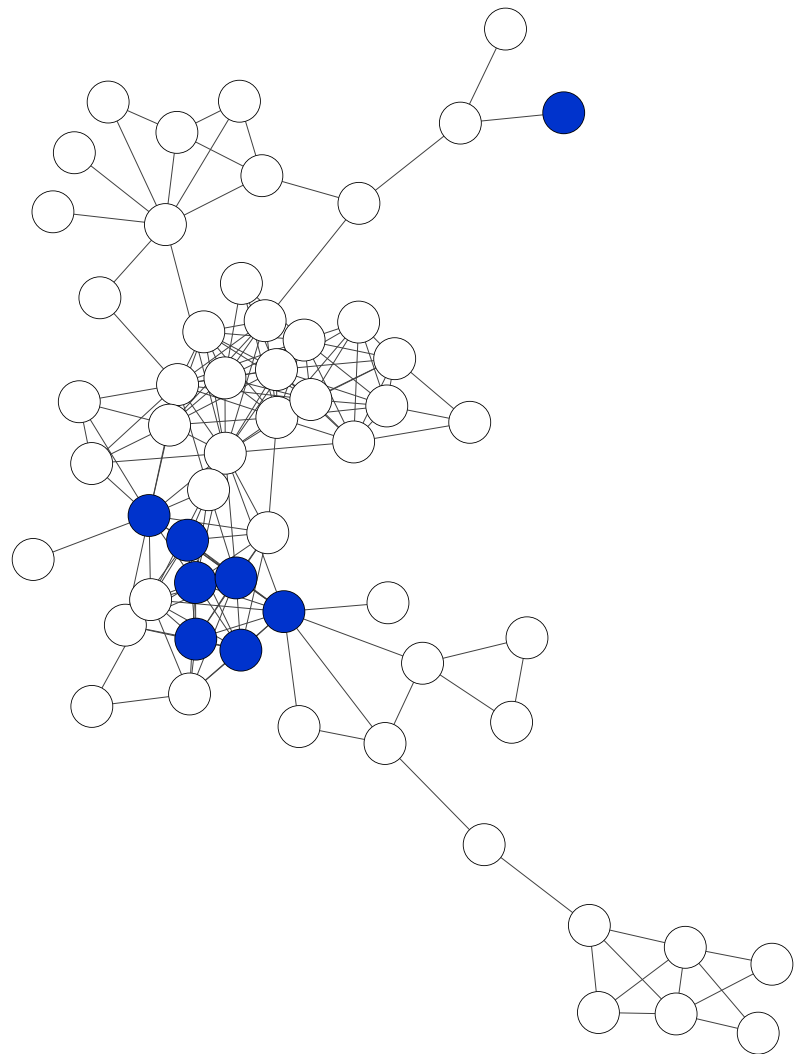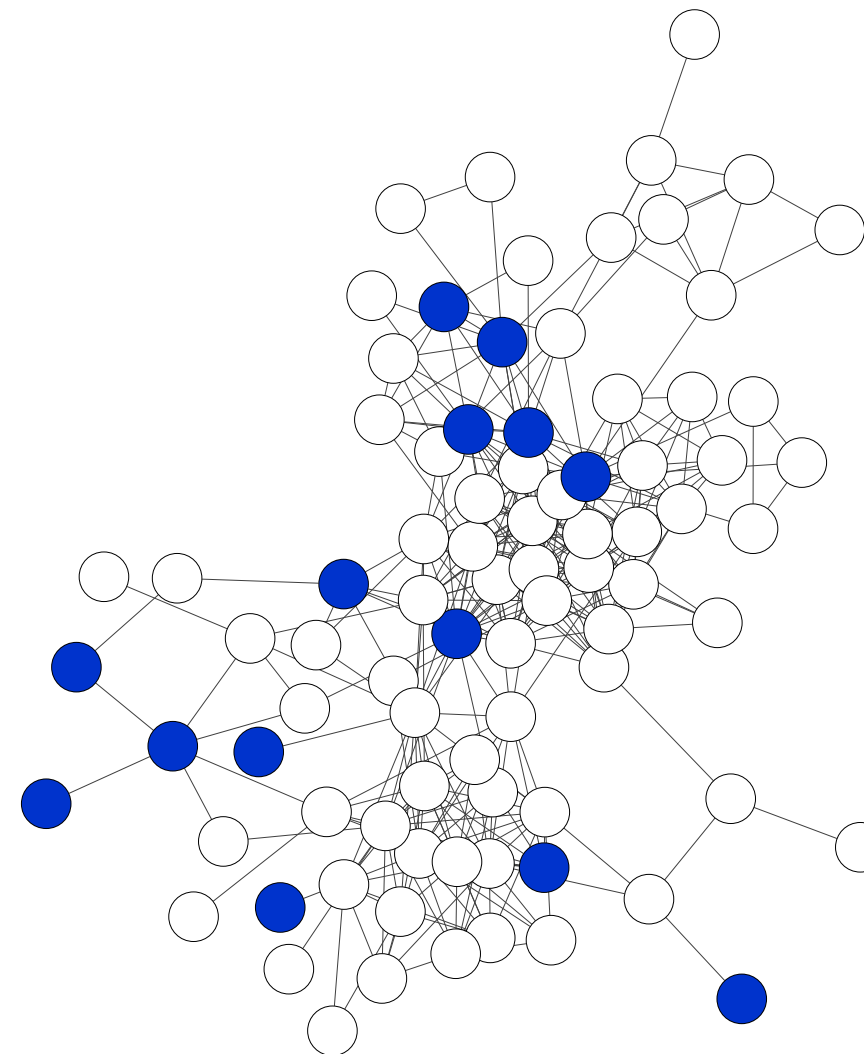**Before optimization**

57 nodes

8 GNPS hits

3 unique library hits

(hydroquinidine, nicotinamide
quinidine)

After optimization

85 nodes

14 GNPS hits

10 unique library hits

(cinchonine, cis-4-hydroxy-D-proline
genistein, hydroquinidine, quinidine,
lolilolide, lupinine, maprotiline HCl,
4-quinoline carboxylate, 12-
hydroxy-6-epi-albrassitriol)