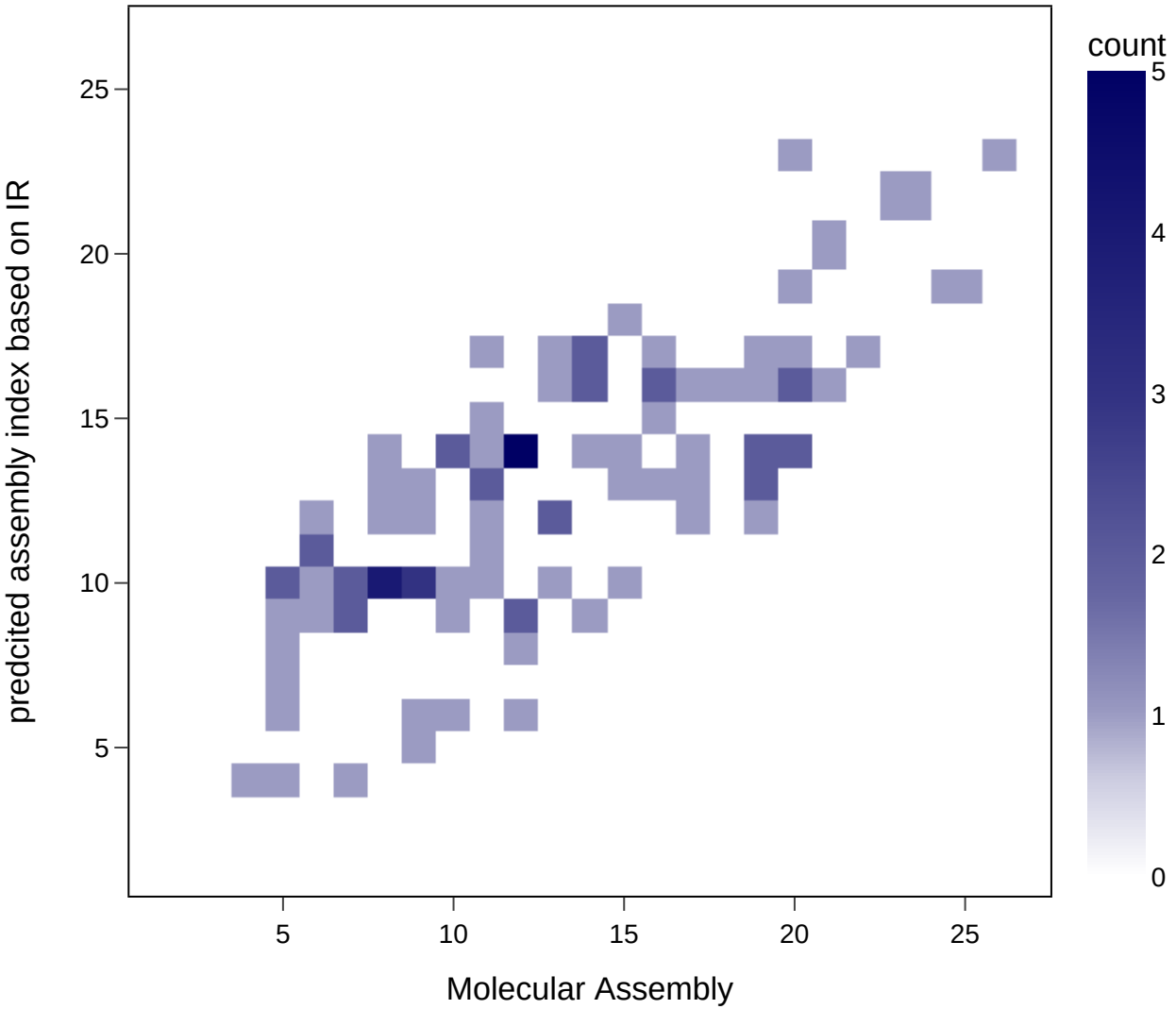predicted assembly index based on experimetal IR