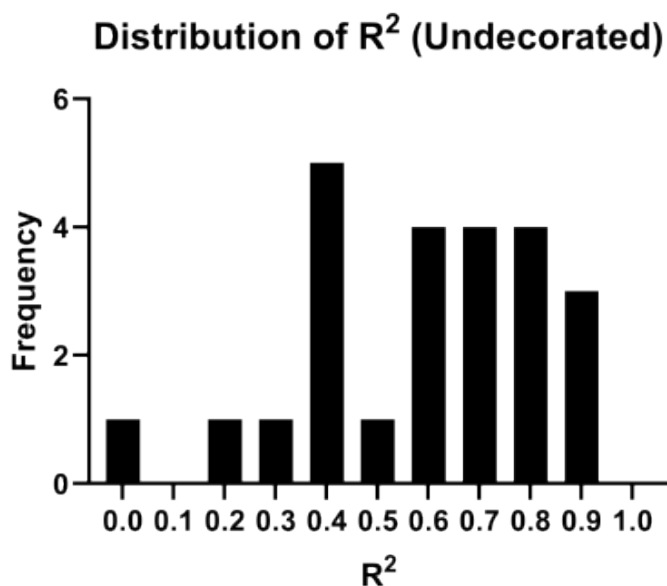


Figure S1. R^2 distribution for high-mannose compounds (total number of compounds = 8).



Distribution of R^2 (Undecorated, >0.1% abundance)

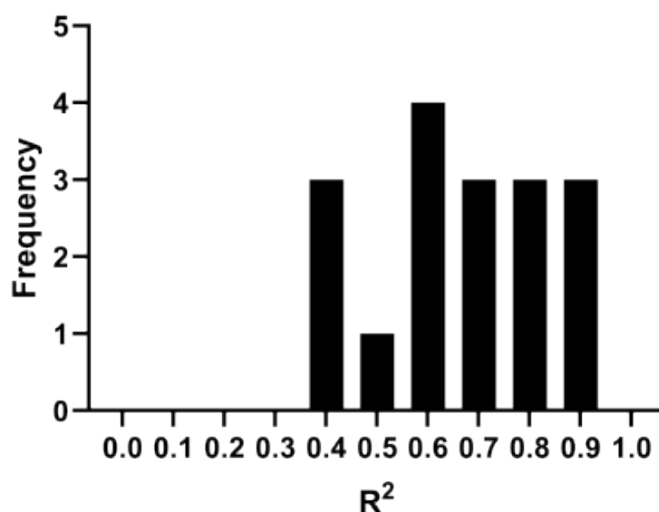


Figure S2. R^2 distribution for undecorated compounds (total number of compounds = 25). Applying an abundance cut-off of >0.1% abundance (total number of compounds = 18) filtered out the models with very poor performance ($R^2 < 0.3$)

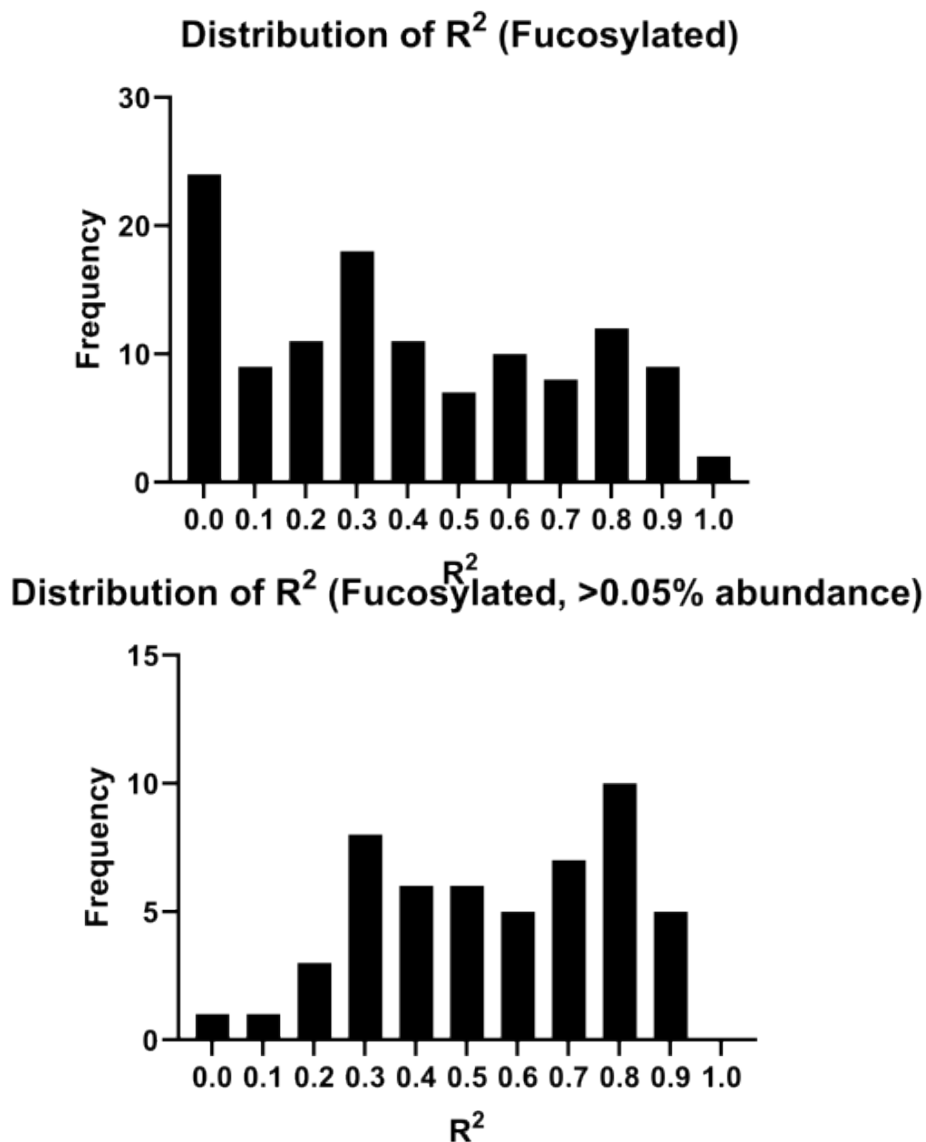


Figure S3. R^2 distribution for fucosylated compounds (total number of compounds = 121). Applying an abundance cut-off of $>0.05\%$ abundance (total number of compounds = 52) filtered out the models with very poor performance ($R^2 < 0.3$)

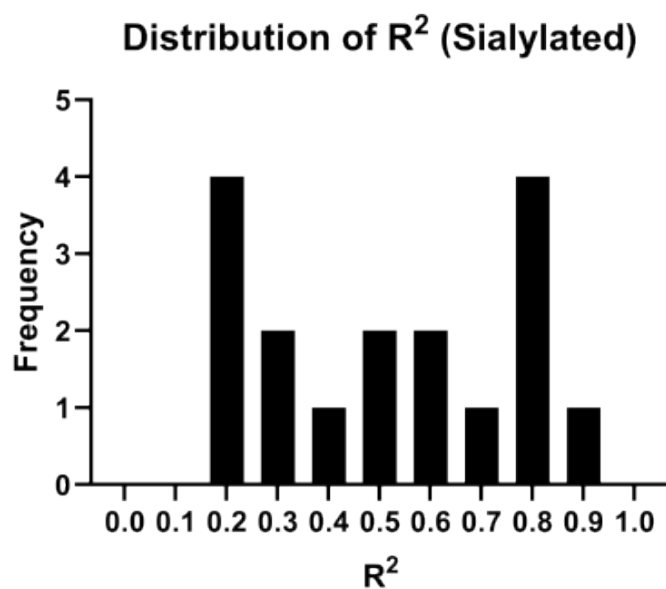
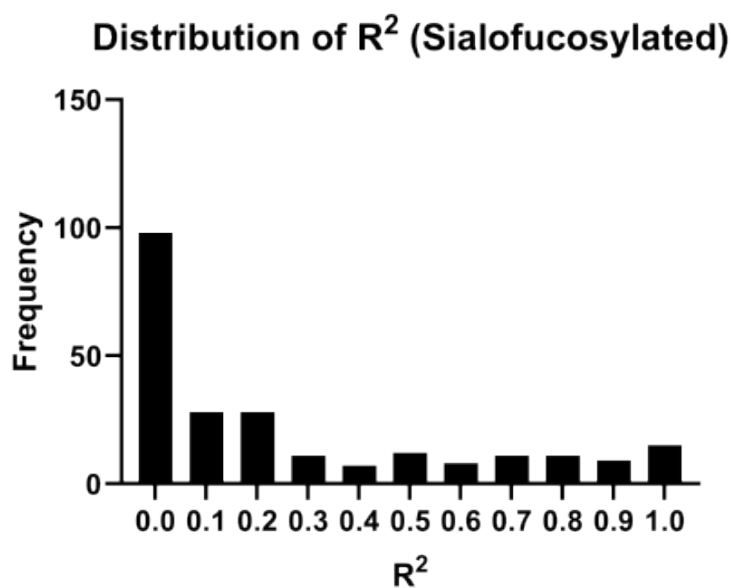


Figure S4. R^2 distribution for sialylated compounds (total number of compounds = 17).



Distribution of R^2 (Sialofucosylated, >0.05% abundance)

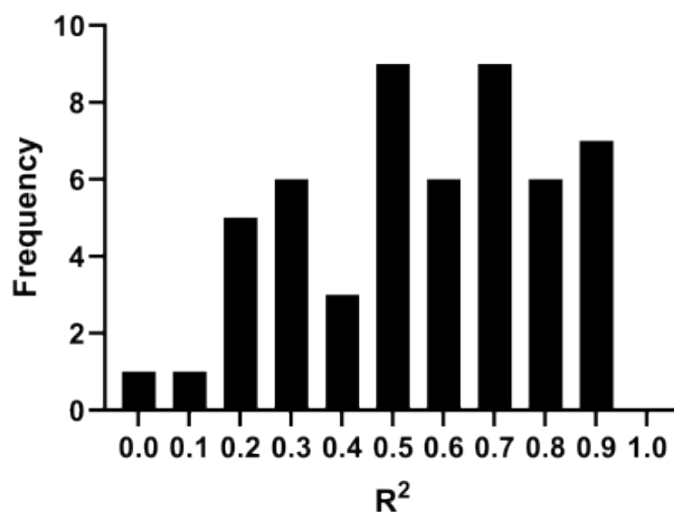


Figure S5. R^2 distribution for sialofucosylated compounds (total number of compounds = 238). Applying an abundance cut-off of >0.05% abundance (total number of compounds = 41) filtered out the models with very poor performance ($R^2 < 0.3$)