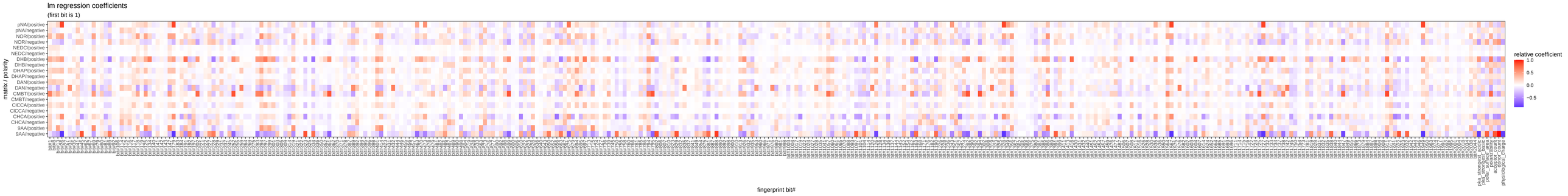
lm regression coefficients
(first bit is 1)
matrix / polarity
pNA/positive
pNA/negative
NOR/positive
NOR/negative
NEDC/positive
NEDC/negative
DHB/positive
DHB/negative
DHAP/positive
DHAP/negative
DAN/positive
DAN/negative
CMBT/positive
CMBT/negative
CICCA/positive
CICCA/negative
CHCA/positive
CHCA/negative
9AA/positive
9AA/negative
fingerprint bit#
relative coefficient
1.0
0.5
0.0
−0.5
pka_strongest_acidic
pka_strongest_basic
polar_surface_area
a_count
a_donor_count
physiological_charge