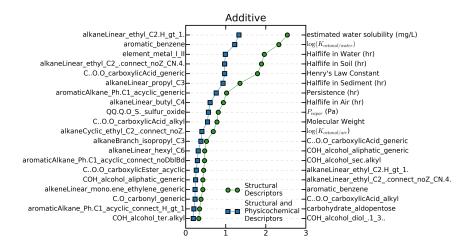
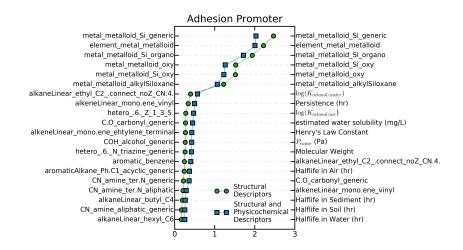
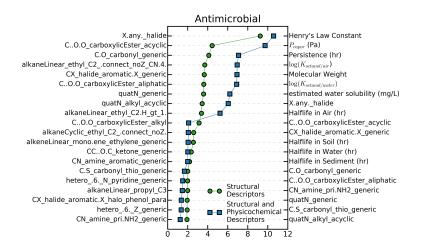
Electronic Supplementary Material (ESI) for Green Chemistry.

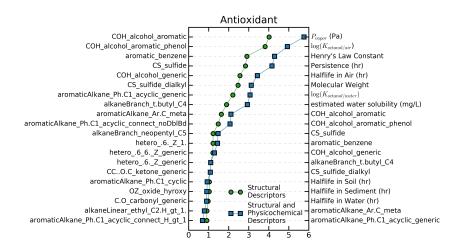
This journal is further Boyal Society of Chemistry 2016 actional Substitutes using Structure-based Classification Models – Supporting



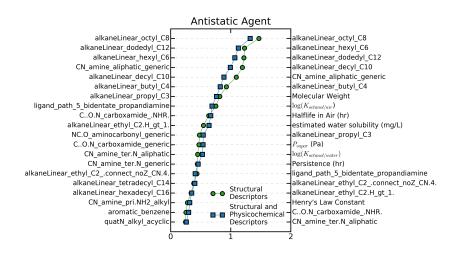


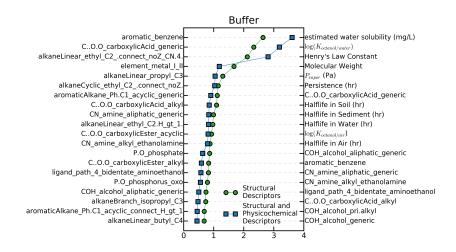


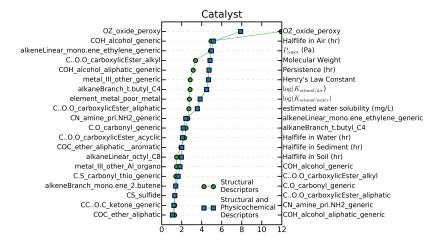


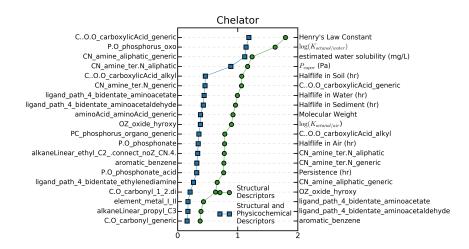


SI Figure 1: Most important variables for additive, adhesion promoter, antimicrobial, and antioxidant QSUR models.

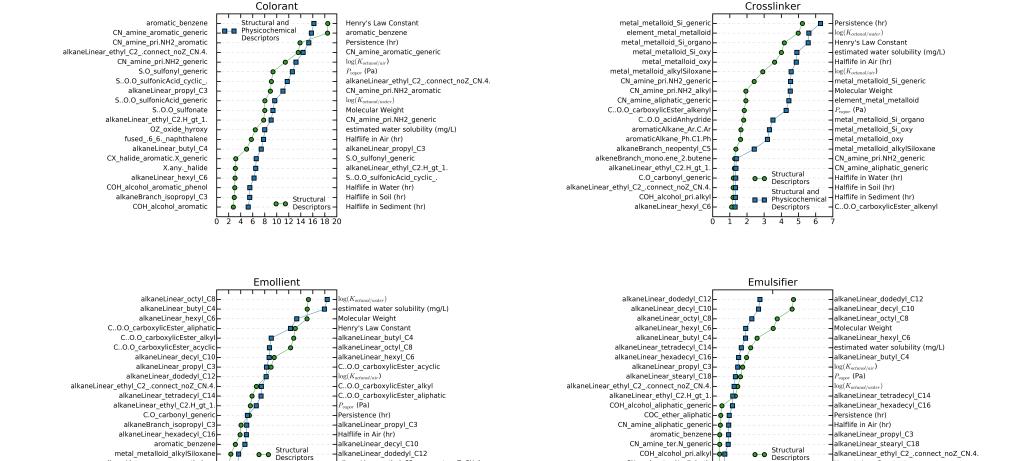








SI Figure 2: Most important variables for antistatic agent, buffer, catalyst, and chelator QSUR models.



SI Figure 3: Most important variables for colorant, crosslinker, emollient, and emulsifier QSUR models.

COH alcohol pri.alkyl

CN_amine_ter.N_aliphatic -

COH alcohol generic

oxy.alkaneLinear_ethyleneOxide_EO2

alkaneLinear dodedyl C12

alkaneBranch_isopropyl_C3

alkaneLinear ethyl C2.H gt 1.

alkaneLinear_ethyl_C2_.connect_noZ_CN.4.

Descriptors

0 1 2 3 4 5 6 7 8 9 10

Structural and

Physicochemical

Descriptors

metal metalloid alkylSiloxane

metal_metalloid_Si_orgar

metal metalloid Si oxy

alkeneLinear_mono.ene_ethylene

alkaneLinear ethyl C2 .connect noZ CN.4.

Henry's Law Constant

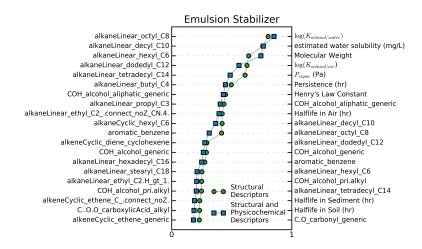
alkaneLinear ethyl C2.H gt 1.

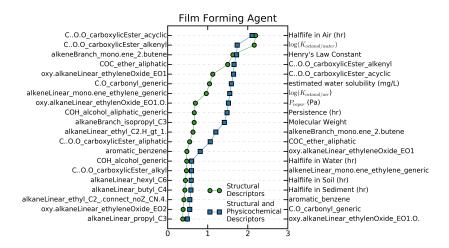
COH_alcohol_aliphatic_generic

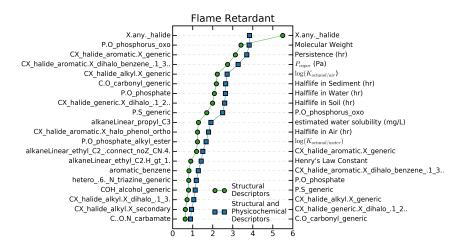
Structural and

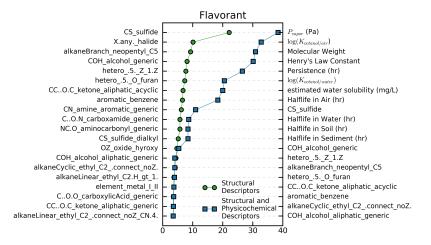
■ Physicochemical

Descriptors

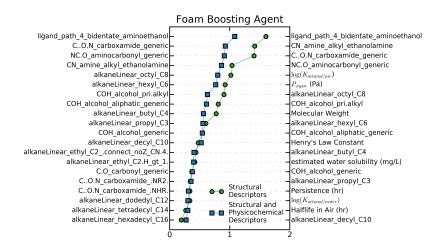


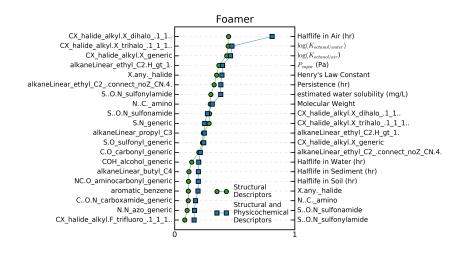


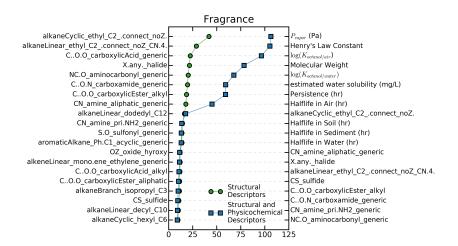


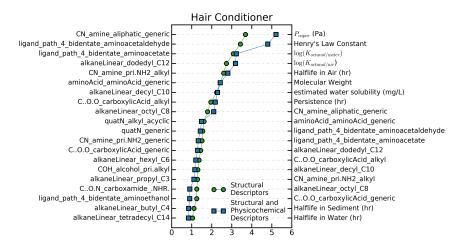


SI Figure 4: Most important variables for emulstion stabilizer, film forming agent, flame retardant, and flavorant QSUR models.

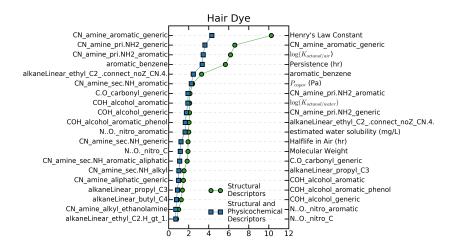


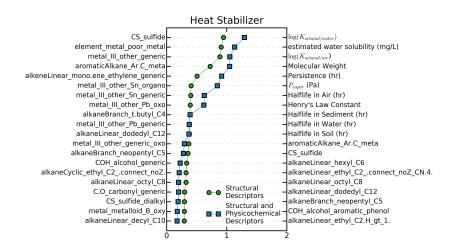


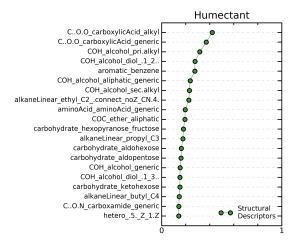


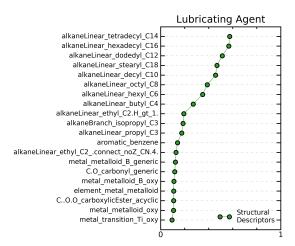


SI Figure 5: Most important variables for foam boosting agent, foamer, fragrance, and hair conditioner QSUR models.

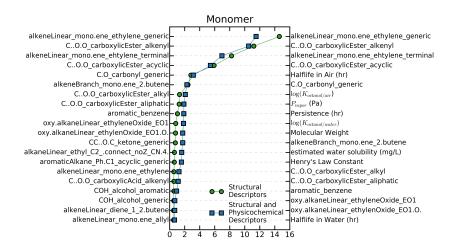


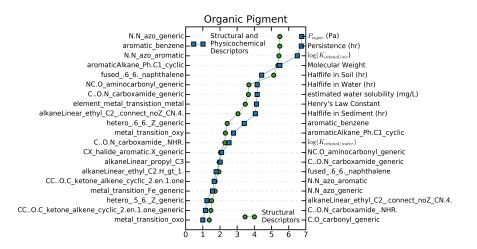


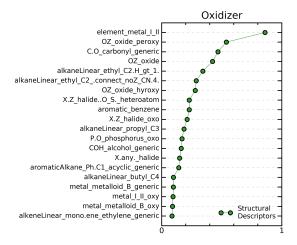


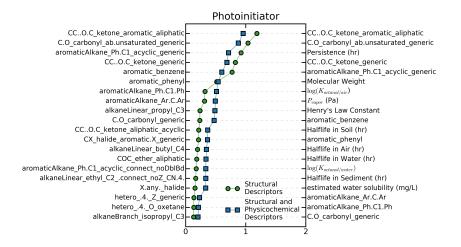


SI Figure 6: Most important variables for hair dve, heat stabilizer, humectant, and lubricating agent OSUR models,

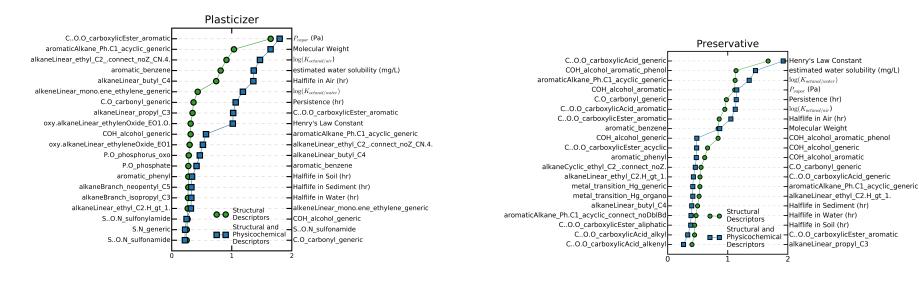


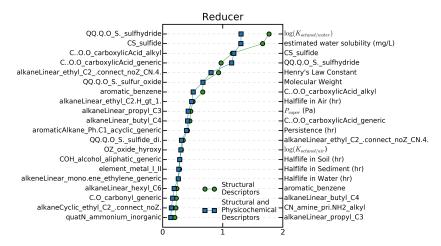


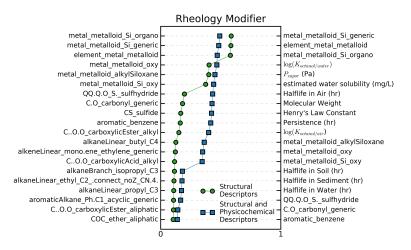




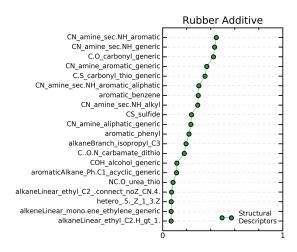
SI Figure 7: Most important variables for valid monomer, organic pigment, oxidizer, and photoinitiator QSUR models.

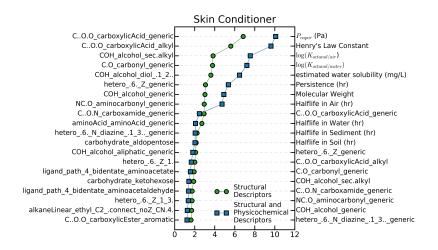


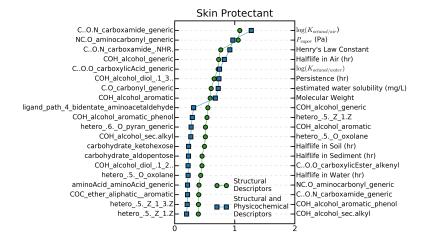


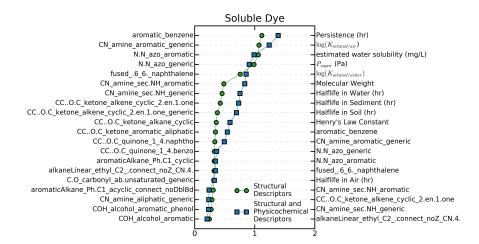


SI Figure 8: Most important variables for plasticizer, preservative, reducer, and rheology modifier QSUR models.

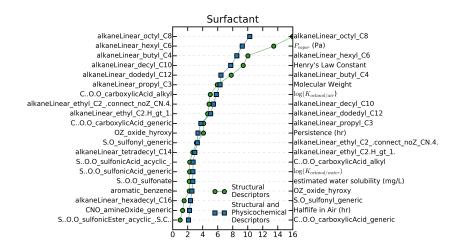


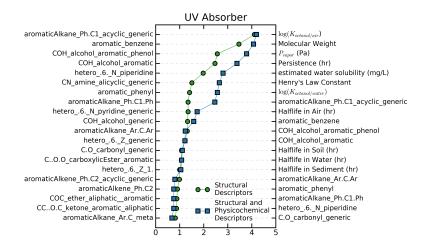


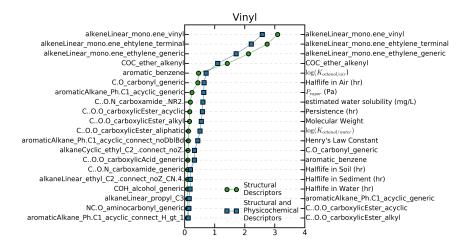


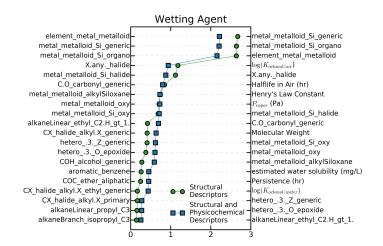


SI Figure 9: Most important variables for rubber additive, skin conditioner, skin protectant, and soluble dye QSUR models.

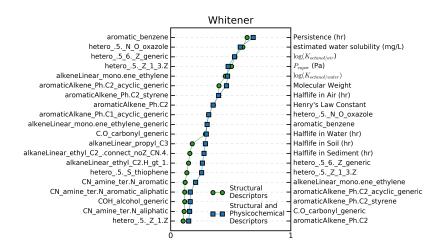








SI Figure 10: Most important variables for surfactant, UV absorber, vinyl, and wetting agent QSUR models.



SI Figure 11: Most important variables for whitener QSUR model.