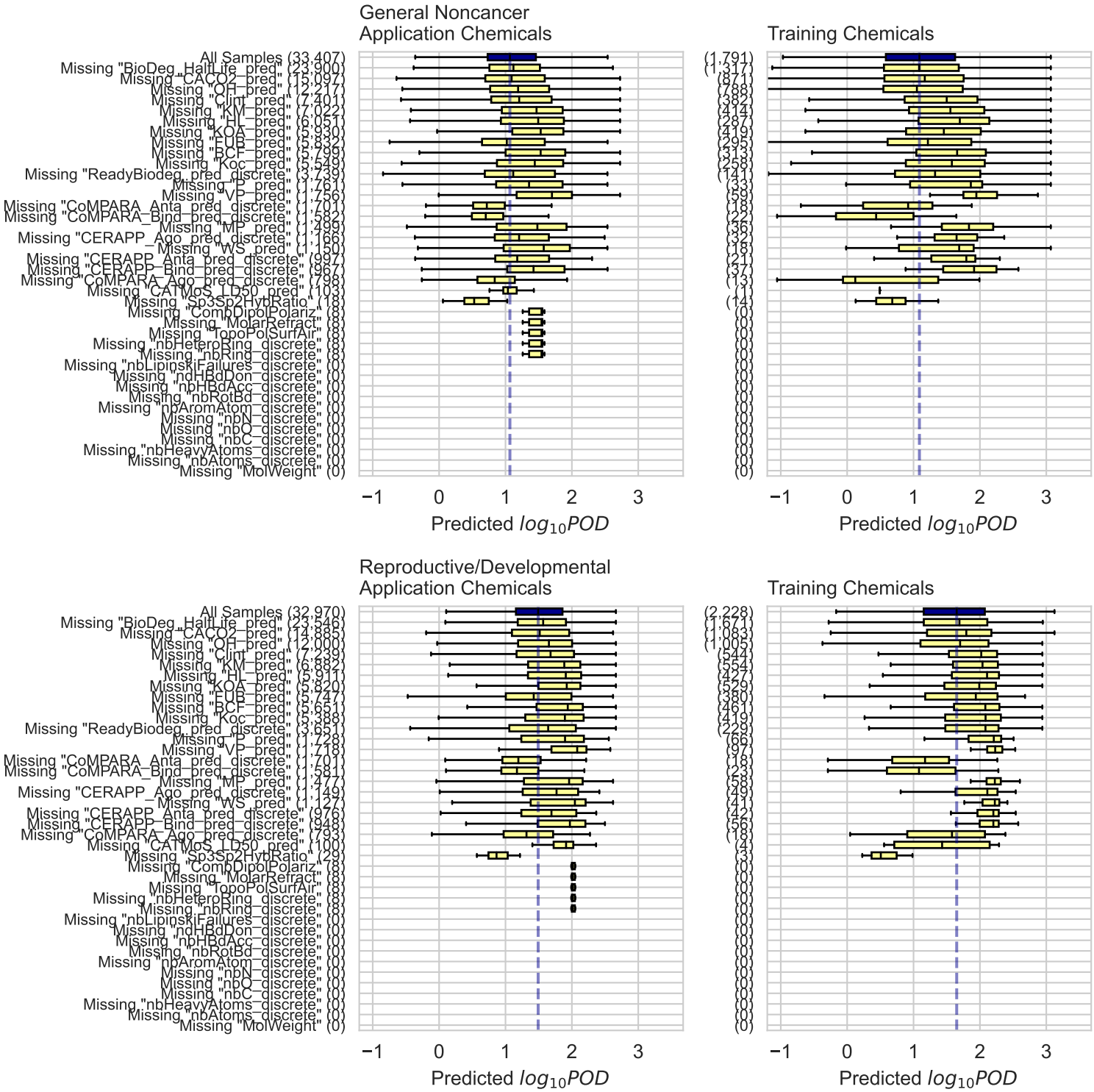
General Noncancer
Application Chemicals
Training Chemicals
All Samples (33,407)
Missing "BioDeg_HalfLife_pred" (23,900)
Missing "CACO2_pred" (15,097)
Missing "OH_pred" (12,217)
Missing "Clint_pred" (7,401)
Missing "KM_pred" (7,022)
Missing "HL_pred" (6,051)
Missing "KOA_pred" (5,930)
Missing "FUB_pred" (5,832)
Missing "BCF_pred" (5,799)
Missing "Koc_pred" (5,549)
Missing "ReadyBiodeg_pred_discrete" (3,739)
Missing "P_pred" (1,761)
Missing "VP_pred" (1,756)
Missing "CoMPARA_Anta_pred_discrete" (1,701)
Missing "CoMPARA_Bind_pred_discrete" (1,582)
Missing "MP_pred" (1,499)
Missing "CERAPP_Ago_pred_discrete" (1,166)
Missing "WS_pred" (1,150)
Missing "CERAPP_Anta_pred_discrete" (997)
Missing "CERAPP_Bind_pred_discrete" (967)
Missing "CoMPARA_Ago_pred_discrete" (798)
Missing "CATMoS_LD50_pred" (103)
Missing "Sp3Sp2HybRatio" (18)
Missing "CombDipolPolariz" (8)
Missing "MolarRefract" (8)
Missing "TopoPolSurfArr" (8)
Missing "nbHeteroRing_discrete" (8)
Missing "nbRing_discrete" (8)
Missing "nbLipinskiFailures_discrete" (0)
Missing "ndHBdDon_discrete" (0)
Missing "npHBdAcc_discrete" (0)
Missing "nbRotBd_discrete" (0)
Missing "npAromAtom_discrete" (0)
Missing "nbN_discrete" (0)
Missing "npO_discrete" (0)
Missing "nbC_discrete" (0)
Missing "nbHeavyAtoms_discrete" (0)
Missing "nbAtoms_discrete" (0)
Missing "MolWeight" (0)
(1,791)
(1,371)
(1,171)
(788)
(382)
(414)
(287)
(419)
(295)
(313)
(258)
(141)
(33)
(59)
(18)
(22)
(36)
(32)
(18)
(21)
(37)
(13)
(14)
−1
0
1
2
3
Predicted $log_{10}POD$
Reproductive/Developmental
Application Chemicals
Training Chemicals
All Samples (32,970)
Missing "BioDeg_HalfLife_pred" (23,546)
Missing "CACO2_pred" (14,886)
Missing "OH_pred" (12,060)
Missing "Clint_pred" (7,239)
Missing "KM_pred" (6,882)
Missing "HL_pred" (5,910)
Missing "KOA_pred" (5,840)
Missing "FUB_pred" (5,747)
Missing "BCF_pred" (5,651)
Missing "Koc_pred" (5,386)
Missing "ReadyBiodeg_pred_discrete" (3,651)
Missing "P_pred" (1,728)
Missing "VP_pred" (1,718)
Missing "CoMPARA_Anta_pred_discrete" (1,701)
Missing "CoMPARA_Bind_pred_discrete" (1,581)
Missing "MP_pred" (1,477)
Missing "CERAPP_Ago_pred_discrete" (1,149)
Missing "WS_pred" (1,127)
Missing "CERAPP_Anta_pred_discrete" (976)
Missing "CERAPP_Bind_pred_discrete" (948)
Missing "CoMPARA_Ago_pred_discrete" (793)
Missing "CATMoS_LD50_pred" (100)
Missing "Sp3Sp2HybRatio" (29)
Missing "CombDipolPolariz" (8)
Missing "MolarRefract" (8)
Missing "TopoPolSurfArr" (8)
Missing "nbHeteroRing_discrete" (8)
Missing "nbRing_discrete" (8)
Missing "nbLipinskiFailures_discrete" (0)
Missing "ndHBdDon_discrete" (0)
Missing "npHBdAcc_discrete" (0)
Missing "nbRotBd_discrete" (0)
Missing "npAromAtom_discrete" (0)
Missing "nbN_discrete" (0)
Missing "npO_discrete" (0)
Missing "nbC_discrete" (0)
Missing "nbHeavyAtoms_discrete" (0)
Missing "nbAtoms_discrete" (0)
Missing "MolWeight" (0)
(2,228)
(1,672)
(1,083)
(1,005)
(544)
(541)
(524)
(415)
(375)
(360)
(360)
(461)
(419)
(229)
(66)
(97)
(18)
(23)
(58)
(49)
(41)
(42)
(56)
(18)
(4)
(3)
−1
0
1
2
3
Predicted $log_{10}POD$