Estimating lithium concentrations in groundwater used as drinking water for the conterminous United States as a Tool for Human Exposure Assessment

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Supporting Information

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Table SI_1 Well and water quality characteristics from wells across the conterminous United States.

Characteristic	Minimum	Median	Average	Maximum	NA
Depth (feet)	3.0	174	303.8	4908	
Lithium (Li) concentration (ug/L)	0.001	6.74	19.42	15000	
pH	3.62	7.30	7.18	10.27	95
Total dissolved solids	150	265	335	1000	1279
Sample date	1989-01-09	2008-06-13	2006-08-25	2020-11-19	

Table SI_2 – Number of wells in each lithium (Li) concentration class used in the classification model to estimate geogenic lithium in drinking-water supply wells throughout the conterminous United States.

Dataset	Class1 (≤4 µg/L)	Class2 (>4 and ≤ 10 µg/L)	Class3 (>10 and ≤30 µg/L)	Class4(>30 µg/L)	Total
Training	5269	2835	3372	2046	13522
Testing	1756	945	1123	681	4505
Total	7025	3780	4495	2727	18027
Percent	39.0	21.0	24.9	15.1	100

Table SI_3 – Predictor variables and relative importance for the overall model used to estimate geogenic lithium in drinking-water supply wells throughout the conterminous United States.

Variable name and data source	Variable description	Relative importance
ppt_91_20[37]	Average annual precipitation from 1991 - 2020	1
WELL_DEPTH[29, 44]	Depth of well	0.6517
LP_9[41]	Lateral position within a watershed for 9th order streams	0.5717
C_Li[40]	Lithium concentration in the soil C horizon	0.5706
Zell_trans[42]	Estimated transmissivity of shallow subsurface	0.5564
C_Calcite[40]	Calcite concentration in the soil C horizon	0.4786
LP_7[41]	Lateral position within a watershed for 7th order streams	0.4683
C_Al[40]	Aluminum concentration in the soil C horizon	0.4554
C_Na[40]	Sodium concentration in the soil C horizon	0.4410
Zell_wc_av[42]	Long term average water content of unsaturated zone	0.4247

LP_5[41]	Lateral position within a watershed for 5th order streams	0.4094
C_Kaolinit[40]	Kaolinite concentration in the soil C horizon	0.3996
C_Amorphou[40]	Amorphous content in the soil C horizon	0.3798
LP_3[41]	Lateral position within a watershed for 3rd order streams	0.3777
C_Mg[40]	Magnesium concentration in the soil C horizon	0.3696
Zell_dtw[42]	Simulated depth to groundwater	0.3671
C_Tot_Clay[40]	Total clay in the soil C horizon	0.3540
C_Quartz[40]	Quartz concentration in the soil C horizon	0.3538
LP_1[41]	Lateral position with a watershed for 1st order streams	0.3495
Zell_tt_to[42]	Unsaturated zone long-term average travel time	0.3463

Table SI_4– Relative importance of variables for lithium (Li) classification 1 (Li ≤4 µg/L). Variable descriptions are provided in Table SI_3.

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Variable	Relative Importance
ppt_91_20	1.0000
WELL_DEPTH	0.5339
C_Li	0.4636
LP_9	0.4234
C_Al	0.4114
C_Calcite	0.3934
Zell_trans	0.3862
C_Kaolinit	0.3226
LP_7	0.3203
C_Na	0.3171
Zell_wc_av	0.2927
C_Amorphou	0.2846
LP_5	0.2680
C_Mg	0.2678
C_Tot_Clay	0.2619
C_Quartz	0.2585
LP_3	0.2519
Zell_tt_to	0.2478
Zell_dtw	0.2312
LP_1	0.2199

Table SI_5 - Relative importance of variables for lithium (Li) classification 2 (Li >4 and ≤ 10 µg/L). Variable descriptions are provided in Table SI_3.

Variable	Relative Importance
WELL_DEPTH	1.0000
ppt_91_20	0.9185
Zell_trans	0.8924
LP_7	0.8460
LP_5	0.7997
LP_9	0.7830
Zell_wc_av	0.7570
C_Na	0.7499
LP_3	0.7118
LP_1	0.6968
Zell_dtw	0.6749
C_Li	0.6467
C_Amorphou	0.5948
C_Kaolinit	0.5842
C_Mg	0.5689
C_Tot_Clay	0.5588
C_Quartz	0.5549
Zell_tt_to	0.5122
C_Calcite	0.4893
C_Al	0.4811

Table SI_6 – Relative importance of variables for lithium (Li) classification 3 (Li >10 and ≤30 µg/L). Variable descriptions are provided in Table SI_3.

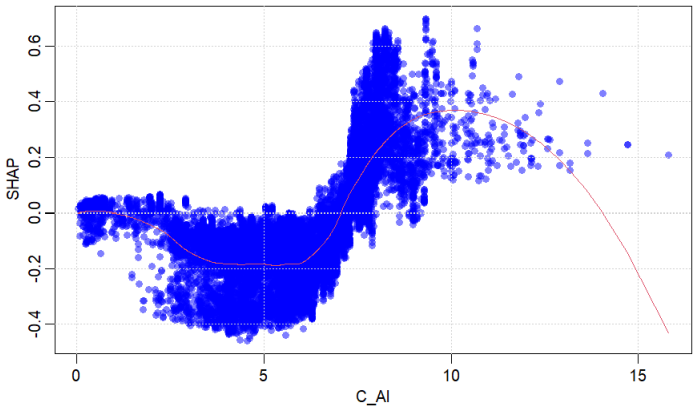
Variable	Relative Importance
ppt_91_20	1.0000
WELL_DEPTH	0.7956
Zell_trans	0.7380
C_Li	0.7317
LP_9	0.6577
LP_7	0.6088
C_Al	0.5868
Zell_wc_av	0.5392
LP_5	0.5286
C_Mg	0.5235
LP_3	0.5187
C_Amorphou	0.5149
C_Na	0.5081

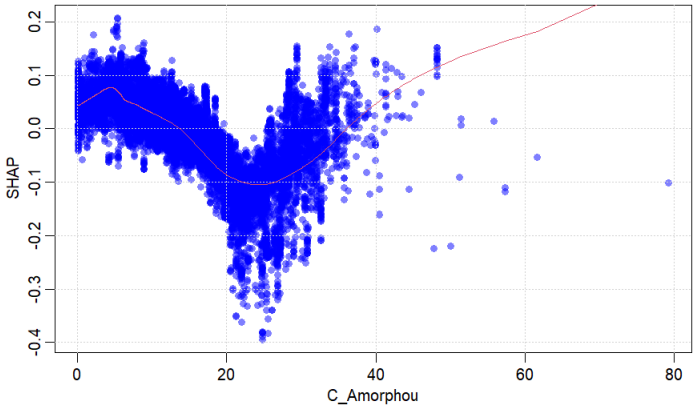
C_Kaolinit	0.5007
Zell_dtw	0.4972
LP_1	0.4874
Zell_tt_to	0.4867
C_Calcite	0.4738
C_Tot_Clay	0.4488
C_Quartz	0.4390

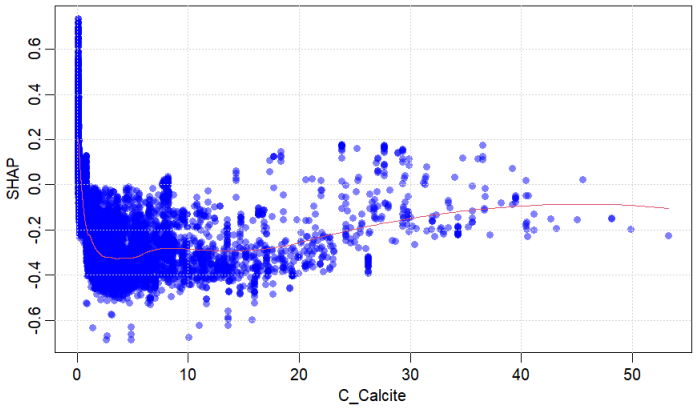
Table SI_7 – Relative importance of variables for lithium (Li) classification 4 (Li > 30 µg/L). Variable descriptions are provided in Table SI_3.

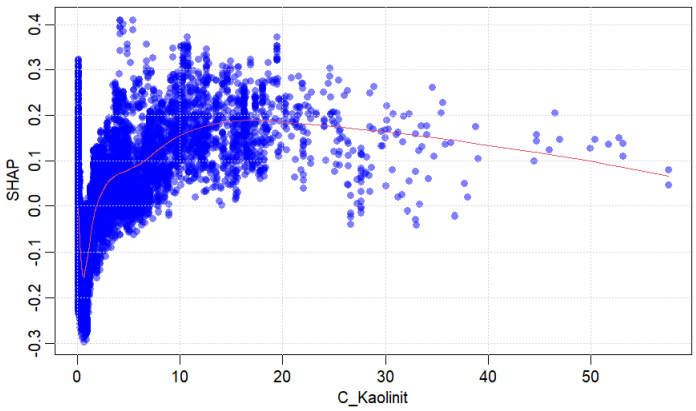
Variable	Relative Importance
ppt_91_20	1.0000
LP_9	0.6195
C_Calcite	0.6032
C_Li	0.5616
WELL_DEPTH	0.5221
Zell_trans	0.4988
C_Na	0.4139
C_Al	0.3933
LP_7	0.3858
Zell_wc_av	0.3621
C_Kaolinit	0.3342
LP_5	0.3282
C_Quartz	0.3257
Zell_dtw	0.3145
C_Tot_Clay	0.3106
C_Amorphou	0.3033
Zell_tt_to	0.2996
C_Mg	0.2985
LP_3	0.2841
LP_1	0.2591

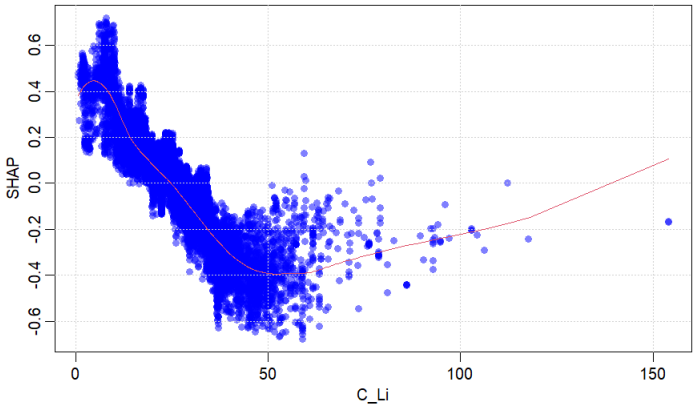
Figure SI_1 Shapley Additive explanation (SHaP) plots for prediction classification of lithium (Li) ≤4 µg/L. Variable descriptions are provided in Table SI_3.

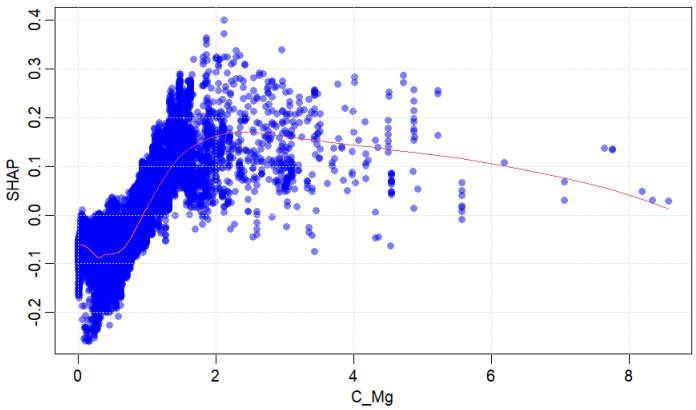


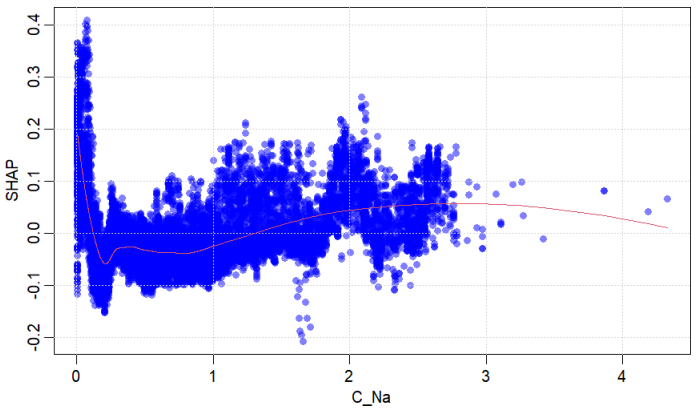


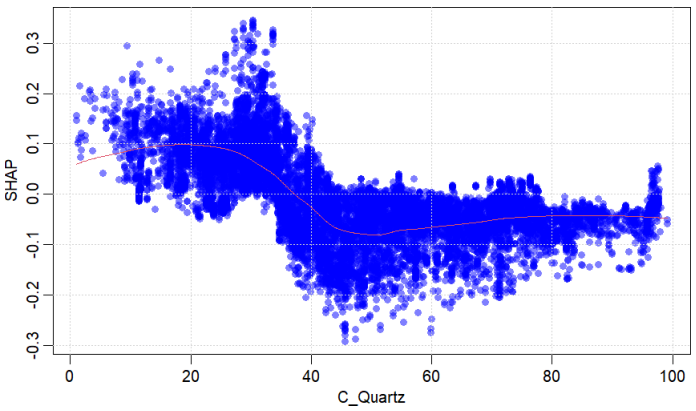












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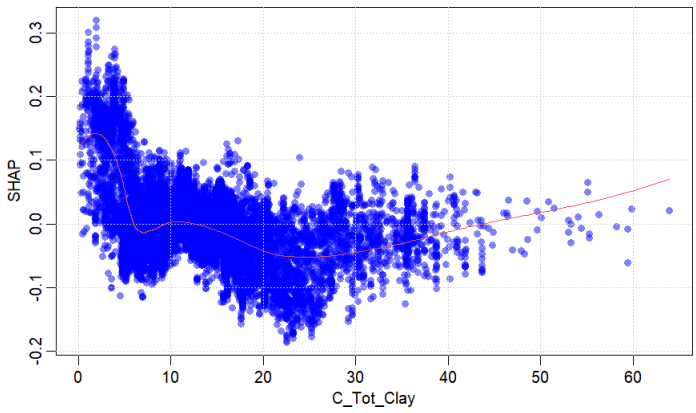

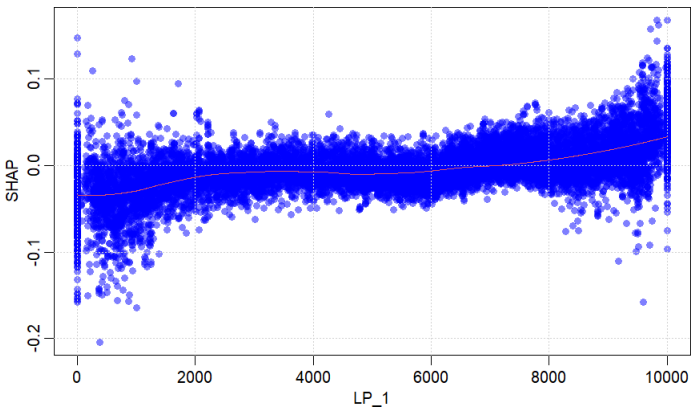

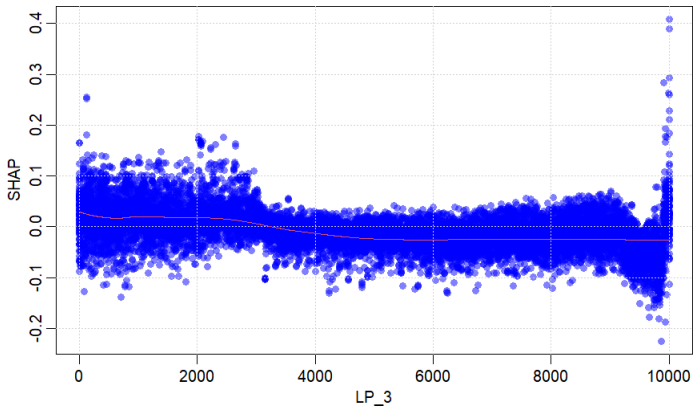

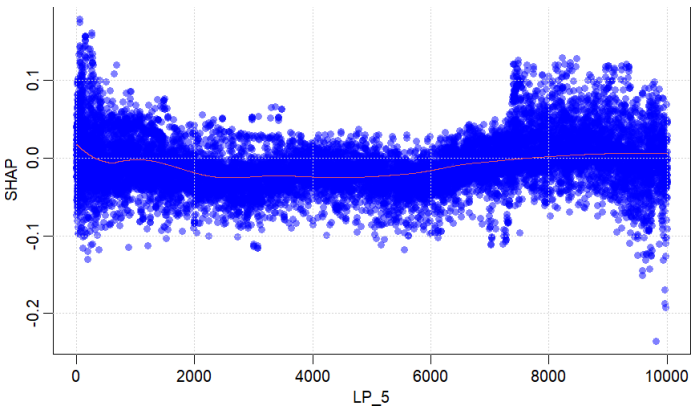

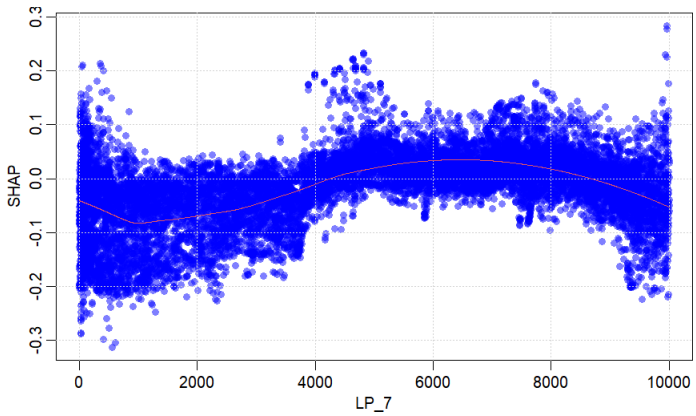

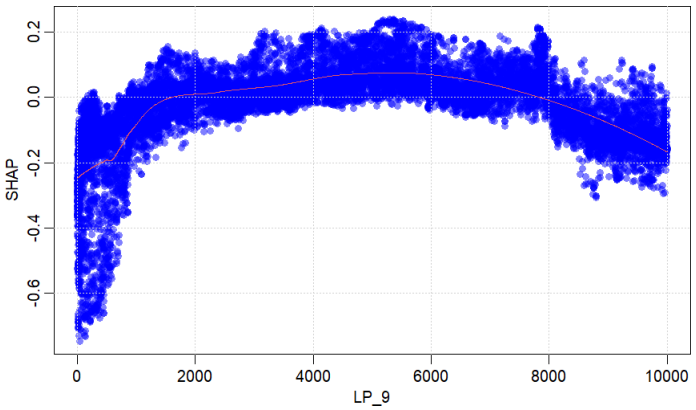

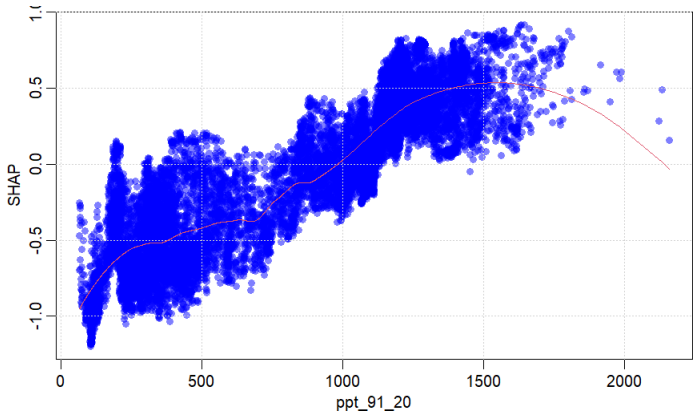

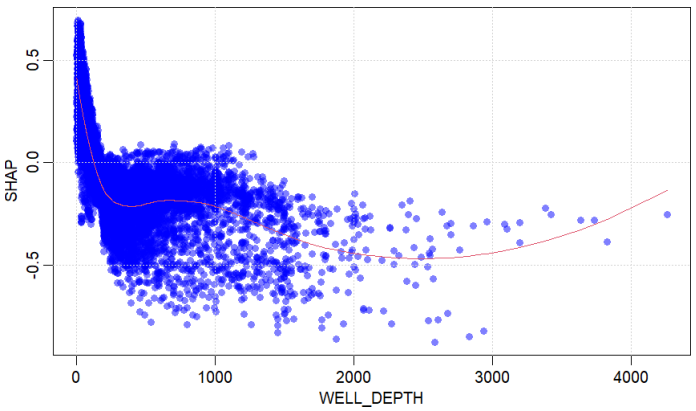

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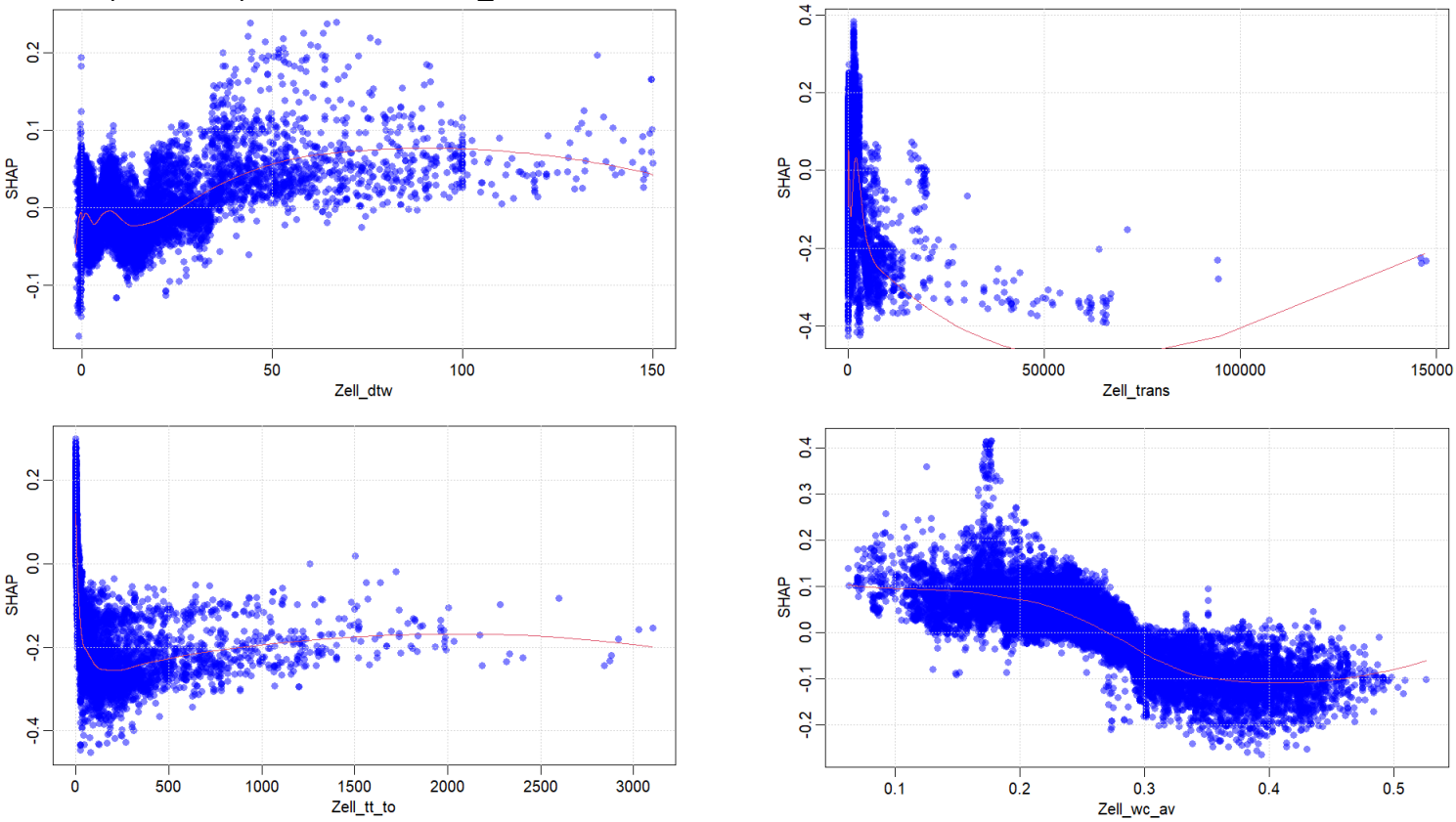
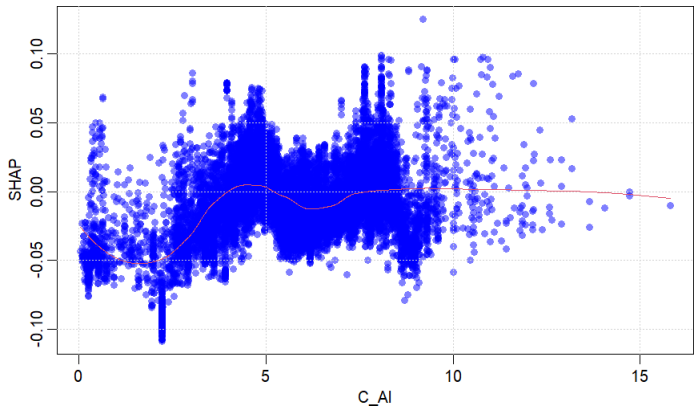
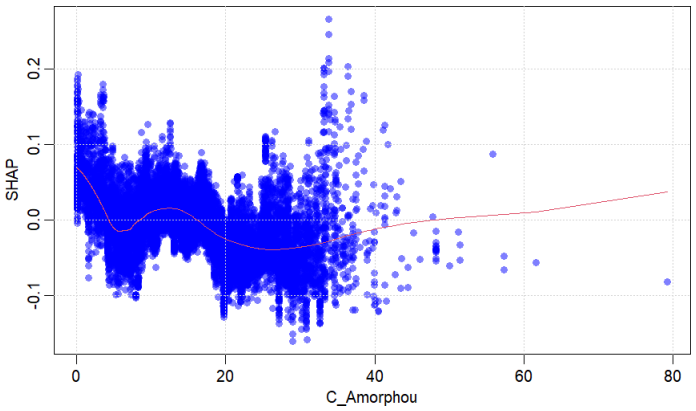
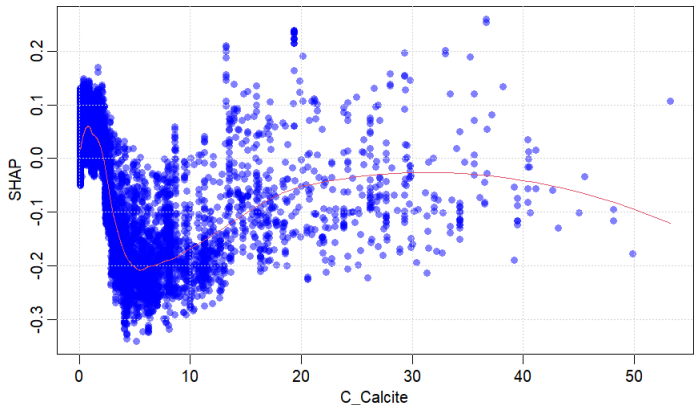
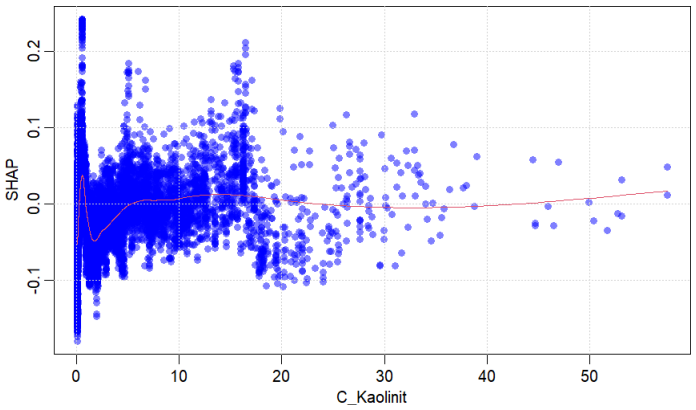


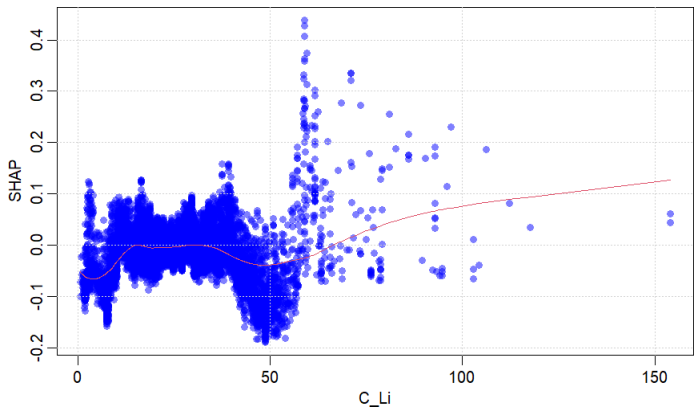
Figure SI_2 Shapley Additive exPlanation (SHaP) plots for prediction classification of lithium (Li) >4 to ≤ 10 µg/L. Variable descriptions are provided in Table SI_3.

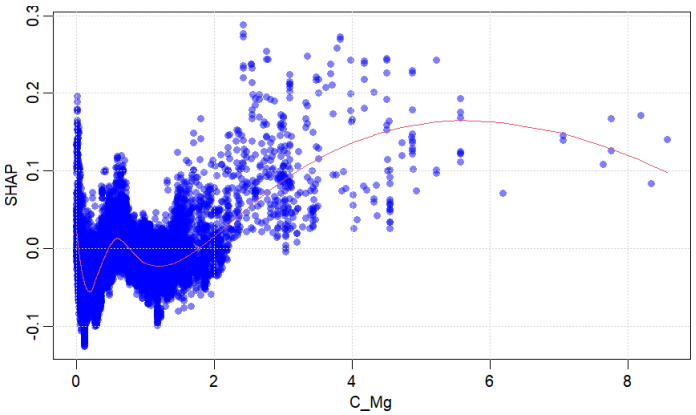


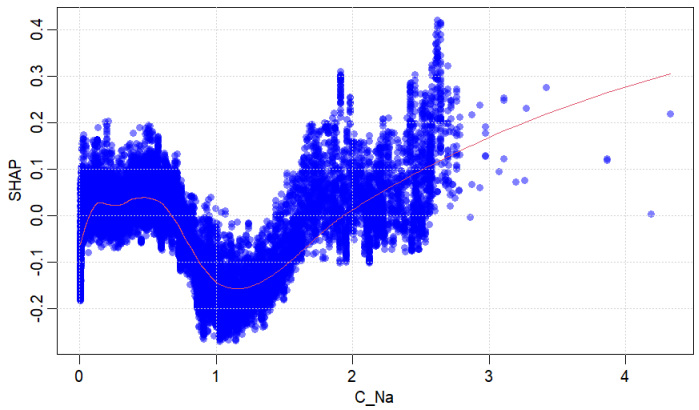












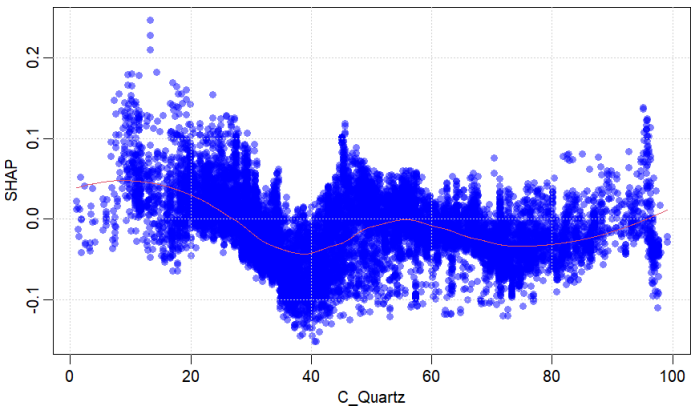
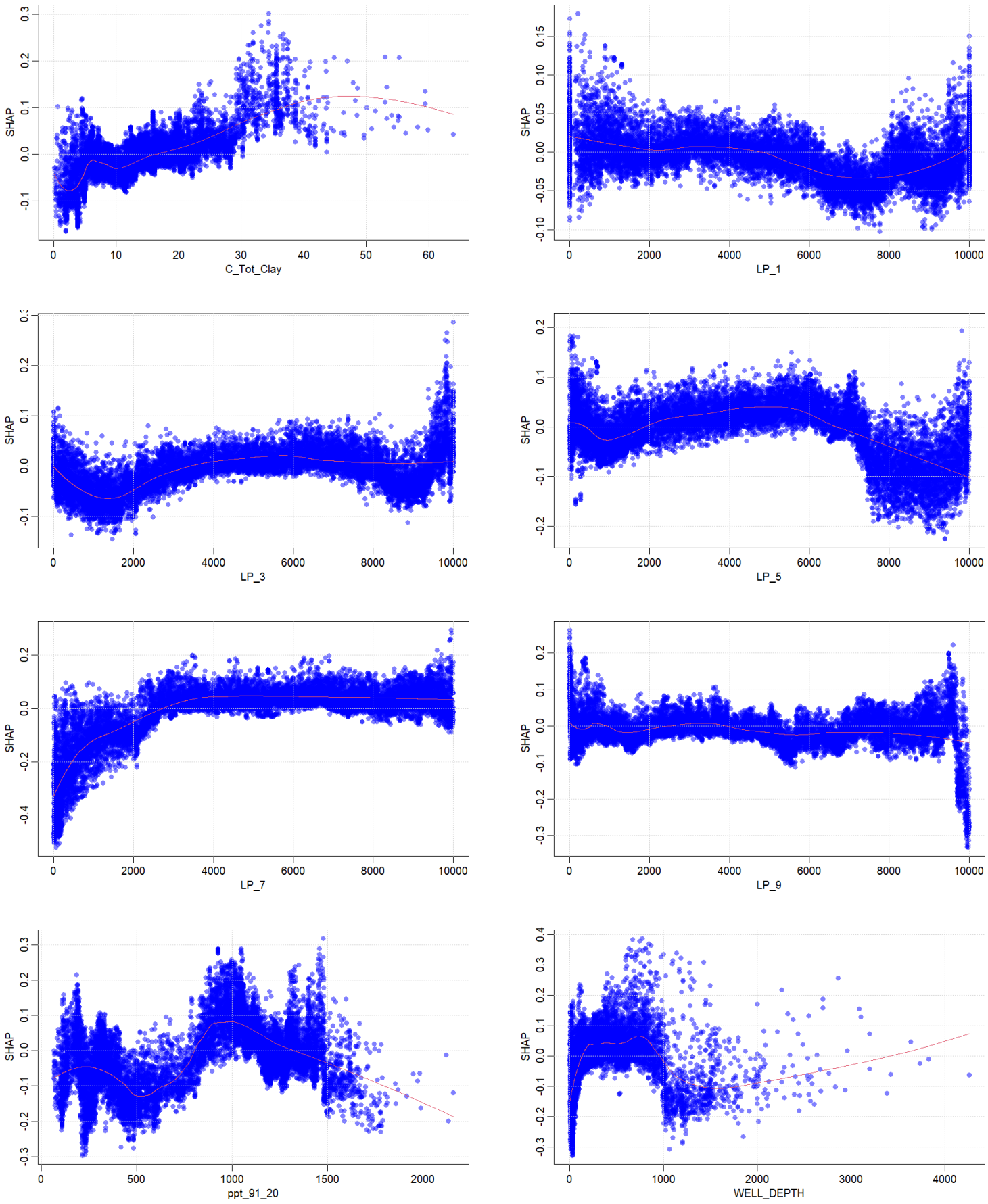


Figure SI_2 Shapley Additive exPlanation (SHaP) plots for prediction classification of lithium (Li) >4 to ≤ 10 µg/L. Variable descriptions are provided in Table SI_3.



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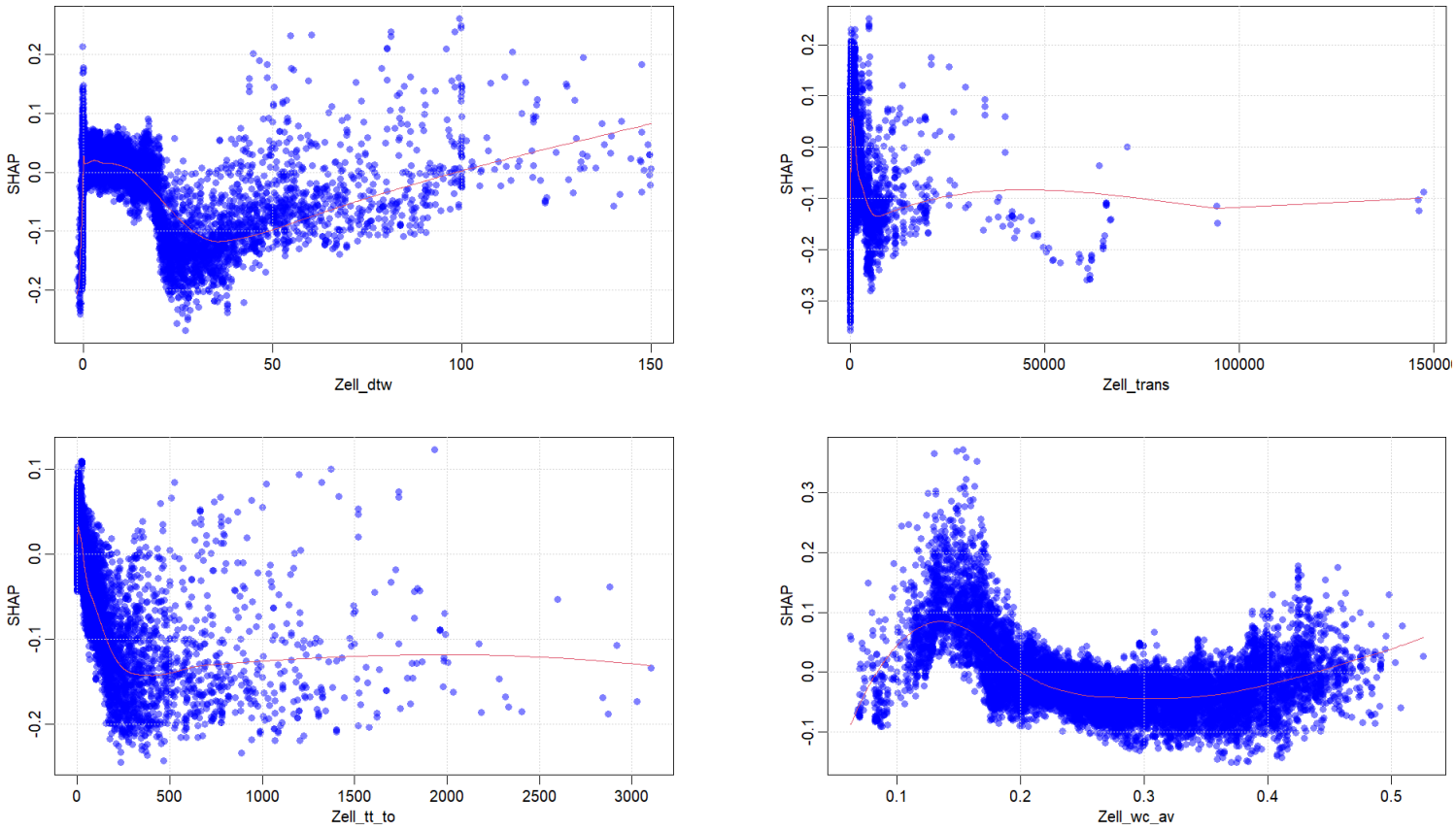
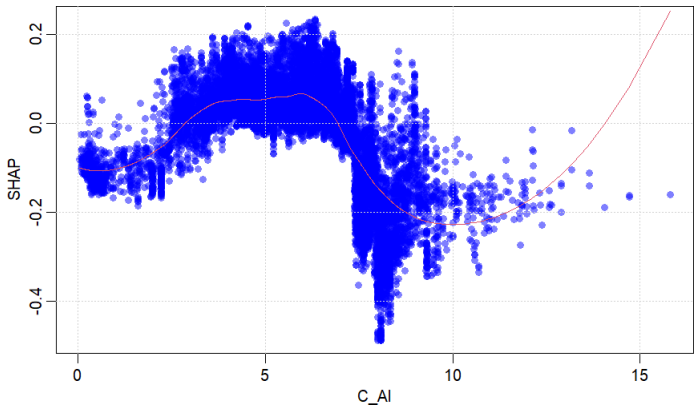
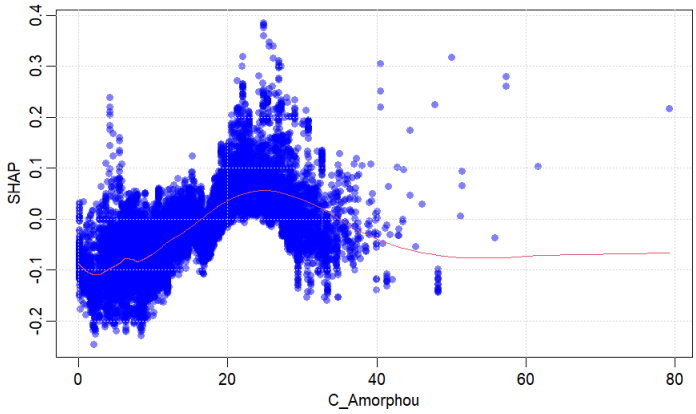
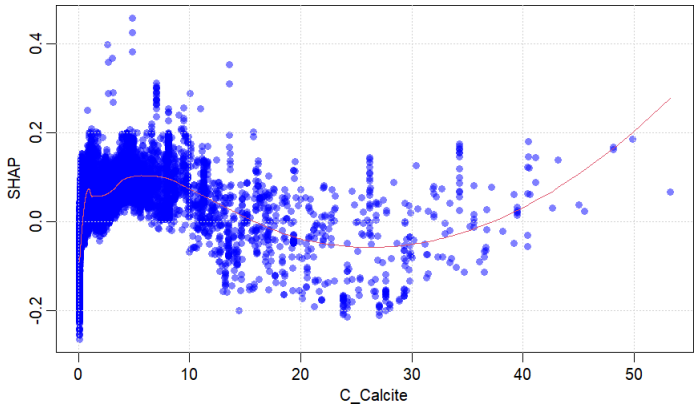
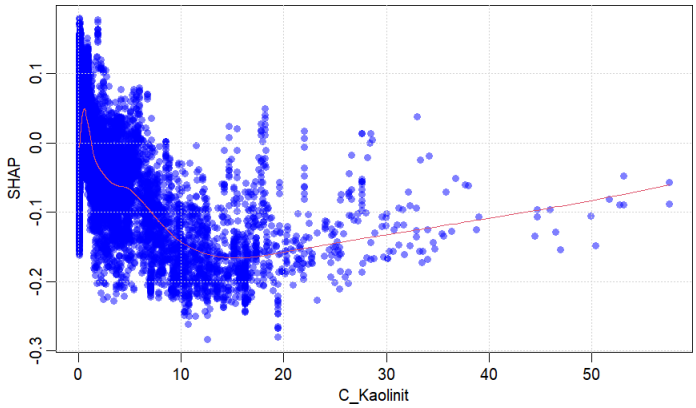


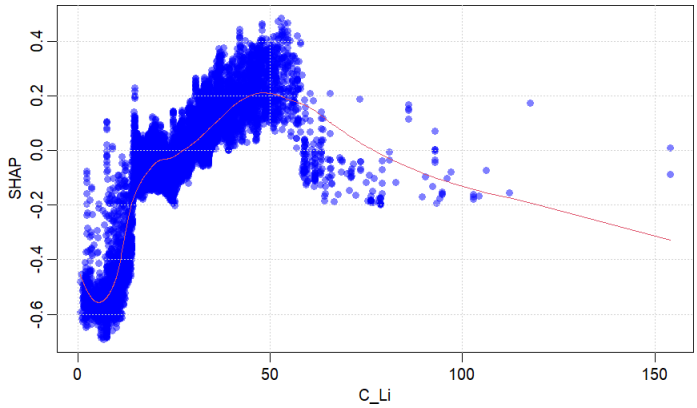
Figure SI_3 Shapley Additive exPlanation (SHaP) plots for prediction classification of lithium (Li) >10 to ≤30 µg/L. Variable descriptions are provided in Table SI_3.

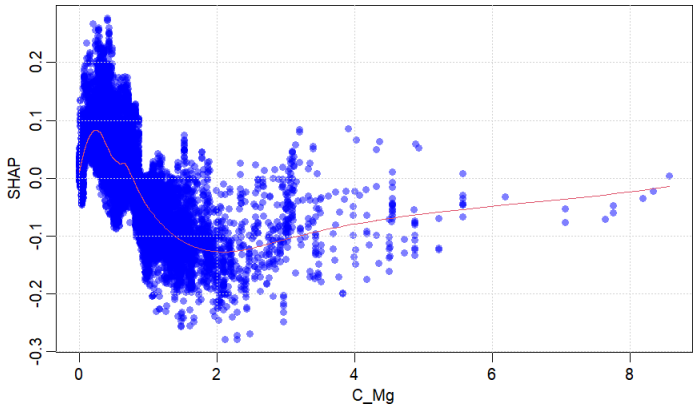


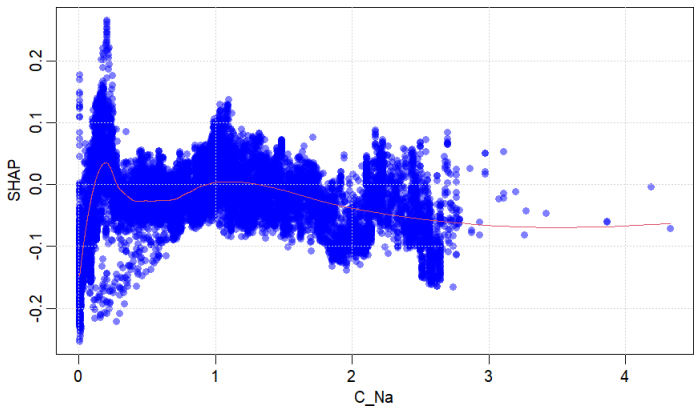












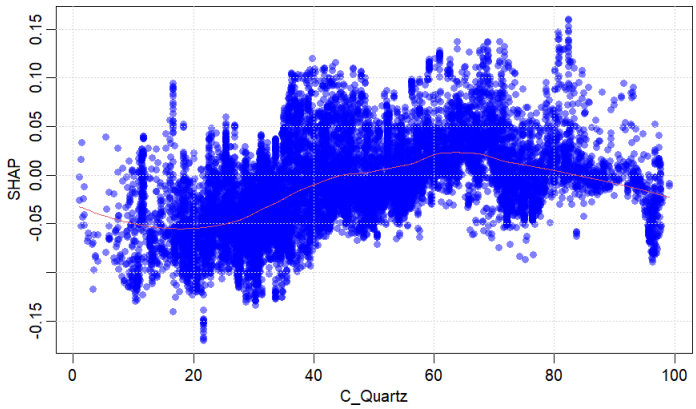


Figure SI_3 Shapley Additive exPlanation (SHaP) plots for prediction classification of lithium (Li) >10 to ≤30 µg/L. Variable descriptions are provided in Table SI_3.

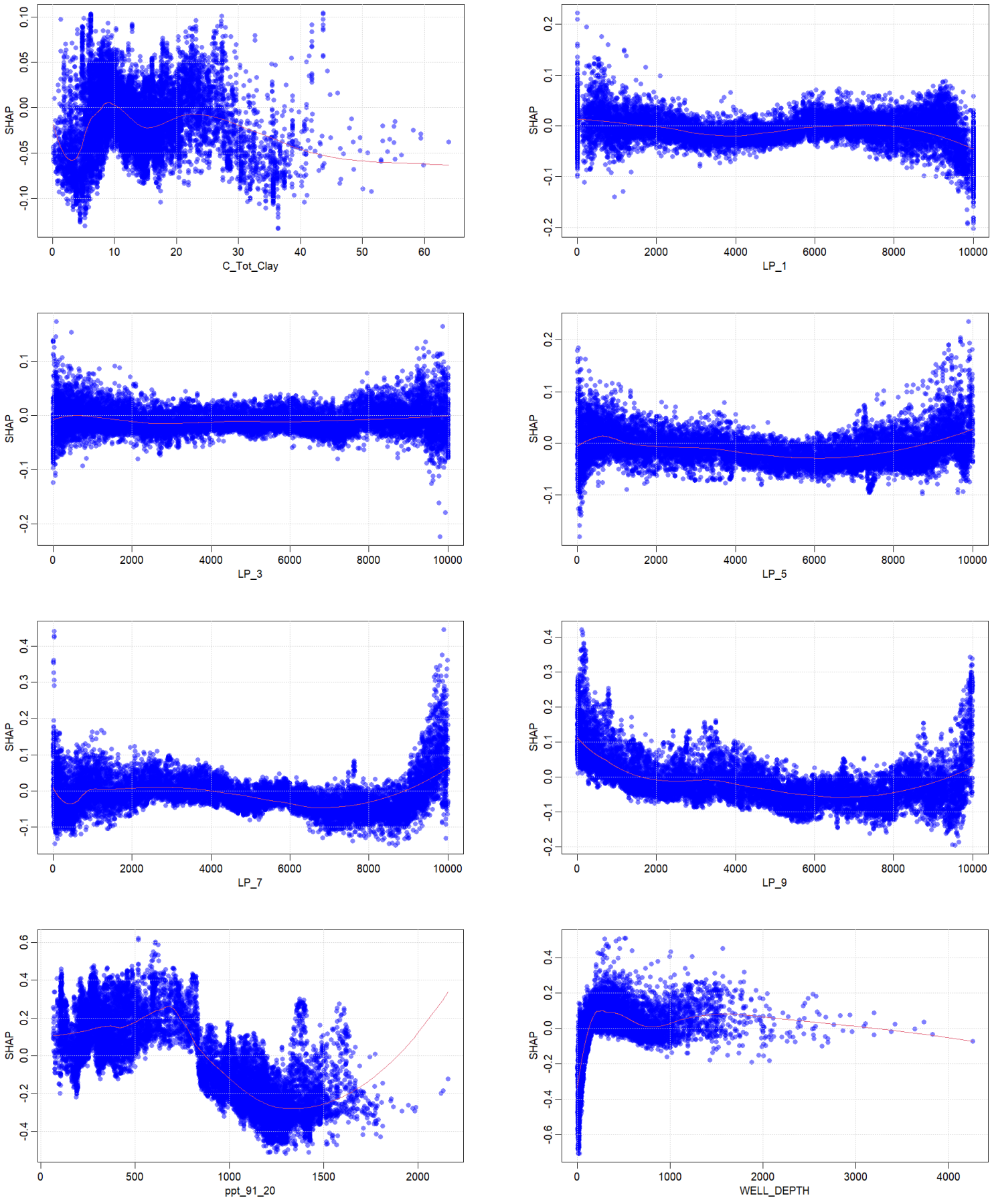
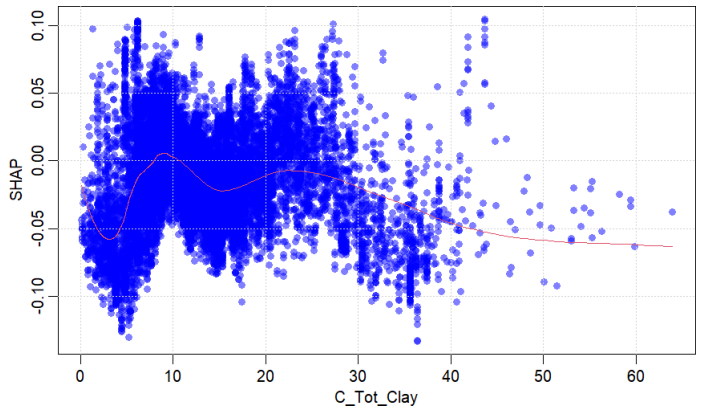
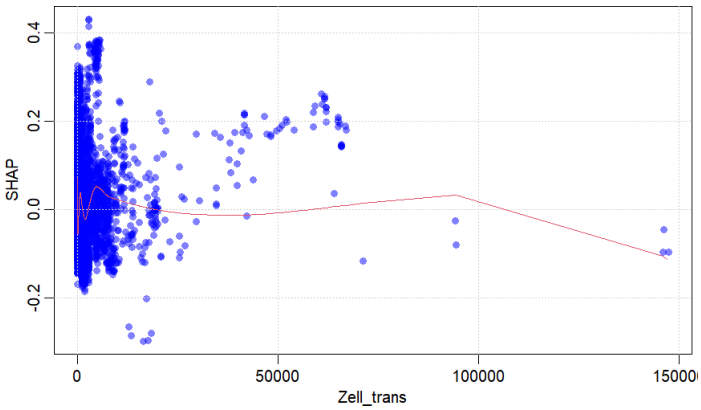
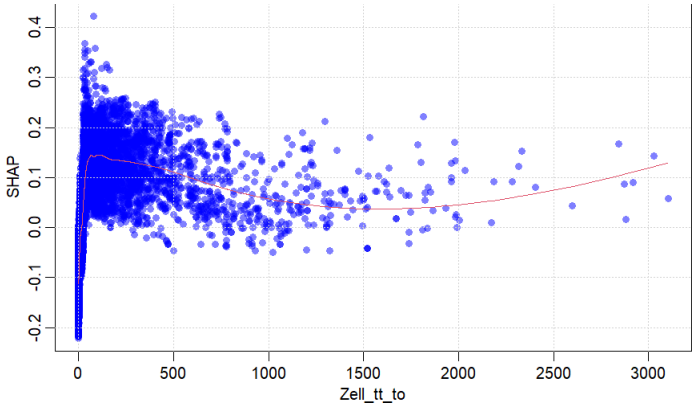


Figure SI_3 Shapley Additive exPlanation (SHaP) plots for prediction classification of lithium (Li) >10 to ≤30 µg/L. Variable descriptions are provided in Table SI_3.







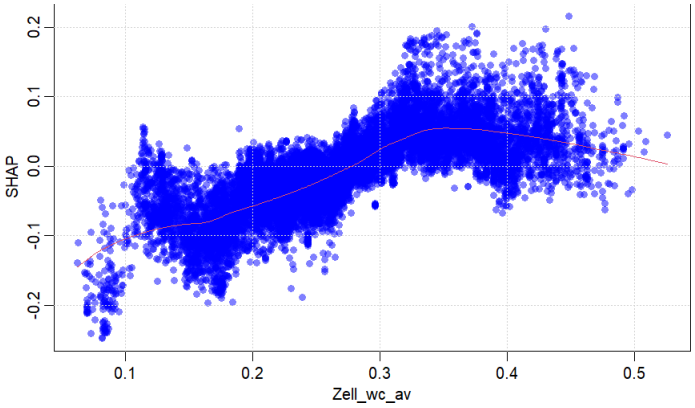
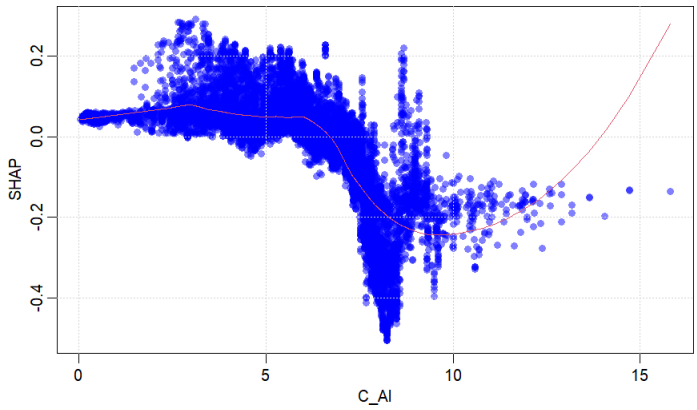
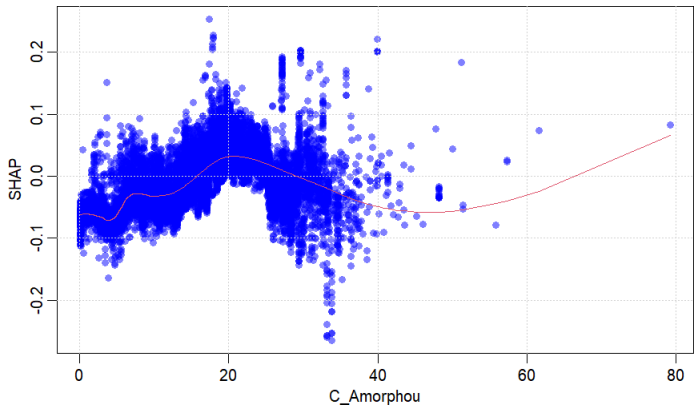
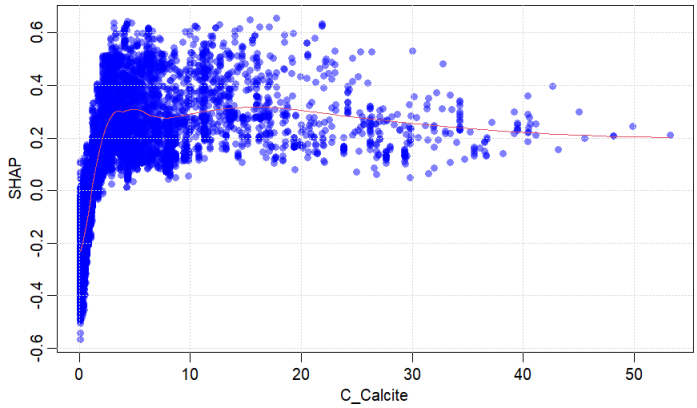
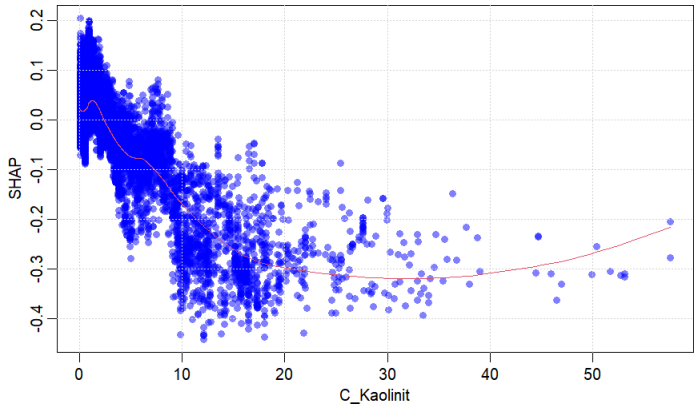


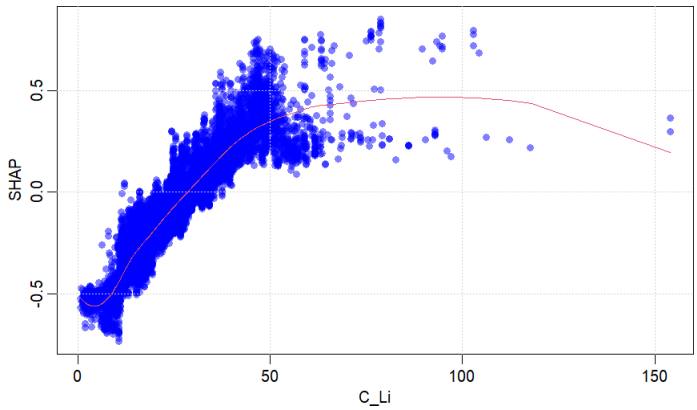
Figure SI_4 Shapley Additive exPlanation (SHaP) plots for prediction classification of lithium (Li) >30 µg/L. Variable descriptions are provided in Table SI_3.

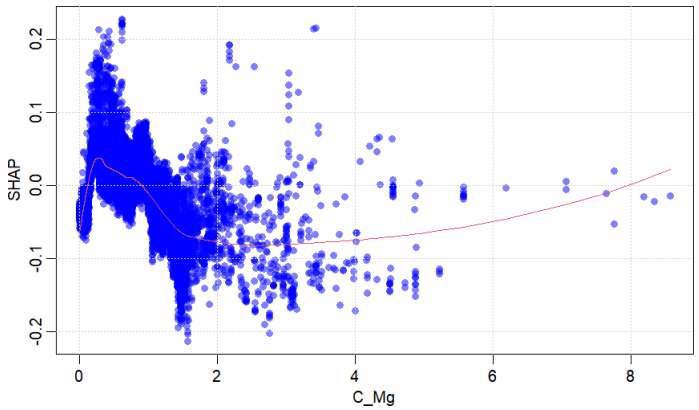


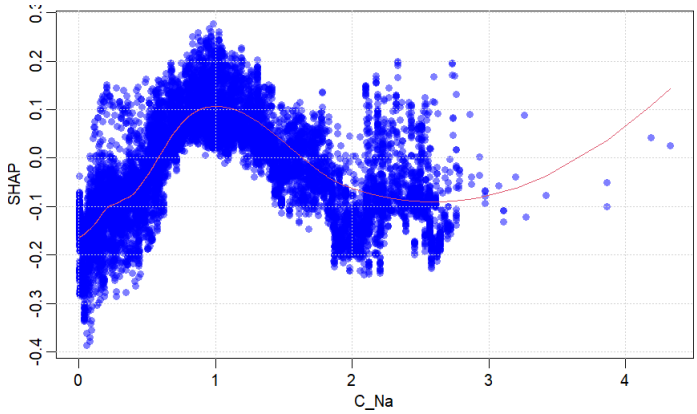












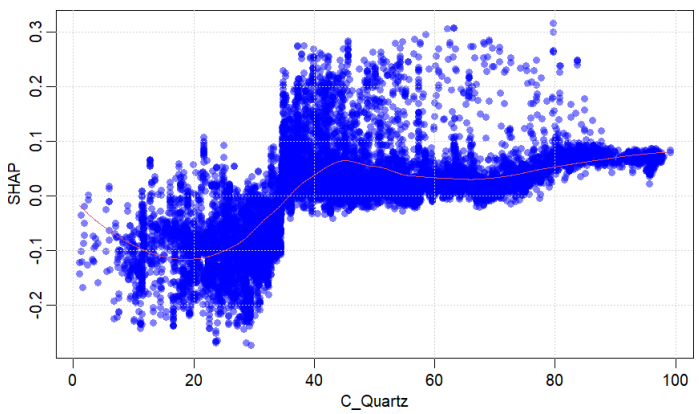


Figure SI_4 Shapley Additive exPlanation (SHaP) plots for prediction classification of lithium (Li) >30 µg/L. Variable descriptions are provided in Table SI_3.

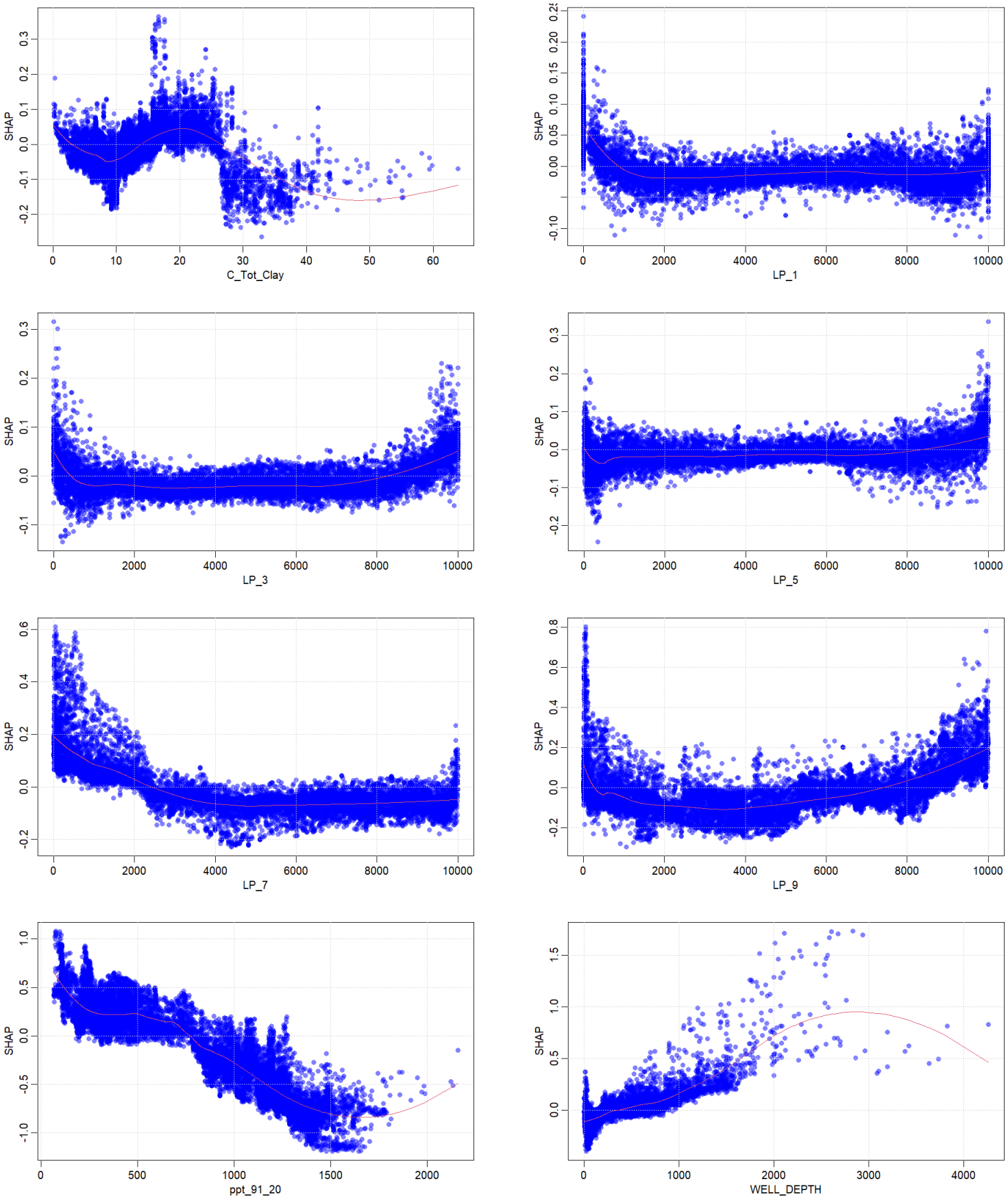


Figure SI_4 Shapley Additive exPlanation (SHaP) plots for prediction classification of lithium (Li) >30 µg/L. Variable descriptions are provided in Table SI_3.

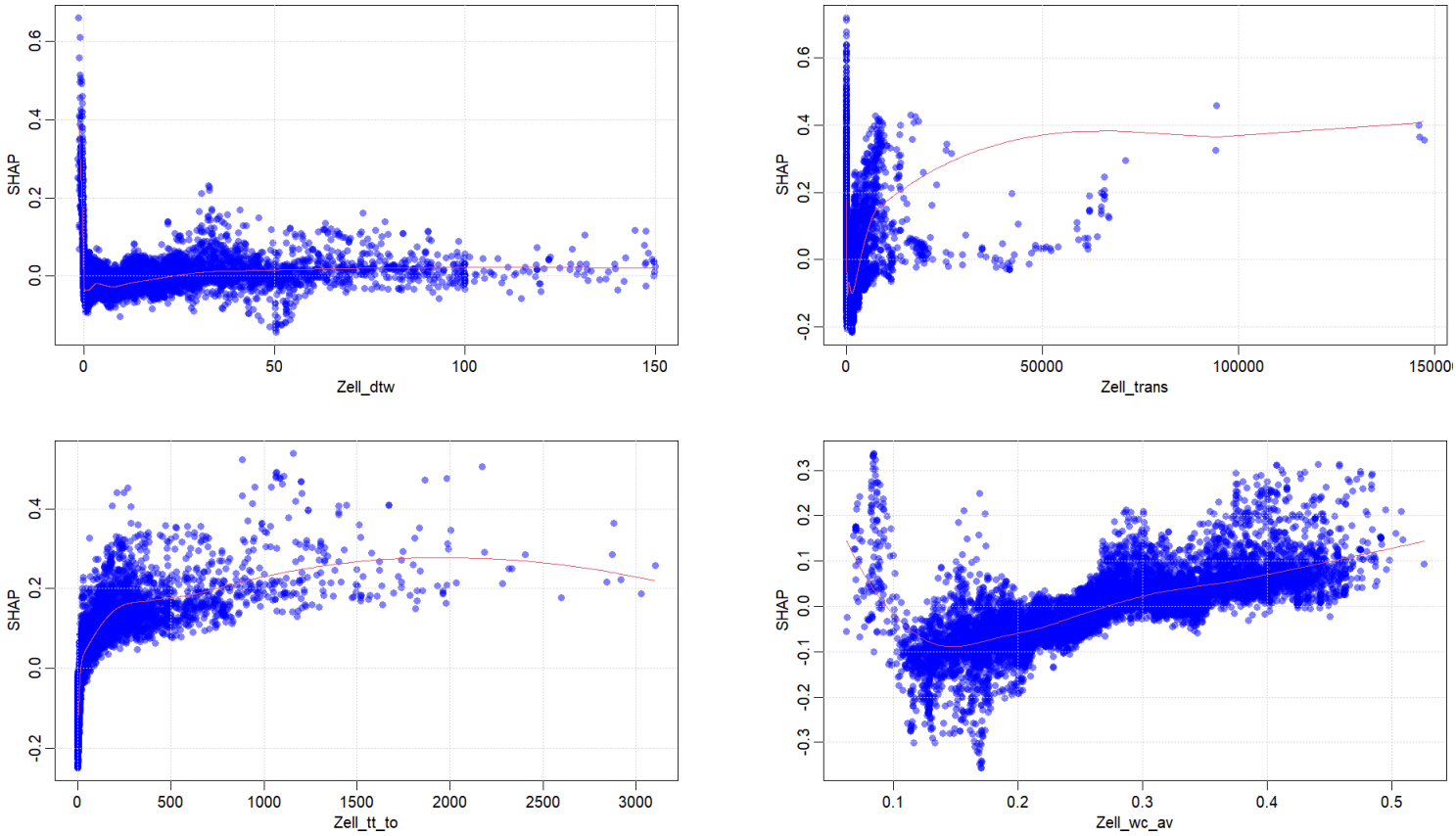


Figure SI_5 Shapley Additive explanation (SHaP) plots for the overall model. Variable descriptions are provided in Table SI_3.

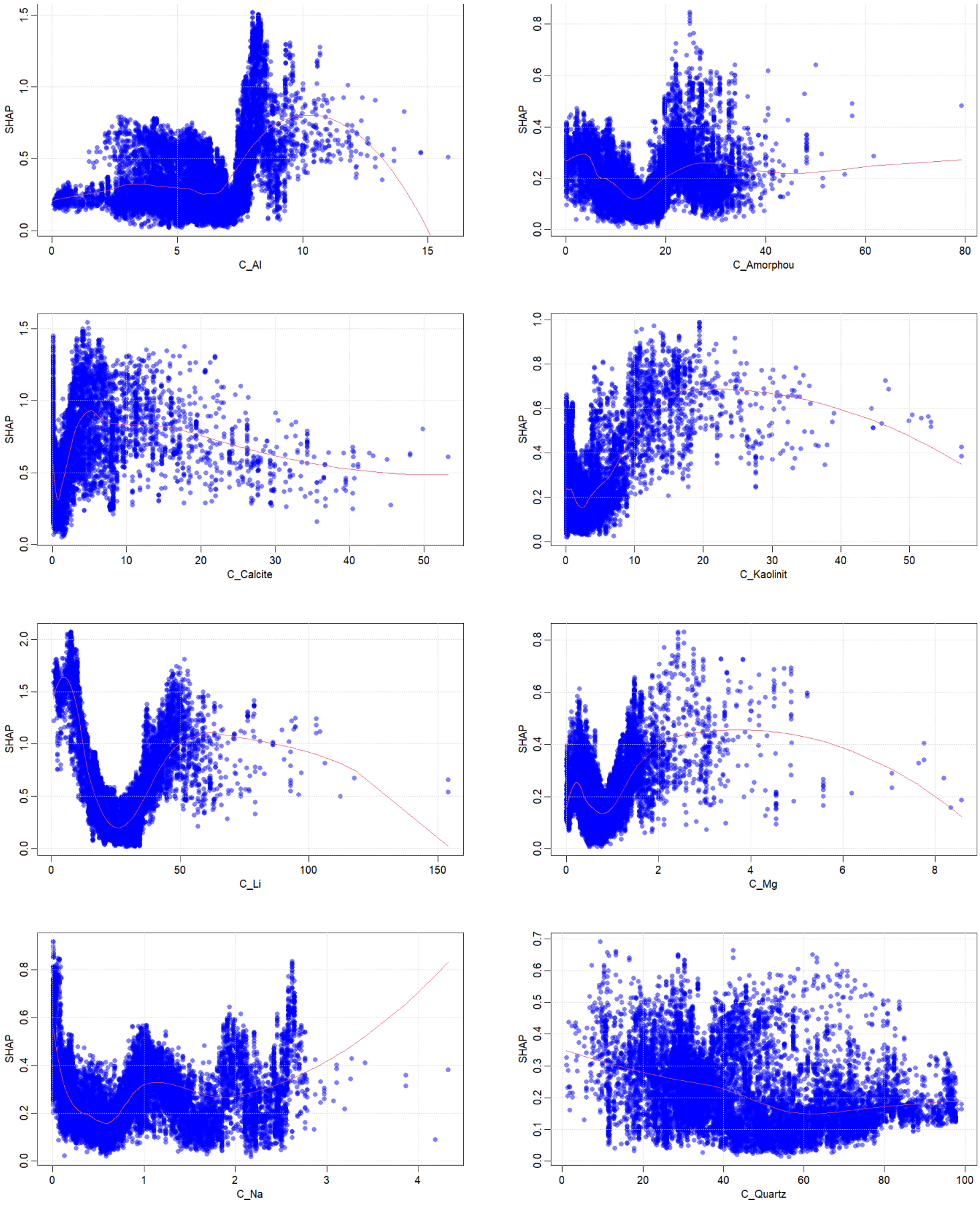


Figure SI_5 Shapley Additive explanation (SHaP) plots for the overall model. Variable descriptions are provided in Table SI_3.

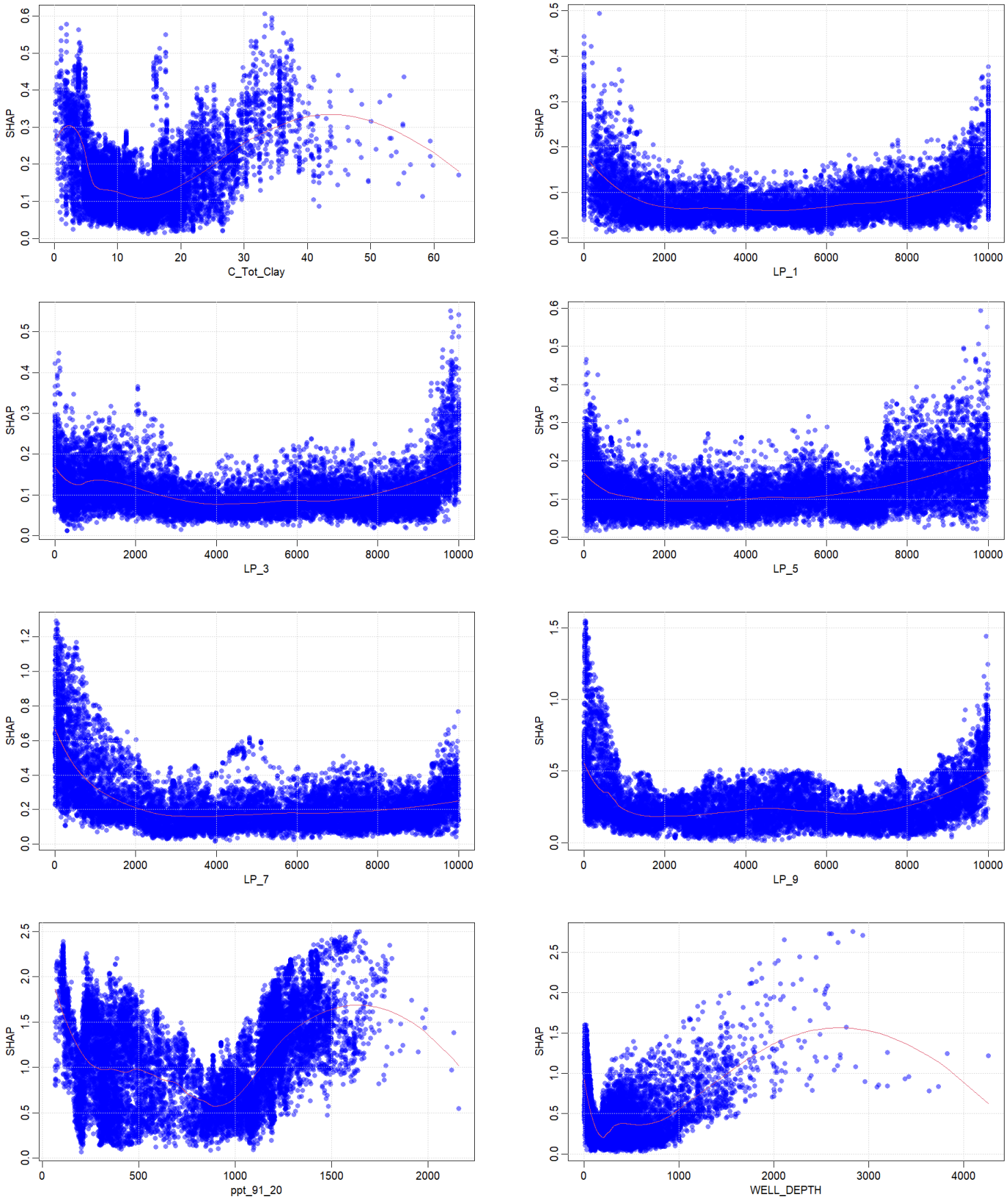
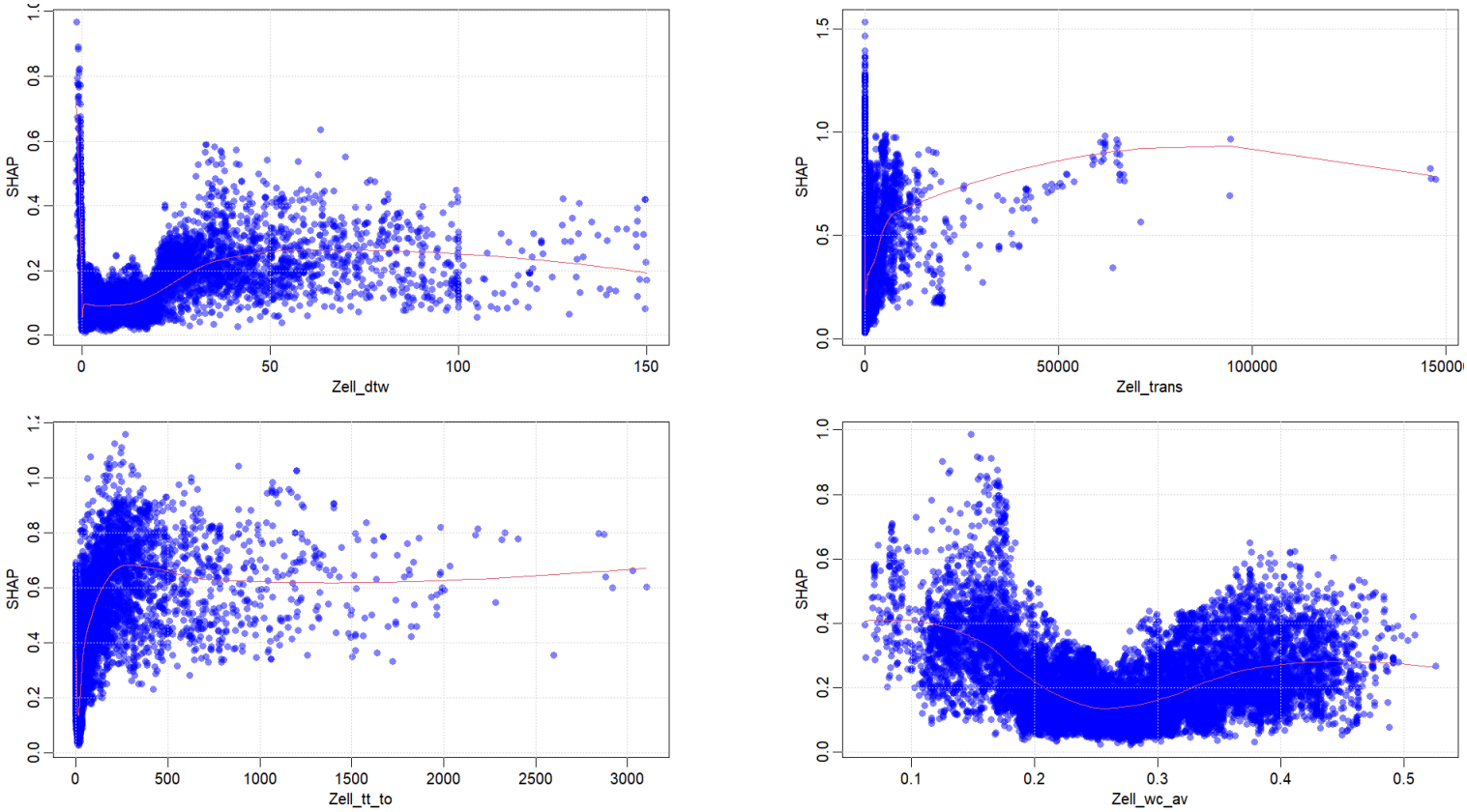


Figure SI_5 Shapley Additive explanation (SHaP) plots for the overall model. Variable descriptions are provided in Table SI_3.



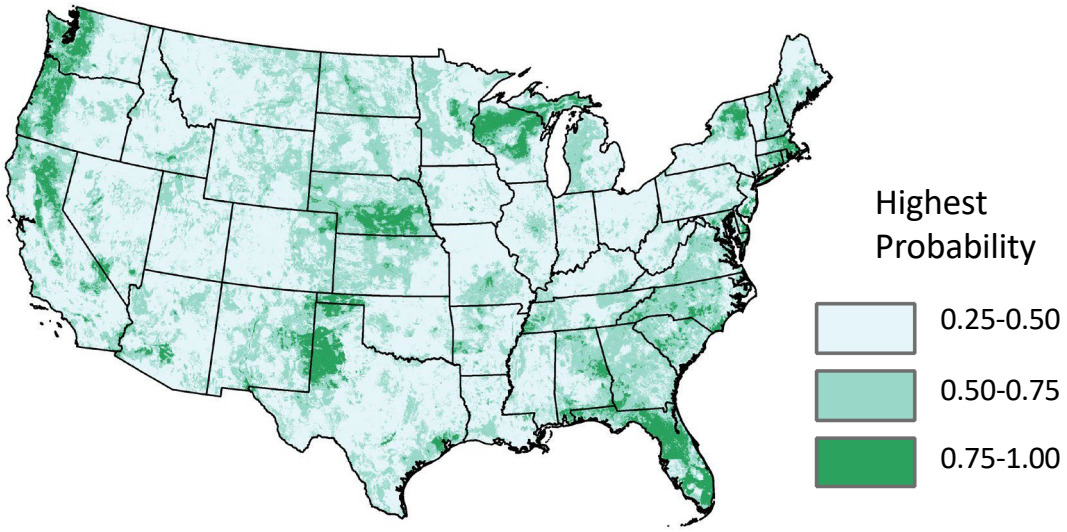


Figure SI_6. Highest probability for each grid classification for public well depth predictions.