

Supplementary materials

Table S1 Correlation analysis of the descriptors used in the built model for COX B1.

	GATS5m	SRW9	RDF40v	Di	VIF
GATS5m	1				2.12
SRW9	0.054172	1			1.064199
RDF40v	-0.7138	0.114092	1		2.210961
Di	-0.11242	0.134276	0.221418	1	1.067301

Table S2 Correlation analysis of the descriptors used to built model for COX B3.

	SdsCH	TDB8u	RNCS	RDF35m	VIF
SdsCH	1				1.101184
TDB8u	-0.18198	1			1.077007
RNCS	0.219084	0.118326	1		1.277192
RDF35m	-0.07567	-0.15256	-0.41559	1	1.224892

Table S3 Correlation analysis of the descriptors used in the built model for PV3.

	MATS4e	MATS5e	GATS6m	SRW9	VIF
MATS4e	1				1.19864
MATS5e	-0.12755	1			1.21407
GATS6m	-0.06769	0.384791	1		1.58936
SRW9	0.32664	0.026567	0.44852	1	1.52319

Table S4 Correlation analysis of the descriptors used in the built model for HRV 14.

	GATS3i	VR3_Dzp	SRW9	RDF130m	VIF
GATS3i	1				1.639311
VR3_Dzp	0.50374	1			4.811878
SRW9	0.196577	0.733338	1		3.766291
RDF130m	0.016252	0.194208	-0.22517	1	1.667856

Table S5 Correlation analysis of the descriptors used in the built model for HRV 21.

	GATS8e	SCH-7	ETA_Shape_Y	E3e	VIF
GATS8e	1				1.263695
SCH-7	0.401276	1			1.750846
ETA_Shape_Y	0.064033	-0.3482	1		1.535758
E3e	0.156837	0.564627	-0.56039	1	1.885641

Table S6 Correlation analysis of the descriptors used in the built model for HRV 71.

	maxssCH2	TDB10u	TDB6i	Di	VIF
maxssCH2	1				1.24509
TDB10u	-0.2099	1			1.63405
TDB6i	0.26925	0.11527	1		1.14754
Di	-0.15514	-0.54558	-0.2713	1	1.64292

Table S7 Y-Randomization test for COX B1.

Model	R	R ²	Q ²
Original	0.990707	0.981501	0.952397
Random 1	0.57103	0.326075	-0.56204
Random 2	0.46309	0.214452	-1.11364
Random 3	0.789257	0.622927	-0.05444
Random 4	0.518721	0.269072	-1.00759
Random 5	0.669565	0.448317	-0.43254
Random 6	0.613679	0.376602	-0.6195
Random 7	0.589219	0.34718	-0.82199
Random 8	0.455719	0.207679	-0.80342
Random 9	0.338477	0.114566	-1.03986
Random 10	0.791526	0.626514	-0.00299
Random Models Parameters			
Average r :	0.580028		
Average r ² :	0.355338		
Average Q ² :	-0.6458		
cRp ² :	0.795698		

Table S8 Y-Randomization test for COX B3.

Model	R	R ²	Q ²
Original	0.989306	0.978727	0.524394
Random 1	0.64493	0.415934	-0.49523
Random 2	0.307174	0.094356	-1.24515
Random 3	0.326217	0.106418	-0.50336
Random 4	0.685098	0.469359	-0.29506
Random 5	0.669228	0.447867	-0.60514
Random 6	0.603617	0.364353	-1.00755
Random 7	0.477457	0.227965	-0.65626
Random 8	0.326778	0.106784	-2.6184
Random 9	0.183833	0.033795	-0.77057
Random 10	0.618556	0.382611	-1.56293
Random Models Parameters			
Average r :	0.484289		
Average r ² :	0.264944		
Average Q ² :	-0.97596		
cRp ² :	0.85344		

Table S9 Y-Randomization test for PV3.

Model	R	R ²	Q ²
Original	0.992078	0.984219	0.958016
Random 1	0.734869	0.540032	-0.0403
Random 2	0.466197	0.21734	-0.65963
Random 3	0.295421	0.087273	-1.41999
Random 4	0.648146	0.420094	-0.3627
Random 5	0.652977	0.42638	-0.34261
Random 6	0.398954	0.159164	-1.35586
Random 7	0.588094	0.345855	-0.15105
Random 8	0.569587	0.324429	-1.61608
Random 9	0.489486	0.239596	-0.88752
Random 10	0.712315	0.507392	-0.35966
Random Models Parameters			
Average r :	0.555605		
Average r ² :	0.326755		
Average Q ² :	-0.71954		
cRp ² :	0.815391		

Table S10 Y-Randomization test for HRV 14.

Model	R	R ²	Q ²
Original	0.990939	0.98196	0.968278
Random 1	0.331271	0.109741	-1.28006
Random 2	0.247508	0.06126	-1.42076
Random 3	0.522696	0.273212	-0.65442
Random 4	0.408621	0.166971	-1.01081
Random 5	0.615903	0.379336	-0.99632
Random 6	0.588511	0.346345	-0.77818
Random 7	0.334671	0.112005	-1.51982
Random 8	0.330163	0.109008	-1.61145
Random 9	0.593043	0.3517	-0.21414
Random 10	0.452129	0.204421	-0.92165
Random Models Parameters			
Average r :	0.442452		
Average r ² :	0.2114		
Average Q ² :	-1.04076		
cRp ² :	0.878643		

Table S11 Y-Randomization test for HRV 21.

Model	R	R ²	Q ²
Original	0.971357	0.943535	0.830363
Random 1	0.621493	0.386254	-1.009
Random 2	0.581182	0.337772	-0.5568
Random 3	0.663908	0.440774	-0.14664
Random 4	0.676541	0.457707	-1.18223
Random 5	0.707401	0.500416	-0.10006
Random 6	0.531382	0.282367	-2.00836
Random 7	0.438971	0.192696	-0.85652
Random 8	0.34876	0.121633	-1.89739
Random 9	0.405657	0.164558	-0.96563
Random 10	0.41794	0.174674	-2.24956
Random Models Parameters			
Average r :	0.539323		
Average r ² :	0.305885		
Average Q ² :	-1.09722		
cRp ² :	0.784737		

Table S12 Y-Randomization test for HRV 71.

Model	R	R ²	Q ²
Original	0.991193	0.982463	0.959806
Random 1	0.392006	0.153669	-0.80457
Random 2	0.700753	0.491054	-0.39966
Random 3	0.431751	0.186409	-0.89757
Random 4	0.7377	0.544201	0.030705
Random 5	0.584026	0.341086	-0.8897
Random 6	0.626657	0.392699	0.029473
Random 7	0.646583	0.41807	-0.50237
Random 8	0.517401	0.267703	-0.76415
Random 9	0.500434	0.250434	-0.41897
Random 10	0.452092	0.204387	-0.60507
Random Models Parameters			
Average r :	0.55894		
Average r ² :	0.324971		
Average Q ² :	-0.52219		
cRp ² :	0.811355		

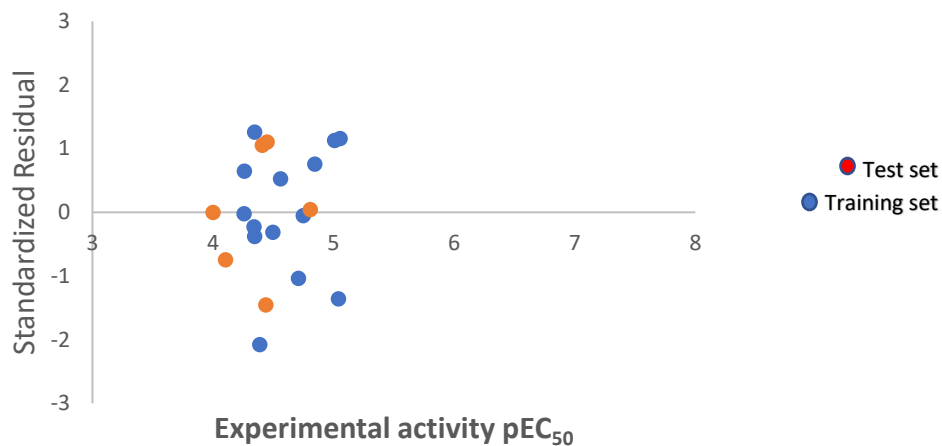


Figure S1 Plot of standardized residual against experimental activity pEC₅₀ for COX B1.

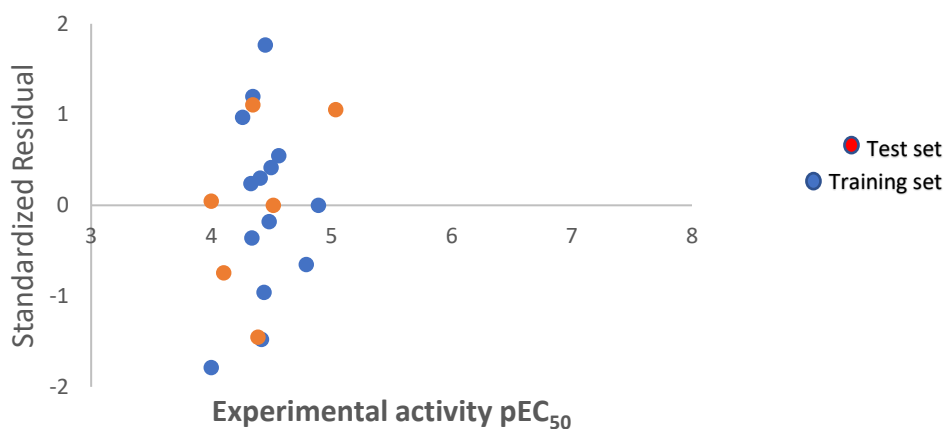


Figure S2 Plot of standardized residual against experimental activity pEC₅₀ for COX B3.

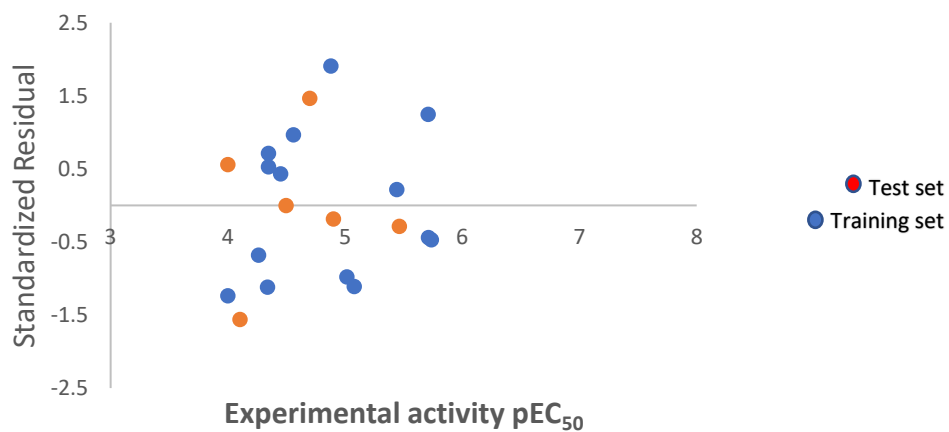


Figure S3 Plot of standardized residual against experimental activity pEC₅₀ for PV3.

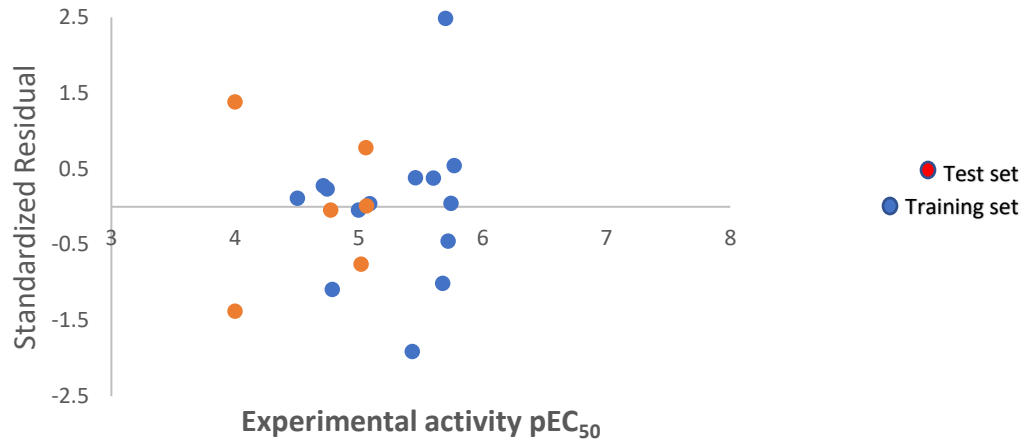


Figure S4 Plot of standardized residual against experimental activity pEC_{50} for HRV 14.

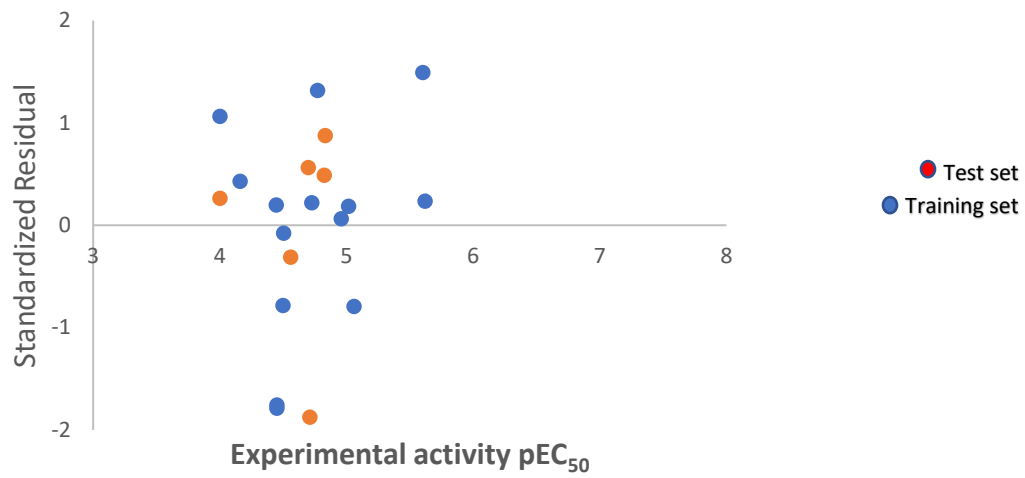


Figure S5 Plot of standardized residual against experimental activity pEC_{50} for HRV 21.

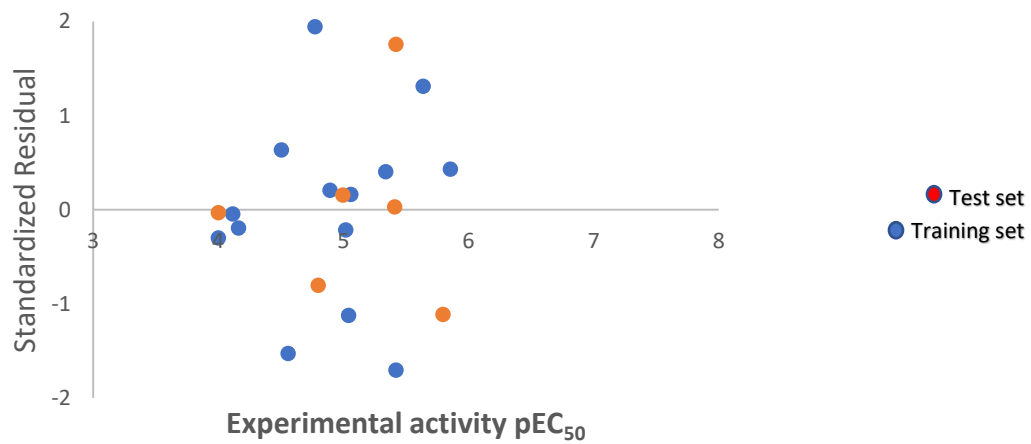


Figure S6 Plot of standardized residual against experimental activity pEC_{50} for HRV 71.

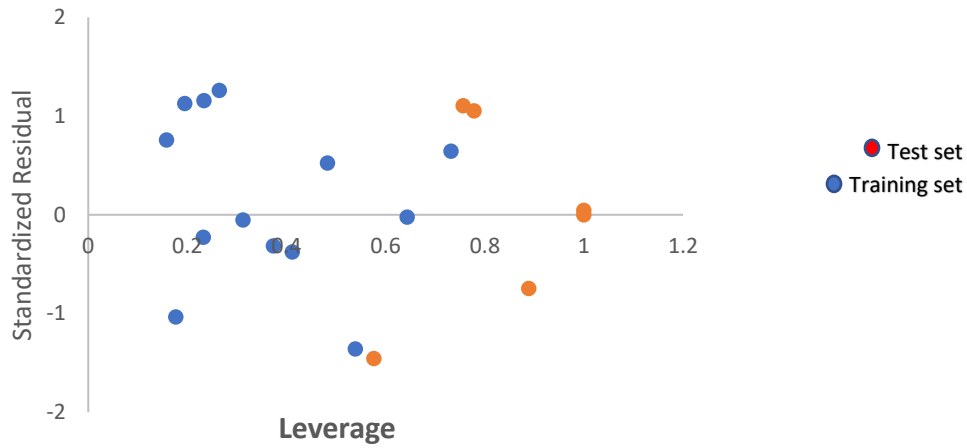


Figure S7 Williams plot of standardized residual against Leverage for COX B1.

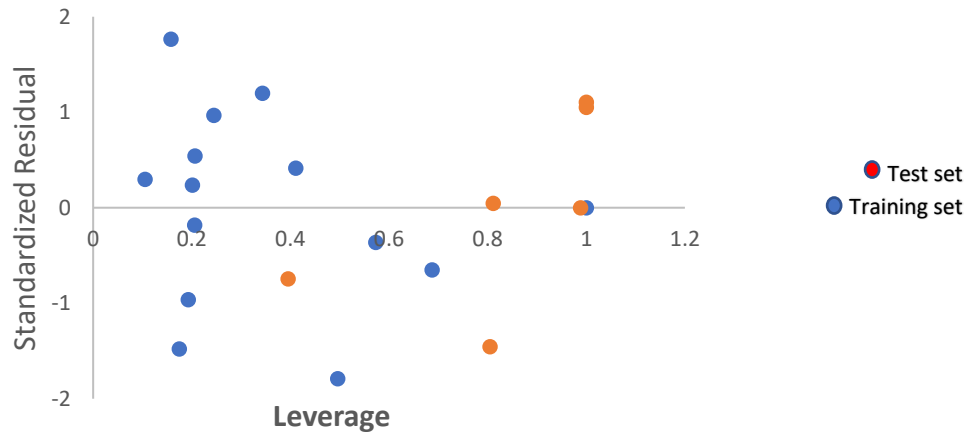


Figure S8 Williams Plot of standardized residual against Leverage for COX B3.

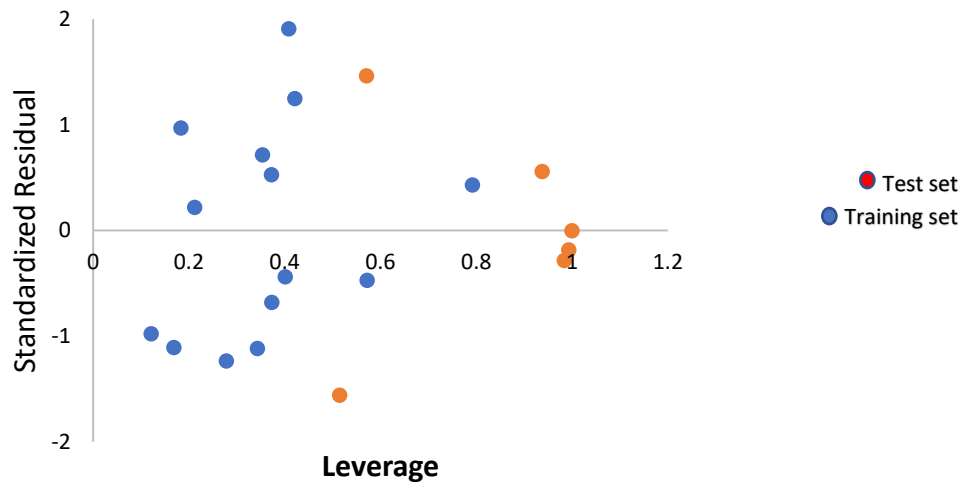


Figure S9 Williams Plot of standardized residual against Leverage for PV3.

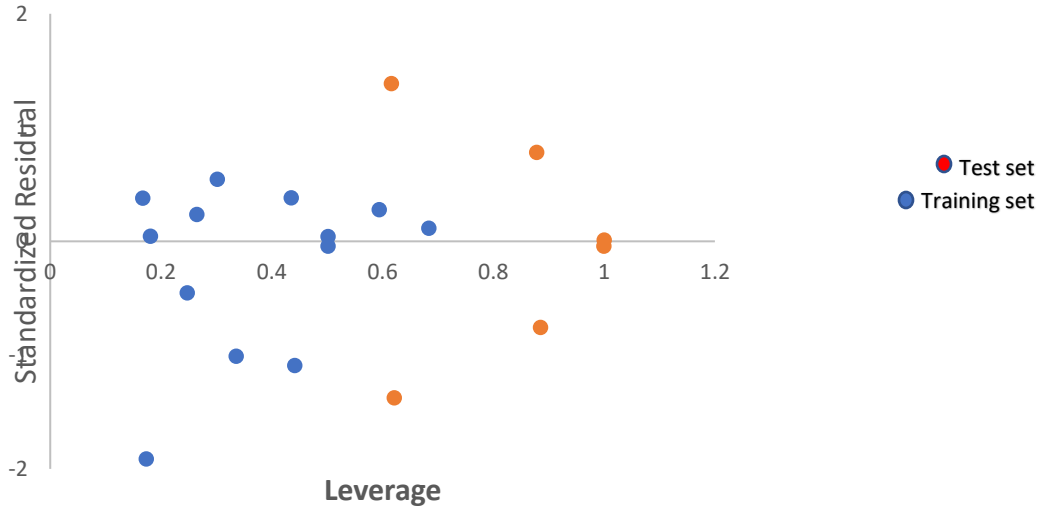


Figure S10 Williams Plot of standardized residual against Leverage for HRV 14.

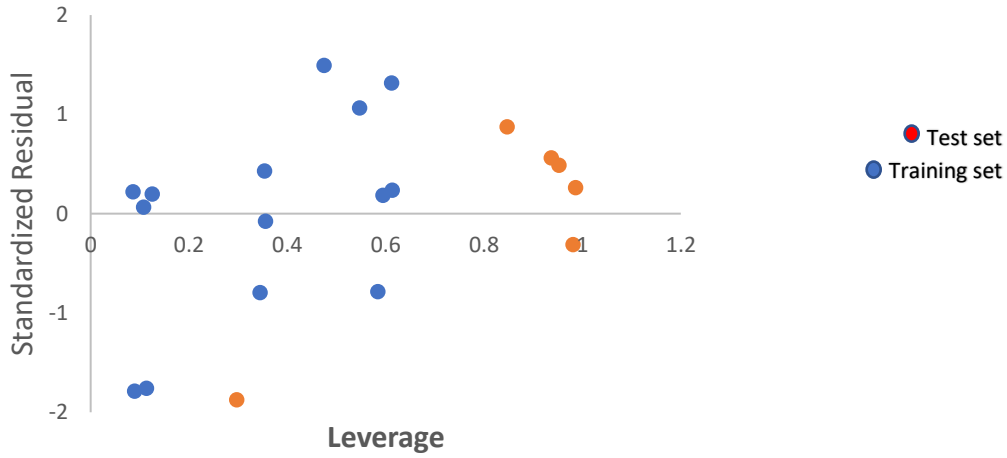


Figure S11 Williams Plot of standardized residual against Leverage for HRV 21.

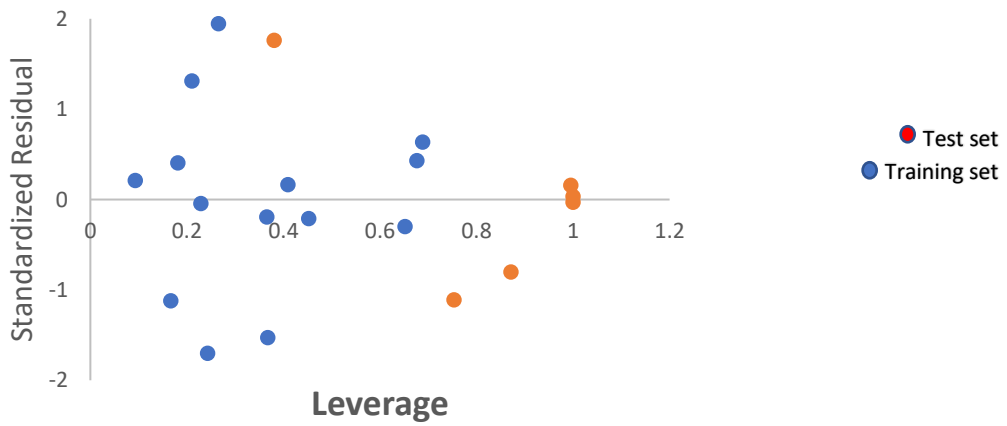


Figure S12 Williams Plot of standardized residual against Leverage for HRV71.