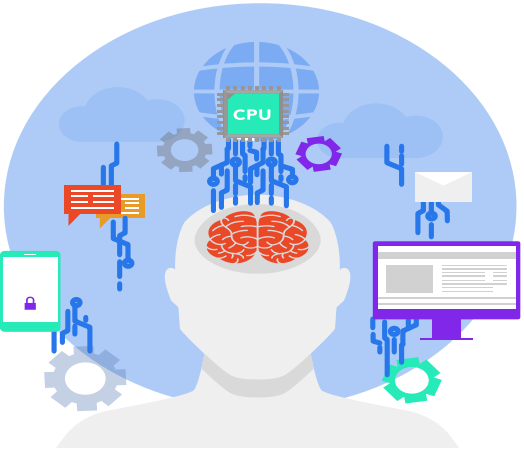
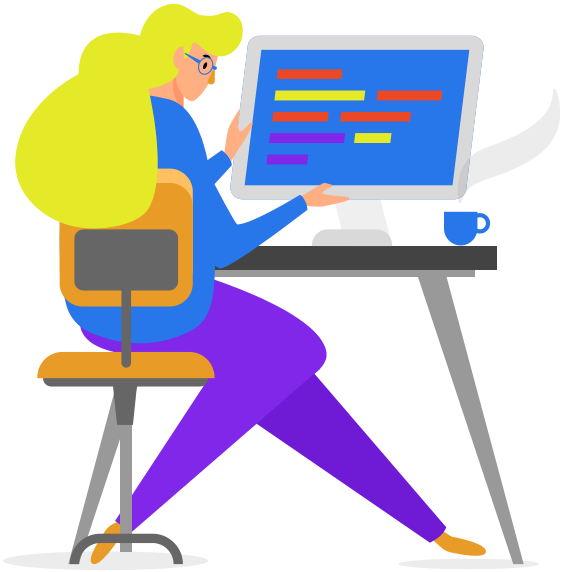


METRICS FOR UNBIASED SELECTION OF MACHINE LEARNING REGRESSION MODELS

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Machine Learning in Predictive Cheminformatics



01 Drug Design

02 Materials property

03 Toxicity screening

04 Nanotechnology

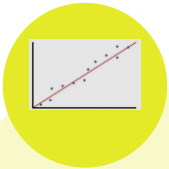
05 Agriculture

06 Food Science

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Mol Divers 29, 3703–3715 (2025)

Machine Learning Modeling



Regression

- For continuous numerical responses values
- Correlation- and error-based metrics
- Examples: Linear regression, Ridge regression, SVR

Vs



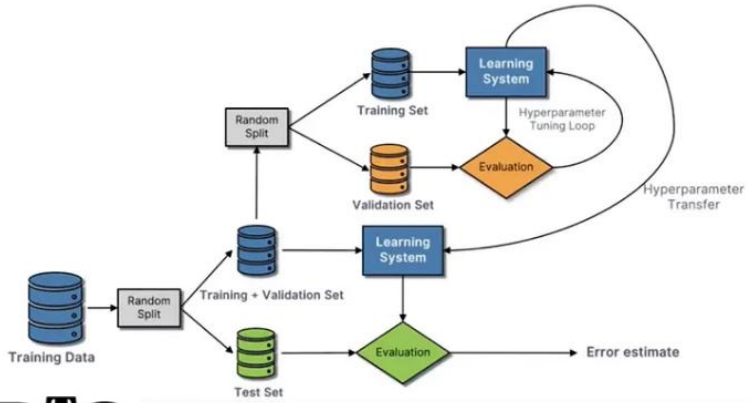
Classification

- For discrete categories or labels
- Metrics like Accuracy, Precision, Recall
- Examples: LDA, Logistic regression, SVC

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Metrics for regression-based models

Regression-based QSAR workflow



Training set statistics — R^2, MAE, RMSEC

Cross-validation statistics — Q^2-LOO, Q^2-LMO, MAE-CV

Test set statistics — Q^2_{F1}, Q^2_{F2}, Q^2_{F3}

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Metrics for regression-based models

$$R^2 = 1 - \frac{\sum \left(Y_{obs(training)} - Y_{cal(training)}\right)^2}{\sum \left(Y_{obs(training)} - \bar{Y}_{training}\right)^2} \quad (1)$$

$$MAE_{training} = \frac{\sum \left|Y_{obs(training)} - Y_{cal(training)}\right|}{n_{training}} \quad (2)$$

$$RMSEC = \sqrt{\frac{\sum \left(Y_{obs(training)} - Y_{cal(training)}\right)^2}{n_{training}}} \quad (3)$$

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Metrics for regression-based models

$$Q^2_{LOO} = 1 - \frac{\sum \left(Y_{obs(training)} - Y_{loo\ predicted(training)}\right)^2}{\sum \left(Y_{obs(training)} - \bar{Y}_{training}\right)^2} \quad (4)$$

$$MAE_{LOO} = \frac{\sum \left|Y_{obs(training)} - Y_{loo\ predicted(training)}\right|}{n_{training}} \quad (5)$$

$$MSE_{LOO} = \frac{\sum \left(Y_{obs(training)} - Y_{loo\ predicted(training)}\right)^2}{n_{training}} \quad (6)$$

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Metrics for regression-based models

$$Q^2_{F1} = 1 - \frac{\sum \left(Y_{obs(test)} - Y_{pred(test)}\right)^2}{\sum \left(Y_{obs(test)} - \bar{Y}_{training}\right)^2} \quad (7)$$

$$Q^2_{F2} = 1 - \frac{\sum \left(Y_{obs(test)} - Y_{pred(test)}\right)^2}{\sum \left(Y_{obs(test)} - \bar{Y}_{test}\right)^2} \quad (8)$$

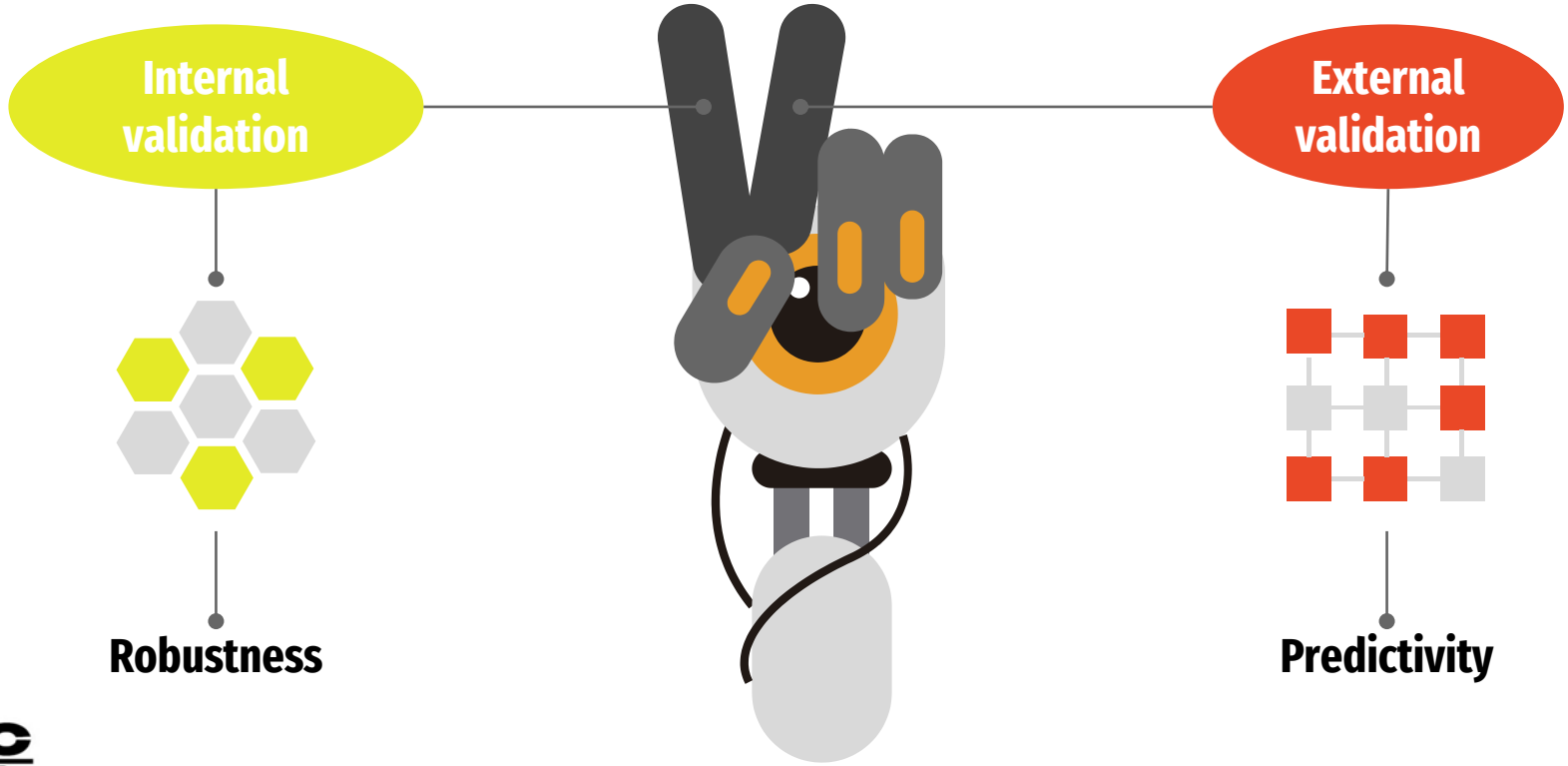
$$Q^2_{F3} = 1 - \frac{\left[\sum \left(Y_{obs(test)} - Y_{pred(test)}\right)^2\right]/n_{test}}{\left[\sum \left(Y_{obs(training)} - \bar{Y}_{training}\right)^2\right]/n_{training}} \quad (9)$$

$$MAE_{test} = \frac{\sum \left|Y_{obs(test)} - Y_{pred(test)}\right|}{n_{test}} \quad (10)$$

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J. Chem. Inf. Model. 2011, 51, 2320−2335

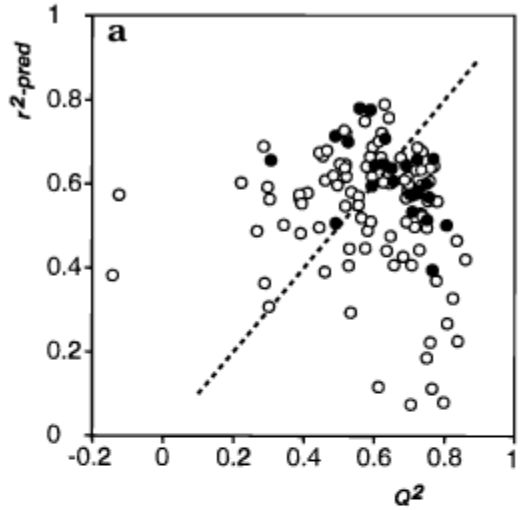
Internal vs. External Validation

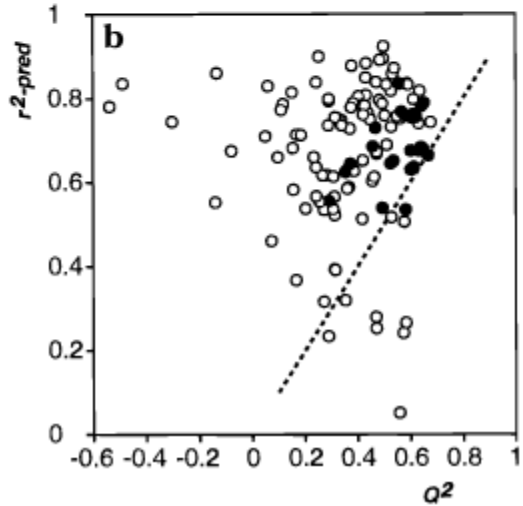


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Internal validation

Robustness





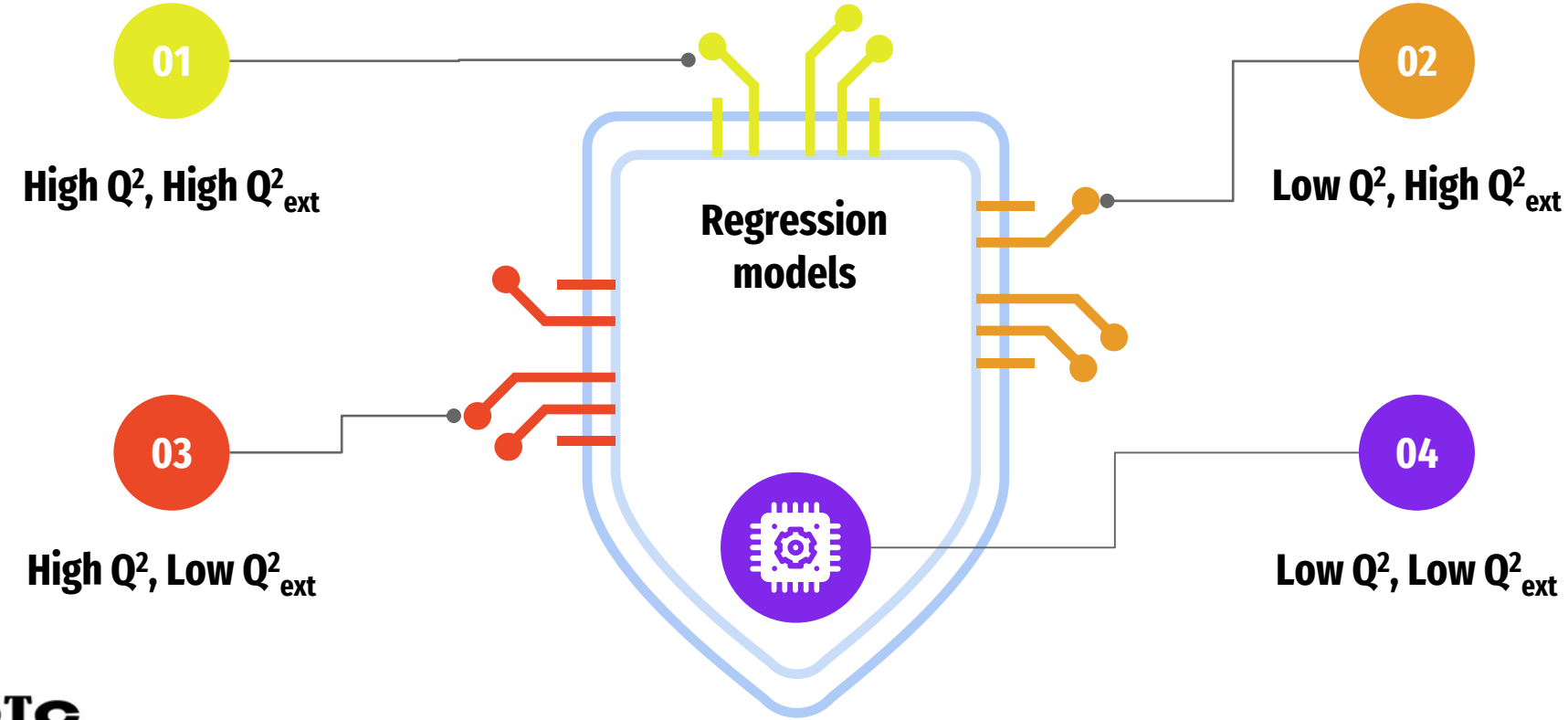
External validation

Predictivity

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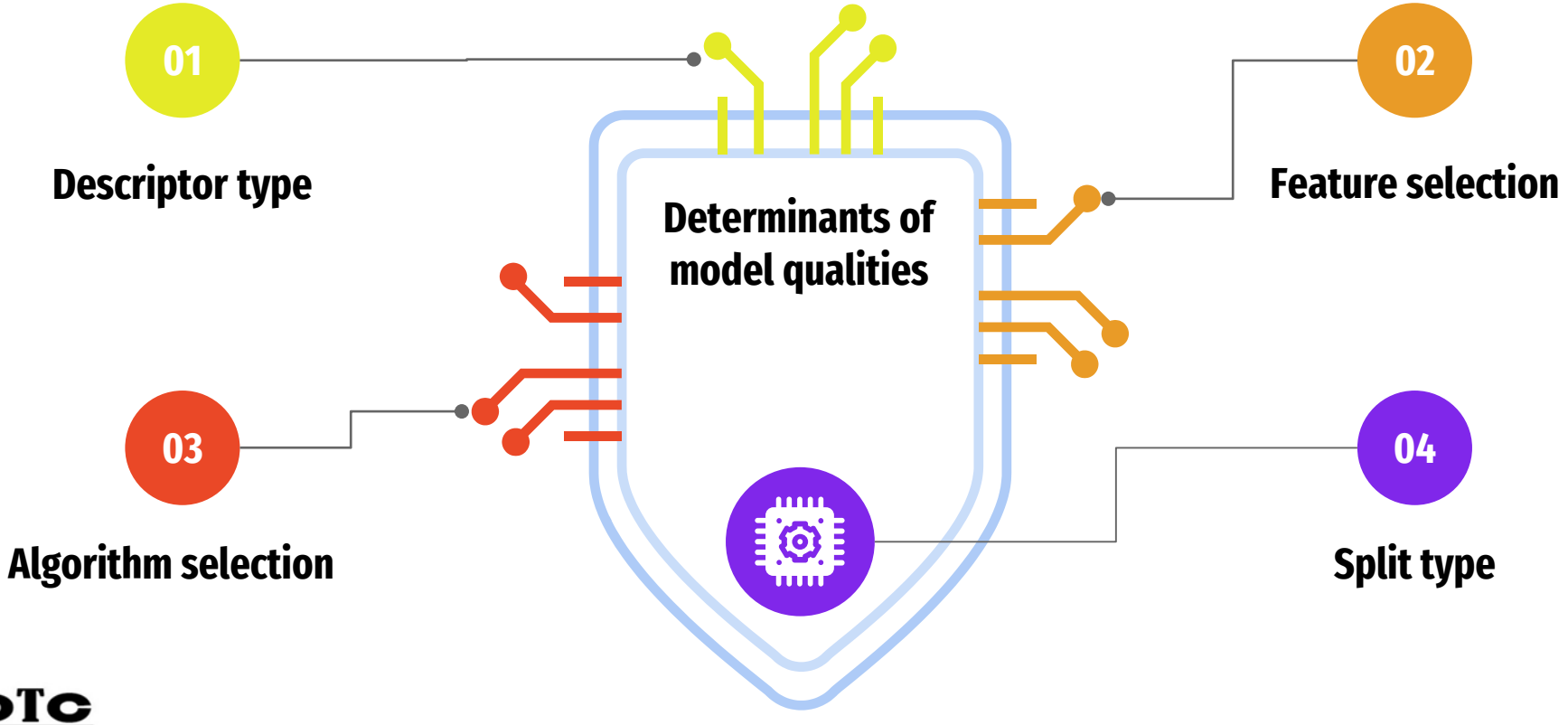
J Med Chem 1998, 41, 2553-2564

Different scenarios



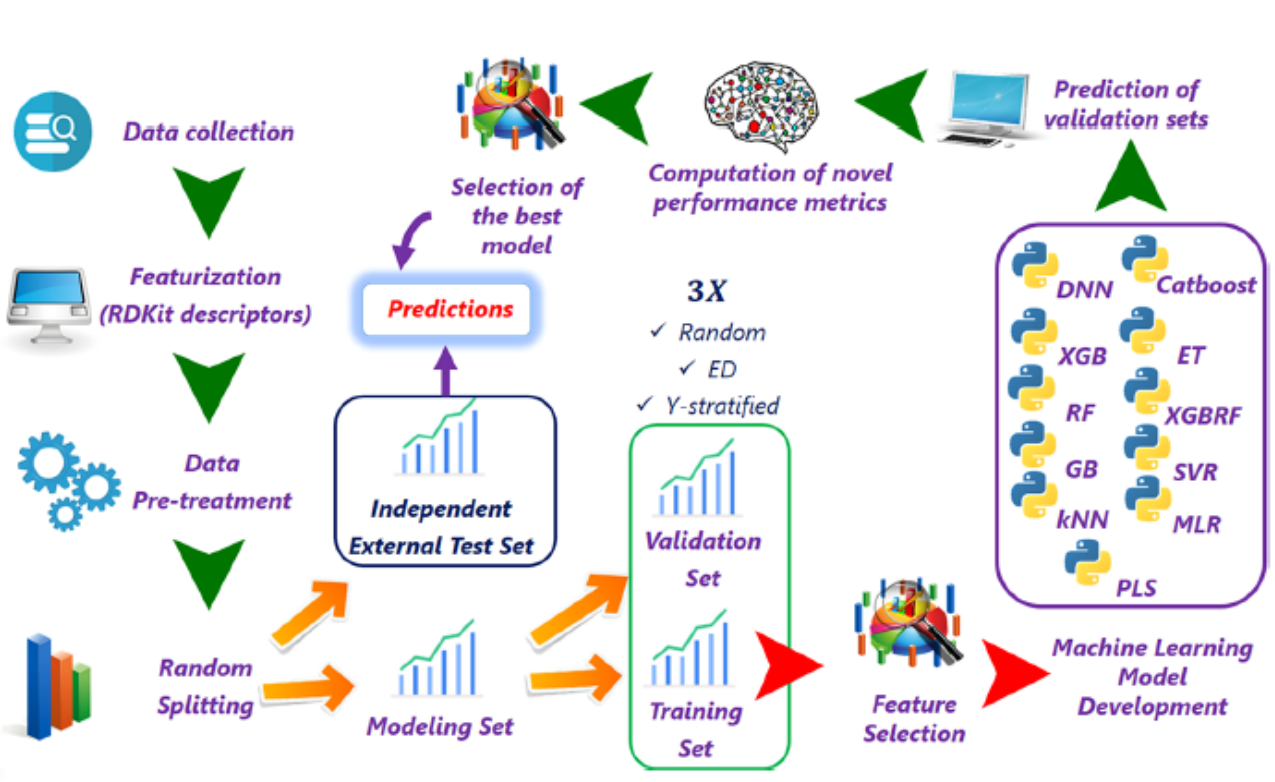
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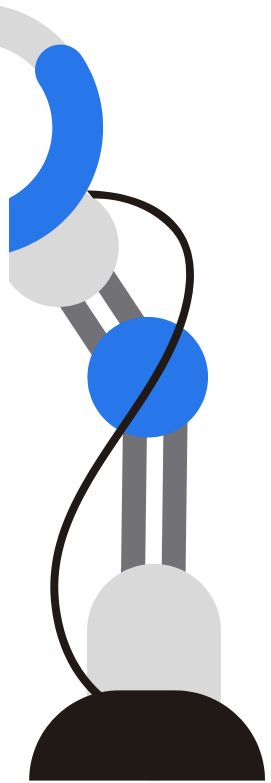
Sources of variations of model qualities



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Machine Learning Regression Workflow





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Data sets/Benchmark data sets

01 Aqueous solubility data

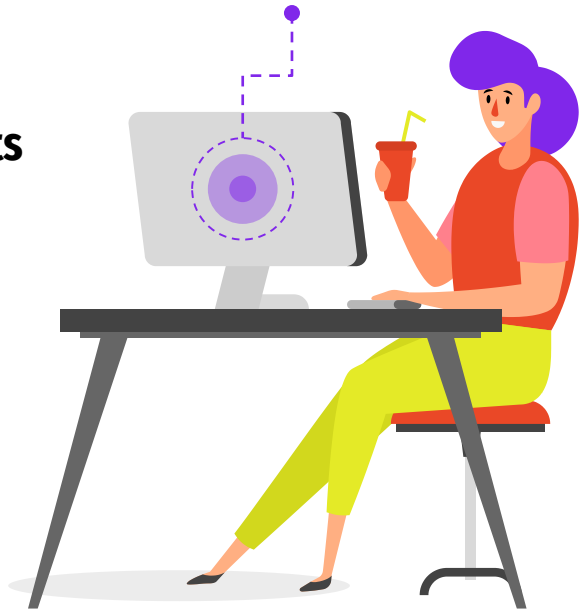
6265 compounds

02 α7nACh Receptor agonists

1453 compounds

03 Reorganization energy

171 structures



logP values 04

13745 compounds

BCF values 05

603 compounds

J. Chem. Inf. Model. 2017, 57, 36−49.

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Novel metrics

$$Q^2_{Robustness} = Q^2_{CV} \times (1 - \sqrt{|R^2_{Train} - Q^2_{CV}|}) \quad (1)$$

$$Q^2_{Generalizability} = Q^2_{F2} \times (1 - \sqrt{|Q^2_{CV} - Q^2_{F2}|}) \quad (2)$$

$$Q^2_{Performance} = \sqrt[3]{Q^2_{Robustness} \times (Q^2_{Generalizability})^2} \quad (3)$$

Toth's criteria: J. Comput.-Aided Mol. Des. 2013, 27, 837−844

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Data set 1

Division	Model	Training and validation set metrics			Novel Q2 metrics			Test set
		R2	Q2-10-fold	Q2F2val	Q2robust	Q2gen	Q2perform	Q2F2ext
Division 1	DNN	0.89	0.81	0.80	0.56	0.72	0.66	0.80
	CatBoost	0.95	0.83	0.83	0.55	0.76	0.68	0.82
	XGBoost	0.99	0.82	0.80	0.48	0.71	0.62	0.81
	ExtraTrees	1.00	0.82	0.81	0.48	0.73	0.63	0.82
	Random Forest	0.97	0.81	0.81	0.48	0.74	0.64	0.82
	XGBRF	0.82	0.78	0.76	0.61	0.68	0.66	0.76
	GB	0.85	0.80	0.79	0.63	0.72	0.69	0.79
	SVR	0.87	0.81	0.81	0.62	0.76	**0.71**	0.81
	kNN	0.85	0.76	0.76	0.53	0.72	0.65	0.75
	MLR	0.76	0.75	0.74	0.71	0.67	0.68	0.73
	PLS	0.76	0.75	0.74	0.71	0.67	0.68	0.73
Division 2	DNN	0.84	0.80	0.78	0.66	0.65	0.66	0.77
	CatBoost	0.94	0.83	0.82	0.55	0.76	0.68	0.82
	XGBoost	0.99	0.81	0.81	0.47	0.75	0.64	0.81
	ExtraTrees	1.00	0.82	0.82	0.48	0.77	0.65	0.82
	Random Forest	0.98	0.82	0.81	0.49	0.75	0.65	0.81
	XGBRF	0.82	0.78	0.77	0.61	0.70	0.67	0.77
	GB	0.85	0.80	0.79	0.63	0.71	0.68	0.80
	SVR	0.87	0.81	0.80	0.62	0.74	**0.70**	0.80
	kNN	0.84	0.75	0.75	0.53	0.68	0.63	0.75
	MLR	0.75	0.75	0.74	0.71	0.65	0.67	0.74
	PLS	0.75	0.75	0.74	0.71	0.65	0.67	0.74
Division 3	DNN	0.78	0.79	0.75	0.73	0.60	0.64	0.73
	CatBoost	0.93	0.81	0.82	0.53	0.75	0.67	0.81
	XGBoost	0.98	0.80	0.81	0.45	0.72	0.62	0.79
	ExtraTrees	1.00	0.80	0.82	0.45	0.70	0.61	0.81
	Random Forest	0.97	0.80	0.82	0.46	0.70	0.61	0.80
	XGBRF	0.81	0.76	0.78	0.60	0.69	0.66	0.76
	GB	0.84	0.79	0.80	0.61	0.73	0.69	0.79
	SVR	0.84	0.80	0.80	0.63	0.77	**0.72**	0.78
	kNN	0.84	0.75	0.76	0.53	0.68	0.62	0.76
	MLR	0.74	0.74	0.73	0.71	0.67	0.68	0.72
	PLS	0.74	0.74	0.73	0.70	0.66	0.68	0.72



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Data set 2

Division	Model	Training and validation set metrics			Novel Q2 metrics			Test set
		R2	Q2-10-fold	Q2F2val	Q2robust	Q2gen	Q2perform	Q2F2ext
Division 1	DNN	0.80	0.54	0.43	0.26	0.29	0.28	0.42
	CatBoost	0.93	0.62	0.57	0.28	0.44	0.38	0.57
	XGBoost	0.99	0.59	0.57	0.22	0.47	0.36	0.52
	ExtraTrees	1.00	0.61	0.54	0.22	0.40	0.33	0.54
	Random Forest	0.95	0.61	0.59	0.26	0.50	0.40	0.56
	XGBRF	0.73	0.55	0.52	0.32	0.43	0.39	0.52
	GB	0.76	0.58	0.55	0.33	0.45	**0.41**	0.52
	SVR	0.72	0.58	0.47	0.36	0.32	0.33	0.46
	kNN	0.70	0.51	0.36	0.29	0.22	0.24	0.42
	MLR	0.53	0.49	0.36	0.40	0.23	0.28	0.40
	PLS	0.53	0.49	0.36	0.40	0.23	0.28	0.40
Division 2	DNN	0.70	0.44	0.53	0.22	0.38	0.31	0.49
	CatBoost	0.95	0.60	0.64	0.24	0.51	0.40	0.55
	XGBoost	1.00	0.57	0.61	0.19	0.48	0.36	0.46
	ExtraTrees	1.00	0.57	0.63	0.20	0.48	0.36	0.49
	Random Forest	0.94	0.59	0.62	0.23	0.50	0.39	0.51
	XGBRF	0.75	0.54	0.56	0.29	0.49	0.41	0.48
	GB	0.78	0.56	0.56	0.30	0.54	**0.44**	0.52
	SVR	0.69	0.54	0.55	0.33	0.49	0.43	0.49
	kNN	0.67	0.46	0.50	0.25	0.40	0.34	0.47
	MLR	0.51	0.37	0.38	0.23	0.34	0.29	0.39
	PLS	0.49	0.41	0.38	0.30	0.32	0.31	0.38
Division 3	DNN	0.66	0.55	0.50	0.36	0.38	0.38	0.48
	CatBoost	0.96	0.64	0.65	0.27	0.58	0.45	0.57
	XGBoost	1.00	0.61	0.58	0.23	0.48	0.38	0.48
	ExtraTrees	1.00	0.64	0.60	0.25	0.50	0.40	0.55
	Random Forest	0.95	0.61	0.63	0.26	0.55	0.43	0.54
	XGBRF	0.72	0.55	0.55	0.32	0.51	0.44	0.46
	GB	0.77	0.57	0.58	0.32	0.53	0.44	0.52
	SVR	0.73	0.58	0.58	0.35	0.54	**0.47**	0.53
	kNN	0.69	0.51	0.47	0.30	0.38	0.35	0.46
	MLR	0.54	0.49	0.45	0.38	0.36	0.36	0.46
	PLS	0.54	0.49	0.45	0.38	0.36	0.36	0.46



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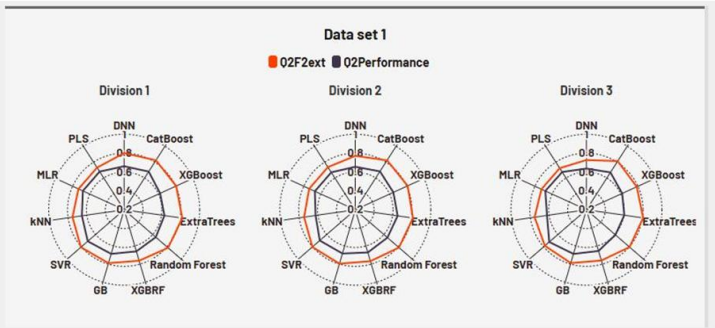
Data set 3

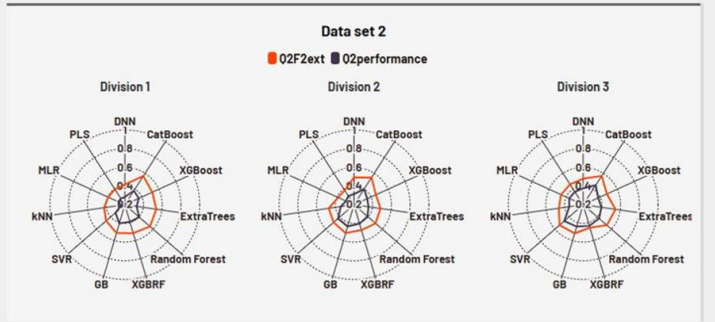
Division	Model	Training and validation set metrics			Novel Q2 metrics			Test set
		R2	Q2-10-fold	Q2F2val	Q2robust	Q2gen	Q2perform	Q2F2ext
Division 1	DNN	0.84	0.63	0.63	0.34	0.58	0.49	0.65
	CatBoost	1.00	0.57	0.65	0.20	0.47	0.35	0.59
	XGBoost	1.00	0.52	0.51	0.16	0.47	0.33	0.51
	ExtraTrees	1.00	0.59	0.55	0.21	0.43	0.34	0.59
	Random Forest	0.94	0.54	0.59	0.19	0.46	0.34	0.55
	XGBRF	0.95	0.49	0.55	0.16	0.41	0.30	0.59
	GB	0.99	0.54	0.73	0.18	0.42	0.32	0.70
	SVR	0.80	0.64	0.60	0.37	0.49	0.45	0.62
	kNN	0.64	0.40	0.43	0.20	0.35	0.29	0.38
	MLR	0.79	0.72	0.70	0.53	0.59	**0.57**	0.72
	PLS	0.78	0.71	0.69	0.53	0.59	**0.57**	0.71
Division 2	DNN	0.72	0.55	0.63	0.32	0.45	0.40	0.60
	CatBoost	0.99	0.51	0.74	0.15	0.38	0.28	0.69
	XGBoost	1.00	0.38	0.72	0.08	0.30	0.19	0.56
	ExtraTrees	1.00	0.56	0.73	0.19	0.43	0.33	0.76
	Random Forest	0.93	0.51	0.69	0.18	0.40	0.31	0.69
	XGBRF	0.95	0.50	0.68	0.16	0.39	0.29	0.65
	GB	0.98	0.52	0.78	0.16	0.38	0.29	0.58
	SVR	0.76	0.61	0.69	0.38	0.50	0.46	0.67
	kNN	0.66	0.43	0.58	0.23	0.36	0.31	0.57
	MLR	0.75	0.71	0.64	0.57	0.47	0.50	0.73
	PLS	0.74	0.70	0.67	0.54	0.57	**0.56**	0.73
Division 3	DNN	0.82	0.69	0.58	0.44	0.38	0.40	0.57
	CatBoost	1.00	0.59	0.64	0.21	0.50	0.38	0.65
	XGBoost	1.00	0.53	0.59	0.17	0.45	0.32	0.57
	ExtraTrees	1.00	0.63	0.65	0.25	0.56	0.42	0.65
	Random Forest	0.95	0.59	0.63	0.24	0.50	0.39	0.63
	XGBRF	0.96	0.58	0.63	0.22	0.48	0.37	0.62
	GB	0.98	0.59	0.65	0.22	0.49	0.37	0.53
	SVR	0.76	0.61	0.62	0.37	0.56	**0.49**	0.62
	kNN	0.72	0.51	0.56	0.28	0.43	0.37	0.47
	MLR	0.80	0.76	0.57	0.60	0.33	0.40	0.67
	PLS	0.80	0.75	0.58	0.60	0.33	0.41	0.67

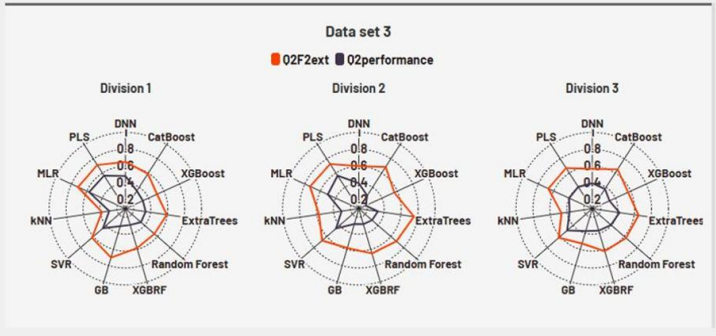


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Data sets 1-3







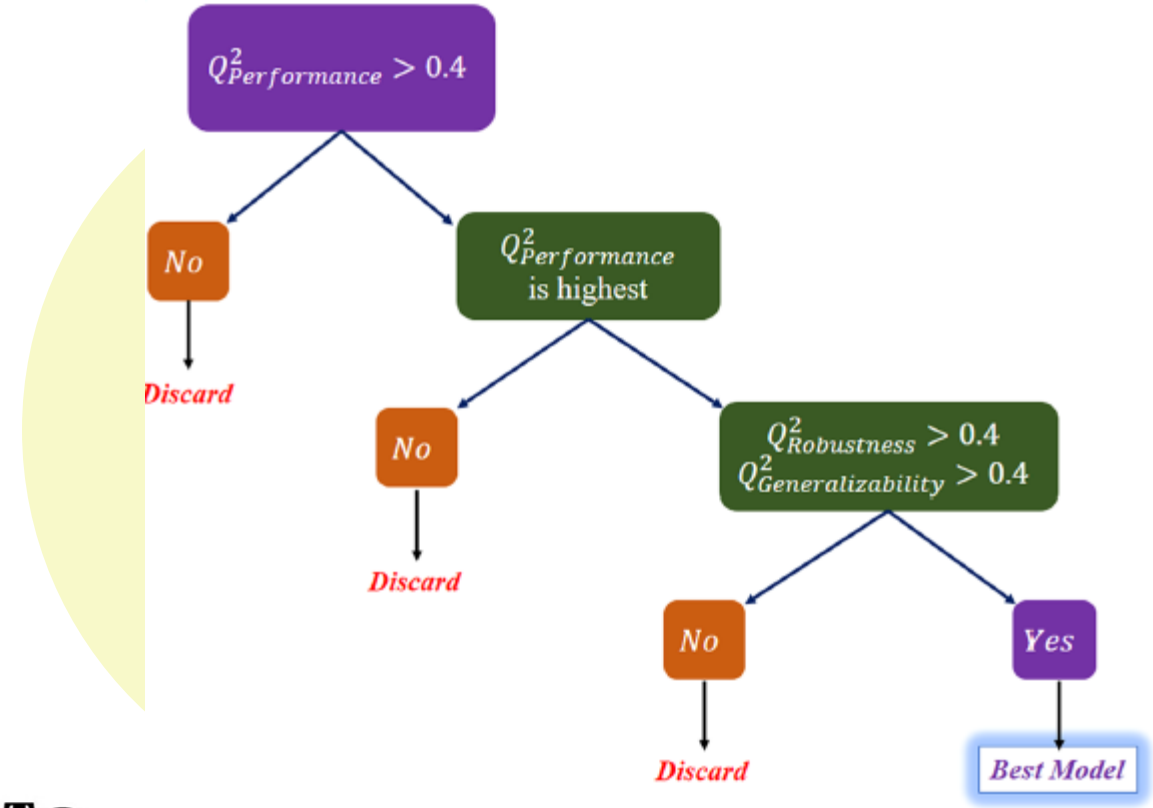
DTC LAB

Data sets 1-3

Set	*Split*	*Model*	$Q^2_{Robustnes}$	$Q^2_{Generalizability}$	$Q^2_{Performance}$	*Stringency Test*	Q^2_{F2Ext}
1	Random	SVR	0.618	0.762	0.710	***Pass***	0.806
	ED	SVR	0.618	0.742	0.698	***Pass***	0.802
	Y-stratified	SVR	0.631	0.772	0.722	***Pass***	0.783
2	Random	GB	0.333	0.454	0.409	**Fail**	0.516
	ED	GB	0.297	0.539	0.442	**Fail**	0.516
	Y-stratified	SVR	0.349	0.541	0.467	**Fail**	0.534
3	Random	MLR	0.533	0.59	0.571	***Pass***	0.715
	ED	PLS	0.544	0.574	0.564	***Pass***	0.727
	Y-stratified	SVR	0.373	0.564	0.492	**Fail**	0.623

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Data sets 1-3



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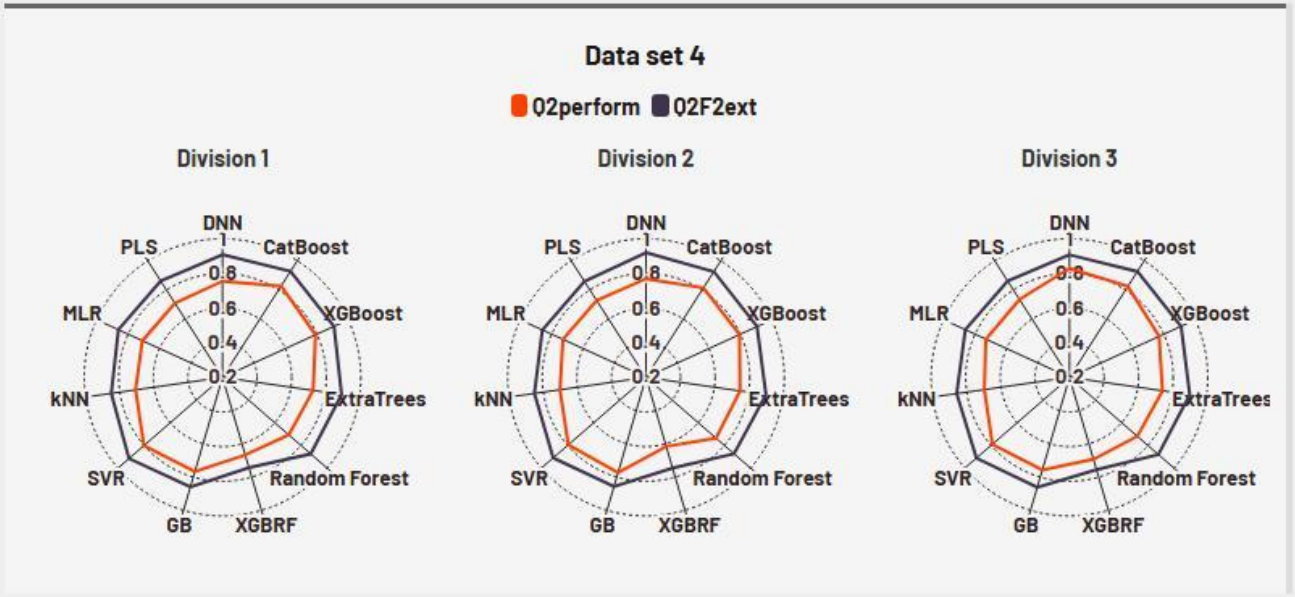
Data set 4

Division	Model	ining and validation set met			Novel Q2 metrics			Test set
		R2	Q2-10-fol	Q2F2val	Q2robust	Q2gen	Q2perform	Q2F2ext
Division 1	DNN	0.93	0.91	0.89	0.78	0.75	0.76	0.91
	CatBoost	0.96	0.92	0.92	0.73	0.88	**0.83**	0.93
	XGBoost	0.98	0.90	0.90	0.65	0.87	0.79	0.91
	ExtraTrees	1.00	0.88	0.89	0.58	0.82	0.73	0.90
	Random For	0.98	0.86	0.87	0.56	0.79	0.71	0.88
	XGBRF	0.76	0.73	0.73	0.60	0.70	0.67	0.74
	GB	0.87	0.85	0.84	0.72	0.79	0.77	0.86
	SVR	0.95	0.91	0.91	0.73	0.84	0.80	0.92
	kNN	0.90	0.83	0.84	0.62	0.76	0.71	0.85
	MLR	0.85	0.85	0.82	0.81	0.66	0.71	0.86
	PLS	0.85	0.85	0.82	0.81	0.66	0.71	0.86
Division 2	DNN	0.95	0.90	0.92	0.71	0.80	0.77	0.92
	CatBoost	0.96	0.92	0.93	0.73	0.86	**0.81**	0.93
	XGBoost	0.98	0.90	0.91	0.65	0.88	0.79	0.91
	ExtraTrees	1.00	0.89	0.89	0.59	0.84	0.75	0.90
	Random For	0.98	0.86	0.87	0.57	0.84	0.74	0.87
	XGBRF	0.76	0.73	0.72	0.61	0.62	0.62	0.75
	GB	0.87	0.84	0.85	0.71	0.81	0.77	0.86
	SVR	0.94	0.90	0.91	0.73	0.83	0.79	0.91
	kNN	0.90	0.83	0.84	0.62	0.75	0.70	0.85
	MLR	0.85	0.83	0.85	0.72	0.73	0.73	0.86
	PLS	0.85	0.83	0.85	0.72	0.73	0.73	0.86
Division 3	DNN	0.92	0.90	0.90	0.78	0.86	**0.83**	0.91
	CatBoost	0.96	0.92	0.92	0.73	0.88	0.82	0.93
	XGBoost	0.98	0.90	0.90	0.64	0.84	0.77	0.91
	ExtraTrees	1.00	0.89	0.90	0.60	0.83	0.74	0.90
	Random For	0.98	0.87	0.87	0.57	0.81	0.72	0.88
	XGBRF	0.77	0.74	0.74	0.61	0.74	0.69	0.76
	GB	0.87	0.85	0.84	0.72	0.78	0.76	0.86
	SVR	0.94	0.91	0.90	0.74	0.82	0.79	0.91
	kNN	0.90	0.83	0.85	0.62	0.74	0.70	0.86
	MLR	0.85	0.83	0.85	0.72	0.74	0.73	0.86
	PLS	0.85	0.83	0.85	0.73	0.74	0.73	0.86



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Data set 4


Data set 4
Q2perform
Q2F2ext
Division 1
Division 2
Division 3
DNN
CatBoost
XGBoost
ExtraTrees
Random Forest
XGBRF
GB
SVR
kNN
MLR
PLS
0.2
0.4
0.6
0.8
1

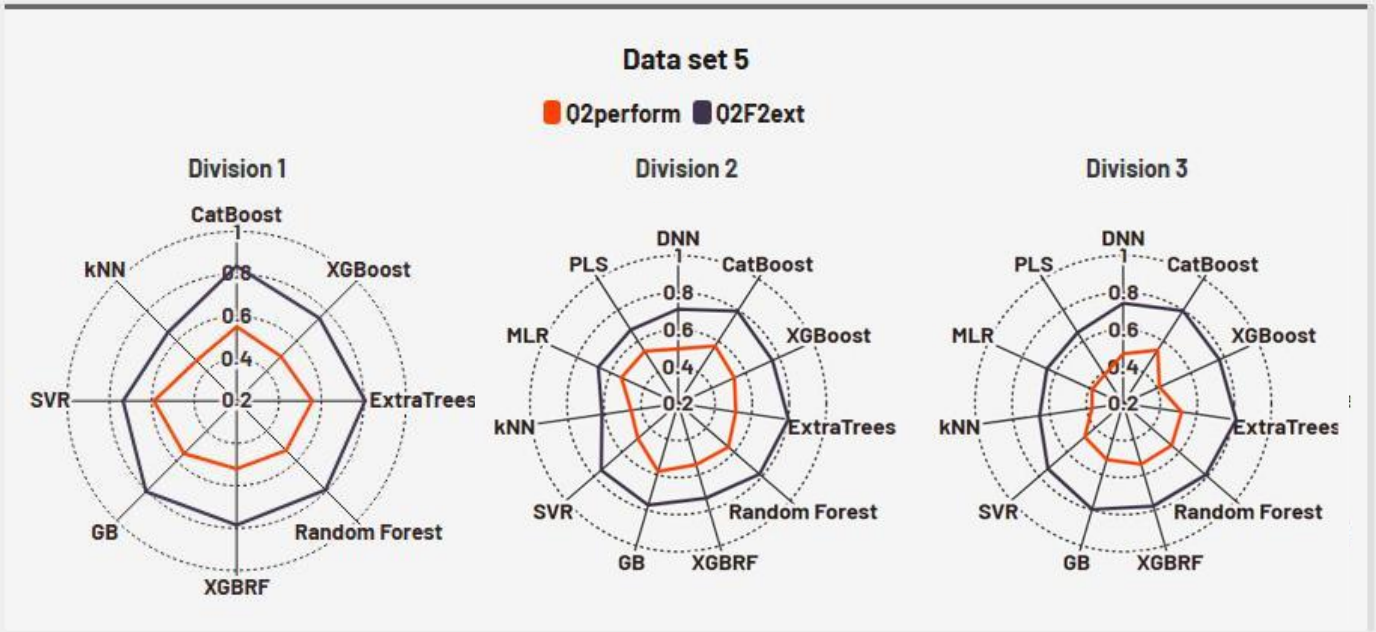
Data set 5

Division	Model	ining and validation set met			Novel Q2 metrics			Test set
		R2	Q2-10-fol	Q2F2val	Q2robust	Q2gen	Q2perform	Q2F2ext
Division 1	DNN	0.85	0.76	<0	0.53	Undefine	Undefined	<0
	CatBoost	0.99	0.79	0.86	0.43	0.62	**0.55**	0.84
	XGBoost	1.00	0.74	0.82	0.36	0.58	0.50	0.75
	ExtraTrees	1.00	0.78	0.84	0.42	0.64	0.56	0.81
	Random For	0.97	0.76	0.84	0.41	0.60	0.53	0.79
	XGBRF	0.94	0.74	0.84	0.42	0.58	0.52	0.79
	GB	0.95	0.77	0.86	0.45	0.61	0.55	0.81
	SVR	0.88	0.75	0.74	0.48	0.65	0.59	0.74
	kNN	0.79	0.66	0.62	0.42	0.49	0.47	0.66
	MLR	0.81	0.77	<0	0.62	Undefine	Undefined	<0
	PLS	0.81	0.77	<0	0.62	Undefine	Undefined	<0
Division 2	DNN	0.87	0.76	0.68	0.51	0.49	0.50	0.71
	CatBoost	0.99	0.79	0.77	0.44	0.65	**0.57**	0.79
	XGBoost	1.00	0.73	0.73	0.34	0.66	0.53	0.76
	ExtraTrees	1.00	0.77	0.73	0.40	0.59	0.51	0.80
	Random For	0.97	0.76	0.75	0.42	0.65	0.56	0.78
	XGBRF	0.91	0.73	0.71	0.42	0.61	0.54	0.73
	GB	0.94	0.75	0.76	0.42	0.69	0.58	0.77
	SVR	0.88	0.75	0.67	0.48	0.49	0.49	0.75
	kNN	0.79	0.64	0.61	0.39	0.49	0.46	0.62
	MLR	0.81	0.78	0.69	0.66	0.48	0.54	0.67
	PLS	0.81	0.78	0.69	0.66	0.48	0.54	0.67
Division 3	DNN	0.88	0.77	0.66	0.52	0.44	**0.47**	0.74
	CatBoost	0.99	0.82	0.76	0.48	0.58	0.54	0.80
	XGBoost	1.00	0.80	0.65	0.45	0.40	0.42	0.77
	ExtraTrees	1.00	0.81	0.74	0.45	0.56	0.52	0.82
	Random For	0.97	0.81	0.76	0.49	0.58	0.55	0.79
	XGBRF	0.95	0.80	0.74	0.49	0.57	0.54	0.78
	GB	0.96	0.82	0.73	0.52	0.52	0.52	0.80
	SVR	0.90	0.77	0.68	0.48	0.47	0.47	0.74
	kNN	0.81	0.68	0.54	0.43	0.34	0.37	0.66
	MLR	0.82	0.78	0.56	0.62	0.30	0.39	0.65
	PLS	0.82	0.78	0.56	0.62	0.30	0.39	0.66



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Data set 5


Data set 5
Q2perform
Q2F2ext
Division 1
CatBoost
XGBoost
ExtraTrees
Random Forest
XGBRF
GB
SVR
kNN
0.2
0.4
0.6
0.8
1
Division 2
DNN
CatBoost
XGBoost
ExtraTrees
Random Forest
XGBRF
GB
SVR
kNN
MLR
PLS
Division 3
DNN
CatBoost
XGBoost
ExtraTrees
Random Forest
XGBRF
GB
SVR
kNN
MLR
PLS

Alternate formula

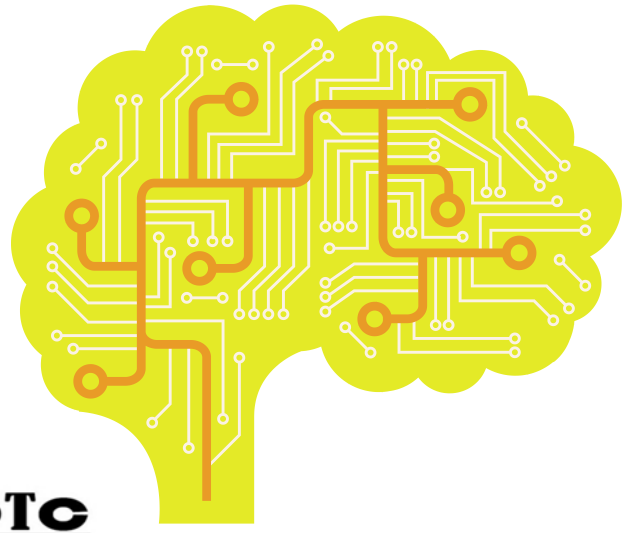
Table 1. Head-to-Head Comparison of Models Selected Using $Q^2_{\text{performance}}$ and "Alternate $Q^2_{\text{performance}}$"

			training		validation		external	
data set/split	model	selection criterion	R^2	$Q^2_{\text{10-fold}}$	Q^2_{F1}	Q^2_{F2}	$Q^2_{\text{F1,ext}}$	$Q^2_{\text{F2,ext}}$
1/1	SVR[a]	$Q^2_{\text{performance}}$	**0.865**	**0.809**	**0.813**	**0.813**	**0.806**	**0.806**
1/1	MLR/PLS	alternate $Q^2_{\text{performance}}$	0.757	0.753	0.743	0.743	0.732/0.731	0.732/0.731
1/2	SVR[a]	$Q^2_{\text{performance}}$	**0.866**	**0.810**	**0.804**	**0.804**	**0.802**	**0.802**
1/2	MLR/PLS	alternate $Q^2_{\text{performance}}$	0.753	0.750	0.737	0.737	0.737	0.737

[a]Best models are highlighted in "bold".

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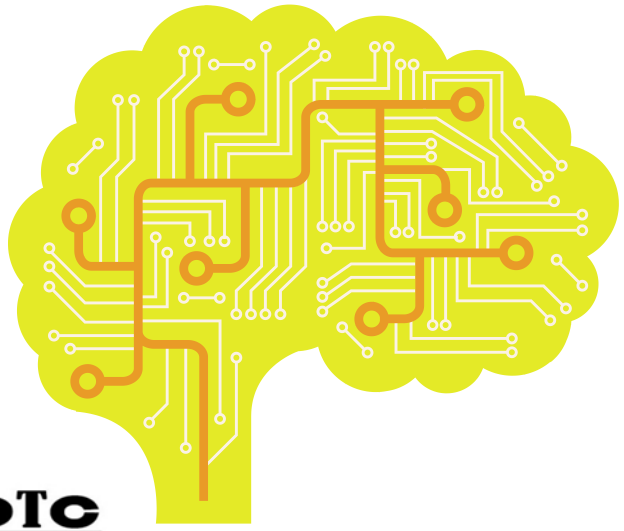
Conclusion



- The proposed framework can be an efficient tool for an unbiased selection of the best model from a set of competing models.
- This framework is neither overdependent on cross-validation performance nor does it exhibit an incorrect dependence solely on external validation performance for model selection.
- A simple quantitative value for a proposed metric can easily guide researchers toward reliable model selection, and the failed cases can prompt the modeler to modify the model development protocol.

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Conclusion



- In fact, a single best model selected from the three best models originating from three training-validation splits (based on the values of $Q^2_{performance}$) can guide the modelers to also select the appropriate data splitting algorithm without using external/test set information.

- In our view, this framework for the unbiased selection of the best model from competing models can be included in the “Best Practices for Model Development, Validation, and Exploitation”

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$Q^2_{performance}$: Toward Unbiased Selection of Machine-Learning Regression Models

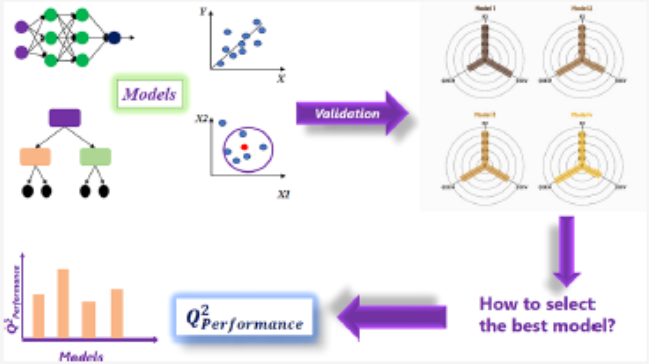
Arkaprava Banerjee* and Kunal Roy*

Cite This: J. Chem. Inf. Model. 2026, 66, 10835−10846

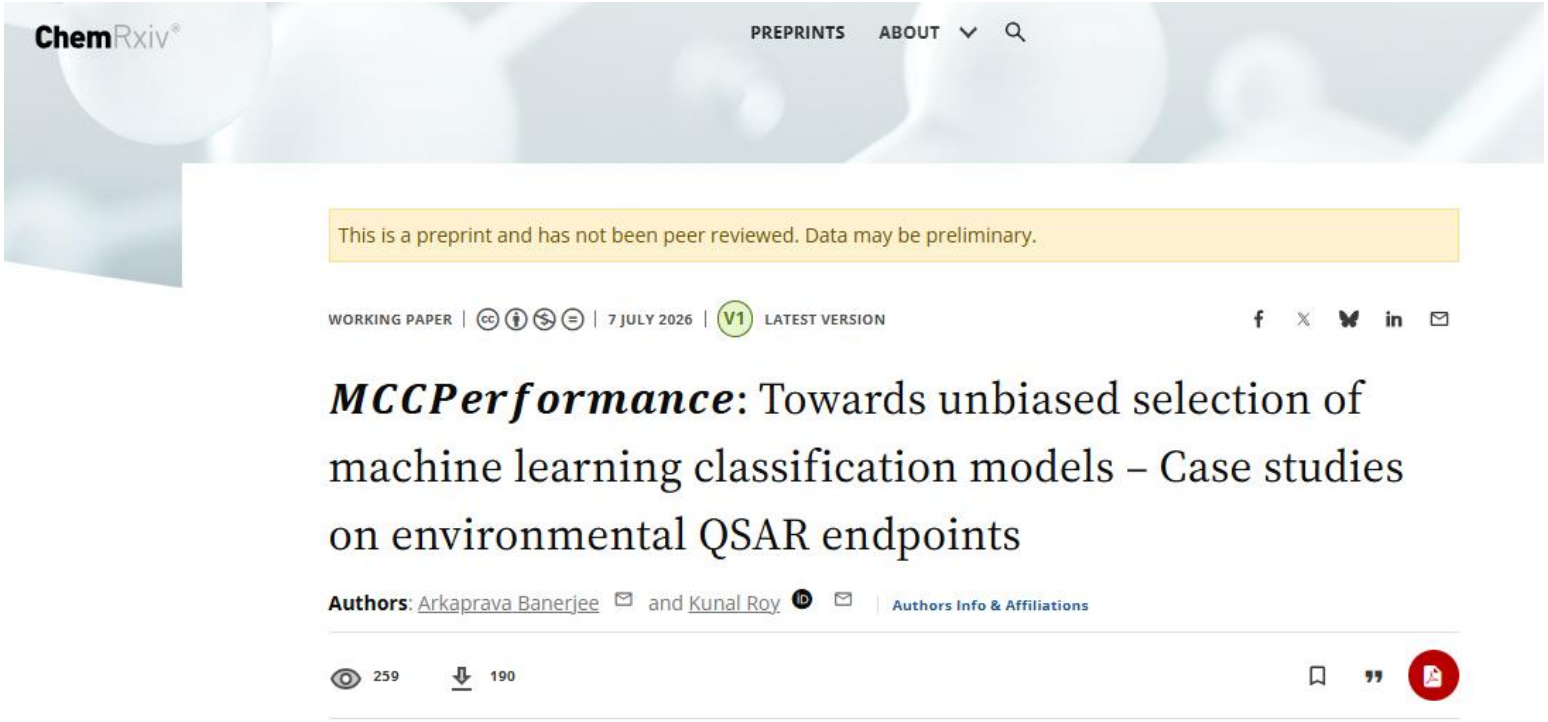
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ABSTRACT: Selecting a single best machine-learning regression model from a set of competing models can be challenging. While models selected based on cross-validation performance do not guarantee good predictions on external data, models selected solely on external validation performance do not ascertain precise predictions for other external sets. Therefore, we propose three quantitative metrics to guide modelers in selecting the best model using the modeling set information only. Three quantitative data sets of varying sizes and complexities were considered. Each data set was randomly split into a modeling set and an independent test set. The modeling set was further split thrice to generate training and validation sets. Various machine-learning models were developed and validated against the validation sets. Our proposed metrics were computed for each model using only training and validation set performances. The novel metric values guided the selection of the best models, which also demonstrated expected performance on the independent test set. Furthermore, successful applications of our framework on two additional benchmark data sets demonstrated its wider generalizability.

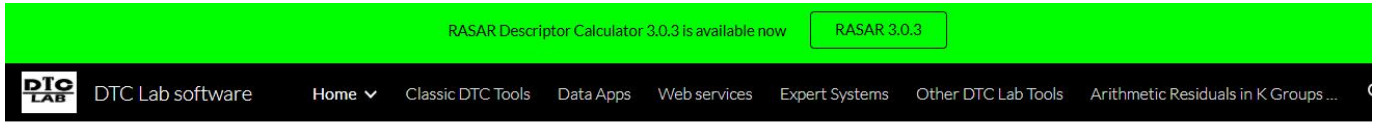


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Thank you



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