CMDWC 2021

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Data Science Framework to Select Corrosion Inhibitors

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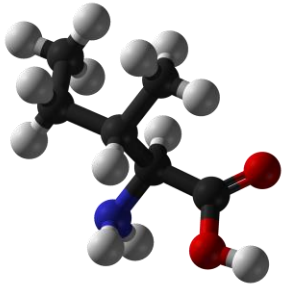
Aim

Selection

Design

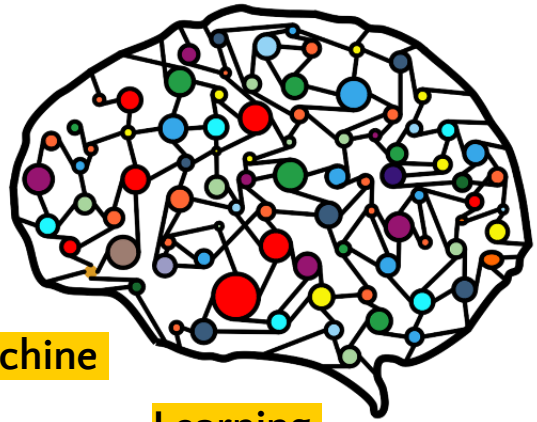
Coatings



Organic Corrosion Inhibitors

Corrosion Protection

Approach



Machine Learning

Data Driven

Web App

1

Selection

Web app

Interactive Corrosion Inhibitor Efficiencies

Metal: Al

Alloy: AA2024, AA7075, Al

Synergistic Inhibitor: None, KI, CaCl2

Mininum Efficiency: 50

Temperature / K: 280 – 370 (280 290 300 310 320 330 340 350 360 370)

pH: -1 – 14 (-1 1 3 5 7 9 11 13 14)

Salt Concentration / M: 0 – 1 (0 1e-7 0.000001 0.0001 0.001 0.01 0.1 1)

Columns to show:

- [x] Inhibitor
- [ ] Mol._weight
- [ ] SMILES
- [x] Metal
- [x] Alloy
- [ ] Time_h
- [x] Temperature_K
- [x] pH
- [ ] Inhib_Concentrat_M
- [x] Salt_Concentrat_M
- [ ] Synergistic_Inhib_type
- [ ] Synergistic_Inhib_M
- [ ] Reference

Show 10 entries — Search:

	Inhibitor	Metal	Alloy	Temperature_K	pH	Salt_Concentrat_M	Efficiency
1	1,2,4-TRIAZOLE	Al	AA2024	298	10	0.1	90
2	1,2,4-TRIAZOLE-3-THIOL	Al	AA2024	298	4	0.1	90
3	1,2,4-TRIAZOLE-3-THIOL	Al	AA2024	298	10	0.1	70
4	1,2,4-TRIAZOLE-3-THIOL	Al	AA7075	298	4	0.1	90
5	1,2,4-TRIAZOLE-3-THIOL	Al	AA7075	298	10	0.1	90
6	1H-IMIDAZO[4,5]PYRAZINE-2-THIOL	Al	AA2024	298	4	0.1	50
7	1H-IMIDAZO[4,5]PYRAZINE-2-THIOL	Al	AA7075	298	4	0.1	70

https://datacor.shinyapps.io/cordata/

Metal

Al

Alloy

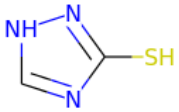
AA2024 AA7075 Al

Synergistic Inhibitor

None KI CaCl2

Mininum Efficiency

50



Temperature / K

280 370

280 300 320 340 360

pH

-1 14

-1 1 3 5 7 9 11 1314

Minimum Salt Concent. / M

0 1

0 1e-07 0.000001 0.0001 0.01 0.1 1

Quickly check the inhibitor structure and the reference

Search for the appropriate conditions

Corrosion Science

Volume 106, May 2016, Pages 229-235

Using high throughput experimental data and *in silico* models to discover alternatives to toxic chromate corrosion inhibitors

D.A. Winkler [a, b, c, d], M. Breedon [a], P. White [a], A.E. Hughes [a, c], E.D. Sapper [e], I. Cole [a]

Columns to show:

- [x] Inhibitor
- [ ] Mol._weight
- [ ] SMILES
- [x] Metal
- [x] Alloy
- [ ] Time_h
- [x] Temperature_K
- [x] pH
- [ ] Inhib_Concentrat_M
- [x] Salt_Concentrat_M
- [ ] Synergistic_Inhib_type
- [ ] Synergistic_Inhib_M
- [ ] Reference

Select and compare different properties

INCLUDE YOUR CORROSION DATA

SUBMIT | GET DATASET | FEEDBACK

Dataset available to contributors

It's free

Data Included

	Al	Cu	Mg	Fe	All
Efficiencies	570	108	257	854	1901
Compounds	108	24	25	40	146
Metal/Alloys	4	3	14	8	29
pH range	[-0.3,11]	[0,13]	[7,8.2]	[-0.5,7.3]	[-0.5,13]
Synergistic Inhib.	Yes	Yes	No	Yes	Yes
References	6	24	3	40	72

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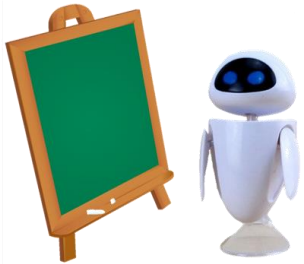
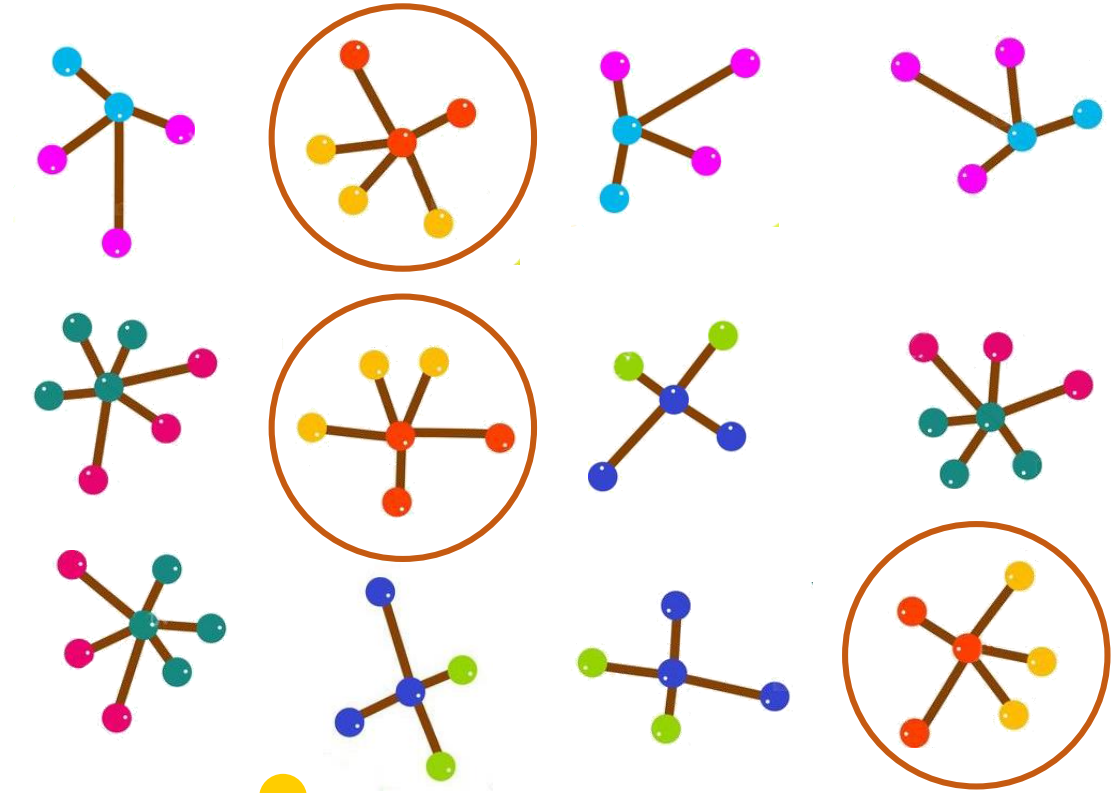
Design

Machine Learning

Identify Inhibitors: Classification





Inhibitors

Efficiency threshold

Non-Inhibitors

Algorithm performance

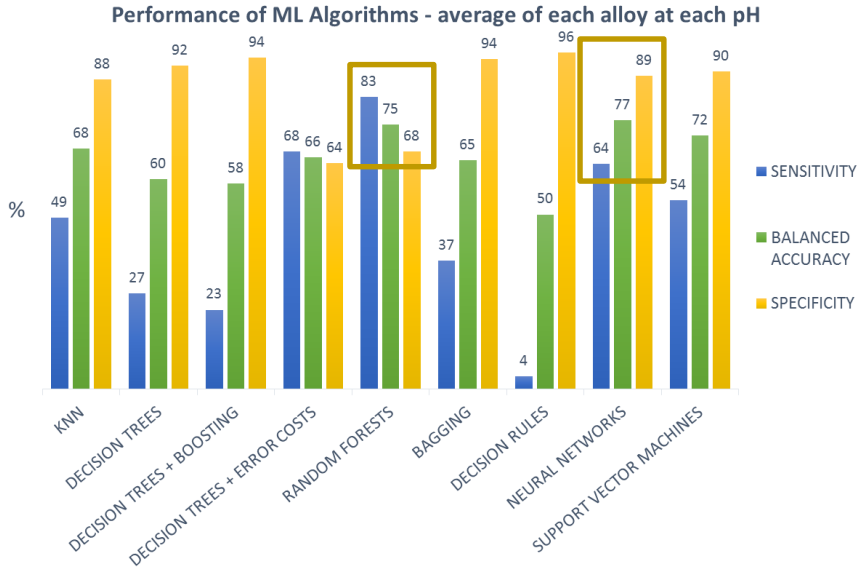
Individual models vs Composite Model

Can we model different conditions in the same model?

D.A. Winkler et al. Corros. Sci. 106 (2016) 229–235.

Algorithm performance

Individual Models



Inhibitors: > 50 % efficiency

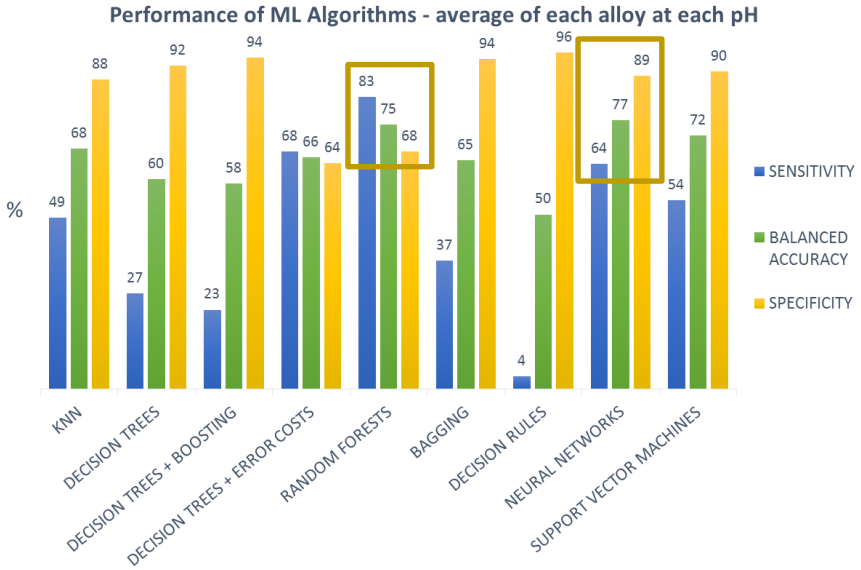
Best methods:

1) Neural Networks
2) Random Forests

T.L.P. Galvão et al., J. Phys. Chem. C 124 (2020) 5624–5635

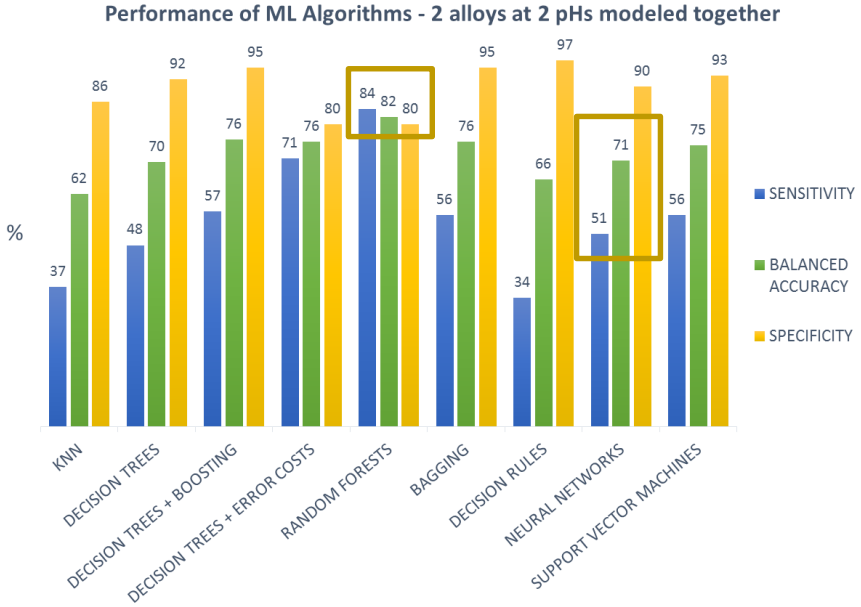
Algorithm performance

Individual Models



Inhibitors: > 50 % efficiency

Composite Model



T.L.P. Galvão et al., J. Phys. Chem. C 124 (2020) 5624–5635

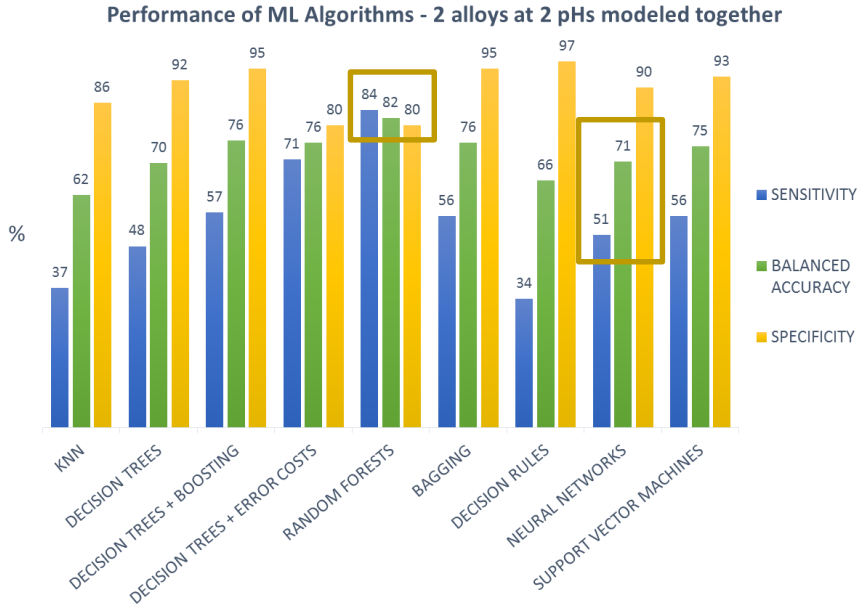
Algorithm performance

Random Forests:

- Best method
- All Tree based methods improve
- Benefits from more data (102 → 408)

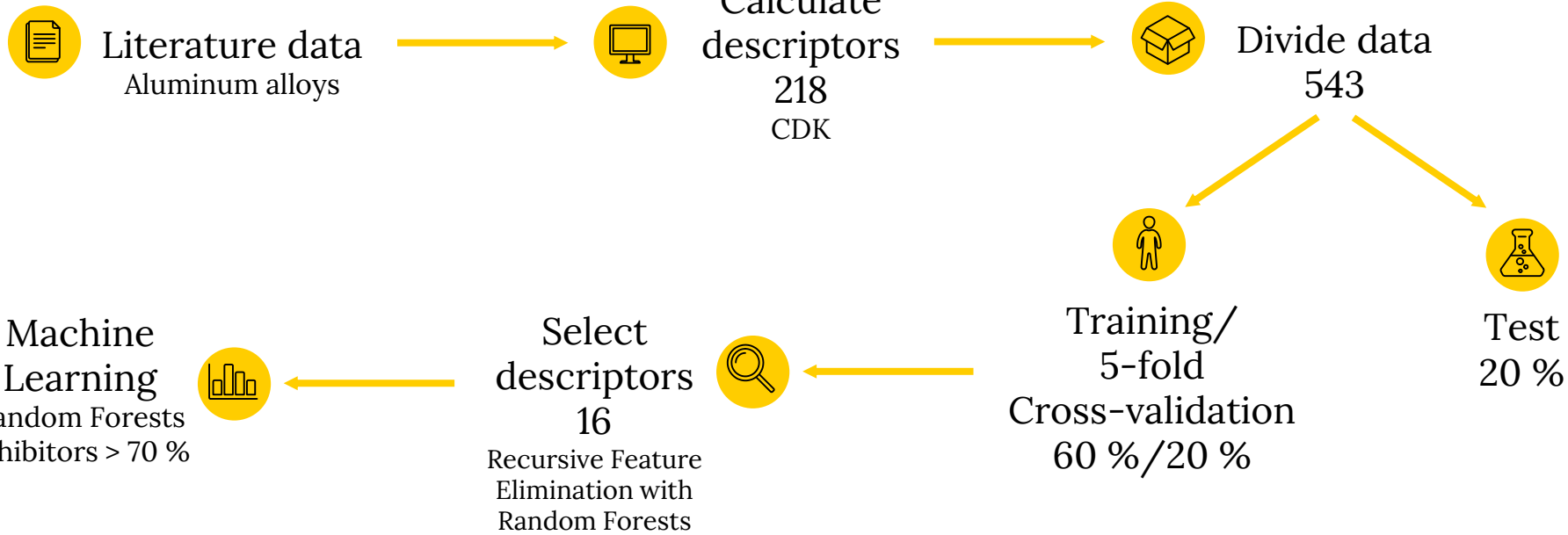
We can model different conditions within the same model

Composite Model

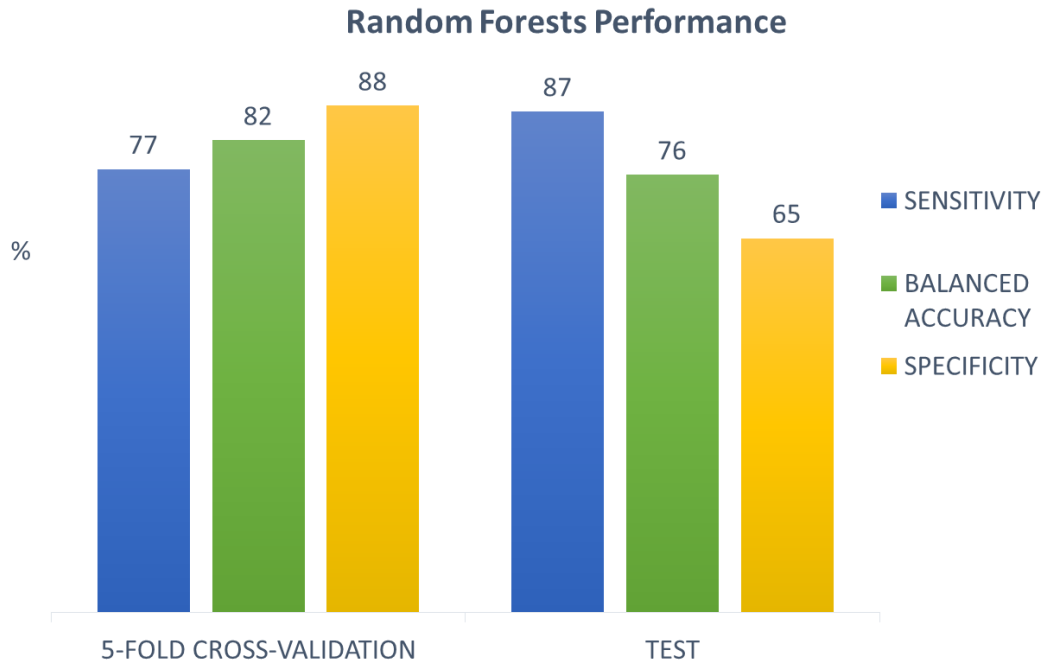


T.L.P. Galvão et al., J. Phys. Chem. C 124 (2020) 5624–5635

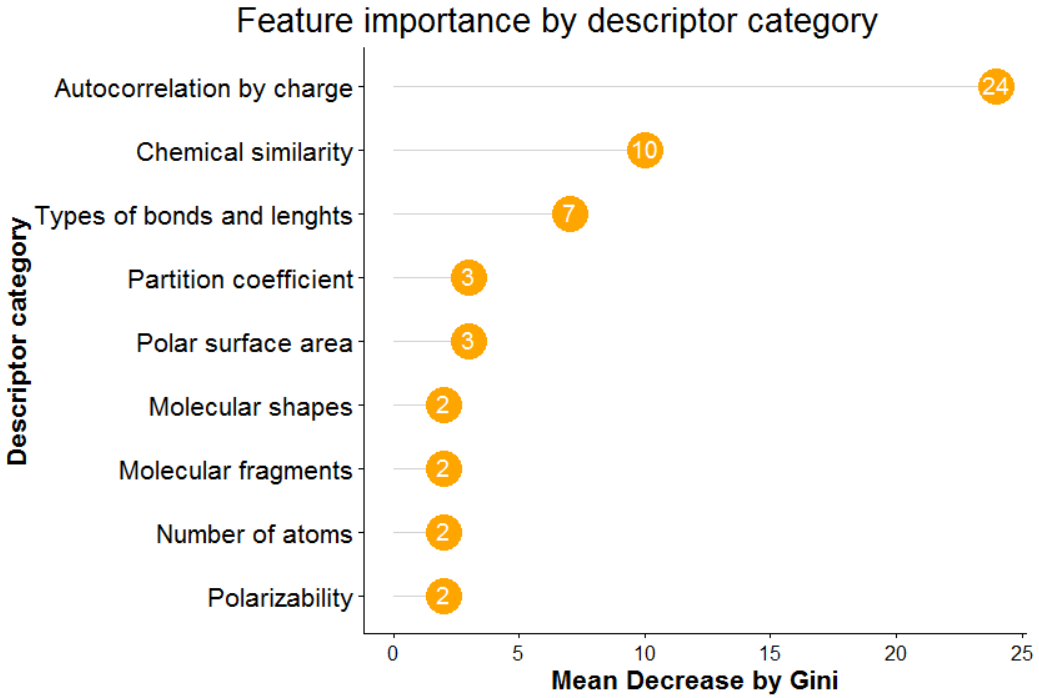
Data from different sources: workflow



Data from different sources: results



Data from different sources: descriptors



Conditions:

- Acidic: pH ≤ 4
- Near neutral: 4 < pH < 10
- Basic: pH ≥ 10

Kolics et al. J. Electro. Soc. 148 (2001) B251

Conclusions

- An open data management web tool is freely available to organize, search and select corrosion inhibition efficiencies of compounds under different conditions.

- A machine learning framework is being developed for aluminum alloys capable of considering data from different sources and making predictions for different pHs.

Acknowledgements

DataCor project

POCI-01-0145-FEDER-030256

PTDC/QUI-QFI/30256/2017)

https://datacorproject.wixsite.com/datacor

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Thank You!

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