

64. Alexander, D.L.J.; Tropsha, A.; Winkler, D.A. Beware of R^2 : Simple, unambiguous assessment of the prediction accuracy of QSAR and QSPR models. *J. Chem. Inf. Model.* **2015**, *55*, 1316–1322, doi:10.1021/acs.jcim.5b00206.
65. Gramatica, P.; Sangion, A. A historical excursus on the statistical validation parameters for QSAR models: A clarification concerning metrics and terminology. *J. Chem. Inf. Model.* **2016**, *56*, 1127–1131, doi:10.1021/acs.jcim.6b00088.
66. Warnes, G.R.; Bolker, B.; Gorjanc, G.; Grothendieck, G.; Korosec, A.; Lumley, T.; MacQueen, D.; Magnusson, A.; Rogers, J. *Gdata: Various R Programming Tools for Data Manipulation*, R package version 2.18.0; 2017.
67. Wickham, H. *Ggplot2: Elegant Graphics for Data Analysis*, 2nd ed.; Springer International Publishing: Cham, Switzerland, 2016; doi:10.1007/978-3-319-24277-4.
68. Wickham, H.; Hester, J.; Francois, R.; Jylänki, J.; Jørgensen, M. *Readr: Read Rectangular Text Data*, R package version 1.1.1; 2017.
69. Wickham, H. Reshaping data with the reshape package. *J. Stat. Softw.* **2007**, *21*, doi:10.18637/jss.v021.i12.



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