

<b>Identifier</b>	Trivial name of herbicide
<b>Name at www.hraclist</b>	<a href="https://hracglobal.com/">https://hracglobal.com/</a> <b>accesed</b>
<b>HRAC2020_class</b>	legacy HRAC classification
<b>ExtendedSet_class</b>	346 HRAC herbicides plus 163 obsolete herbicides whose class (mode of action) has been assigned bysed on the structural similarity
<b>SET</b>	sets used in ML modelling
<b>HRAC2020_MODELLING_SETS</b>	sets used in ML modelling
<b>SMILES</b>	SMILES representation of compounds
<b>MW</b>	Relative molecular mass, Molecular Weight
<b>logP</b>	lipophilicity coefficient
<b>logD_7.4</b>	distribution coefficent at pH 7.4
<b>HBA</b>	number of H-bond accepting atoms (N or O)
<b>HBD</b>	number of H-bond accepting atoms (NH or OH)
<b>TPSA</b>	topological polar surface area
<b>RelPSA</b>	relative polar surface area (calculated by DataWarrior)
<b>FormalCharge</b>	net charge at pH 7.4
<b>max_RF_prob</b>	RF probability maximum value for a given herbicide (definition of applicability domain, AD for MoA models)
<b>min_Jaccard_dist</b>	Jaccard distance minimum valeu for a given herbicide (definition of AD for MoA models)
<b>Predicted_MoA_RF</b>	Predicted Mode of Action (MoA) by the Random Forest model
<b>Predicted_MoA_SVM</b>	Predicted MoA by the SVM model
<b>Application_stage</b>	Application stage for a given herbicide
<b>Weed_Selectivity_WS</b>	Herbicides selective for broad-leaved or grass weeds , and non-selective (NS) herbicides
<b>WS_modelling_sets</b>	Sets used for ML modelling for weed selectivity (WS)
<b>Min_Euclidian_dist</b>	Euclidian distance minimum value for a given herbicide (definition of AD for WS models)
<b>Max_RF_logP_WS</b>	RF probability maximum value for a given herbicide (definition of AD for WS models)
<b>RF_logP_WS</b>	Predictions of RF model with logP as a descriptor, for WS
<b>SVM_logP_WS</b>	Predictions of SVM model with logP as a descriptor, for WS
<b>Natural source</b>	Organism from which a molecules, a natural product (NP) is isolated
<b>Class</b>	Kingdom of an organism from which a NP is isolated