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Applying machine learning to discriminate host rock of quartz using its trace element chemistry– potential application to sedimentary provenance

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Quartz is a ubiquitous mineral found in a wide range of igneous, metamorphic, and sedimentary rocks. As the mineral survives sedimentary recycling, detrital grains can retain the signatures of the P-T-X conditions during their crystallization/precipitation from magma/fluid. The trace element composition of quartz can, therefore, potentially reflect the genetic information of its host rock. Previous studies on using quartz chemistry for petrogenetic discrimination have either used bivariate or ternary discrimination diagrams (e.g., Ti-Al; Ti-Al/10-10*Ge), considering a limited number of elements [1, 2] or have used machine learning-based approaches to classify specific ore-genetic environments [3]. Here, we have compiled published 11,567 trace element analyses of quartz grains from 14 different types of host rocks: granitoids (A-, S-, I- types), volcanic rocks (A-, S-, I- types), granitic pegmatites (A-, S-, I- types), greisen (altered A-, S- type granitoids), hydrothermal veins (associated with A-, S-, I- type magma), and metamorphic rocks. A rigorous machine learning tool has been applied to discriminate the large and high dimensional database of quartz hosted in different rock types, taking into account 50 trace elements. Our result shows that two supervised machine learning classifiers, i.e., XGBoost and LightGBM models, are able to discriminate quartz trace element data with an average accuracy of 95.5% and 95.8%, respectively. For both models, the normalized confusion matrix shows that each class (host rock) can be correctly predicted with more than 82% accuracy, except for metamorphic (~74%) and I-type pegmatite (33%). Additionally, the Shapley Additive exPlanations (SHAP) algorithm shows that Ti, Li, Ge, Al, Si, B, and P contents in quartz exert significant control in discriminating host rock types. These classifier tools can be used to identify the provenance of detrital quartz grains using their trace element chemistry.

[1] Rusk (2012), Am. Mineral. **91**, 1300–1312. [2] Breiter et al. (2020), Ore Geol. Rev. **125**, 103674. [3] Wang et al. (2021), J. Geophys. Res. Solid Earth **126**, e2021JB021925.