

1 Correction of MS 8083R

2 **Olivine in picrites from Continental Flood Basalt provinces**  
3 **classified using machine learning**

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13 Picrites, dominantly composed of highly forsteritic olivine, can serve as

14 important constraints on primary magma composition and eruption

15 dynamic processes in global Continental Flood Basalt (CFB) provinces.

16 Picrites are commonly divided into high-Ti and low-Ti groups based on

17 whole-rock TiO<sub>2</sub> content or Ti/Y ratio. Here, we use an Artificial Neural

18 Network (ANN) to classify the individual olivine in picrites from global

19 CFB provinces according to whether their parental magma is high-Ti or

20 low-Ti to better understand the primary origin and magmatic processes.

21 After training the ANN on one thousand olivine major element

22 compositions data points, the network was able to differentiate chemical

23 patterns for high-Ti and low-Ti olivine, and classify olivine into correct

24 types with an accuracy of >95 %. Moreover, we find that two types of

25 olivine mix in some single samples from Etendeka, Emeishan, and Karoo

26 CFB provinces. Combining the results with chemical markers of source

27 lithology, we suggest that the two types of olivine originate from two  
28 different sources and their olivine populations mixed during the ascent.  
29 This mixing then makes the spatial and temporal variation of picrites types  
30 in some CFB provinces unclear.

31 **Keywords:** Olivine; Machine Learning; Picrites; Chemical Composition;  
32 Classification

33

### 34 **PICRITE IN CONTINENTAL FLOOD BASALT PROVINCES**

35 High-Ti (HT) and low-Ti (LT) types of picrites are commonly observed in  
36 Continental Flood Basalts (CFBs) or Large Igneous Provinces (LIPs). The  
37 classification is based on the values of  $\text{TiO}_2$  or  $\text{Ti/Y}$  of whole-rock  
38 compositions (e.g. [Ewart et al., 2004](#); [Kamenetsky et al., 2017](#); [Peate et al.,](#)  
39 [1999](#); [Xiao et al., 2004](#); [Xu et al., 2001](#)). Both types are found either in  
40 separate locations or within the same succession of a CFB. For example,  
41 in Karoo province, LT picrites ( $\text{TiO}_2 < 1.5$  wt%) are found mainly south of  
42  $26^\circ \text{S}$ , whereas HT picrites predominate north of this latitude ([Galerne et](#)  
43 [al., 2008](#)). The different locations may indicate the two types were  
44 produced from different magmatic sources (e.g. [Heinonen et al., 2013](#);  
45 [Heinonen and Luttinen, 2008](#); [Howarth and Harris, 2017](#); [Kamenetsky et](#)  
46 [al., 2012](#)). On the other hand, in Emeishan province, the two types are  
47 found within the Binchuan succession (e.g. ([Cheng et al., 2014](#); [Xu et al.,](#)  
48 [2001](#))). Why the two types of picrites occur in many LIPs is unclear.

49 Neither is it clear why the two types occur both separately and together.  
50 Since picrites are predominantly composed of highly forsteritic olivine, HT  
51 samples possibly consist of HT olivine and LT samples consist of LT  
52 olivine. In addition to HT and LT samples, some picrites have intermediate  
53 Ti/Y value (IT), and do not show clear characteristics of either HT or LT  
54 in Emeishan LIP ([Kamenetsky et al. 2012](#)). Existence of IT samples may  
55 indicate mixing of multiple olivine populations which should be confirmed,  
56 because the composition of picrite are usually used to constrain on the  
57 source composition (e.g., [Zhang et al., 2006](#)). Source compositions cannot  
58 be constrained correctly from multiple olivine populations.  
59 To address these issues, we need to analyse the chemical patterns of olivine  
60 in picrites. For this study, we have compiled thousands of compositions of  
61 olivines from published picrites samples and built an Artificial Neural  
62 Networks (ANN) to investigate the chemical characteristics of olivine from  
63 HT and LT picrites. Further, we determined the links between olivine  
64 populations and their sources and answered whether olivine populations  
65 mixed during magmatic processes.

66

## 67 **DATABASE OF OLIVINE COMPOSITIONS IN PICRITES**

68 We have collected thousands of major elements data points of olivine as  
69 well as their whole-rock compositions of picrites from six CFBs (Emeishan  
70 LIP, Etendeka province, Ethiopian CFB, Karoo LIP, North Atlantic

71 province, and Siberia CFB) from the open-access and comprehensive  
72 global petrological database GEOROC ([http://georoc.mpch-](http://georoc.mpch-mainz.gwdg.de/georoc/)  
73 [mainz.gwdg.de/georoc/](http://georoc.mpch-mainz.gwdg.de/georoc/)). These CFB provinces are located in different  
74 parts of the earth, and have been well studied (Fig. 1). Within the data, Ti/Y  
75 values of picrites range from 250 to 1400 (Fig. 2). The picrites from the  
76 Ethiopian province have the highest Ti/Y values of 1400, while the  
77 maximal values of other CFBs are around 800 (Fig. 2). Although Xu et al.  
78 (2001) suggested that the Ti/Y value boundary between HT and LT is 500  
79 for the Emeishan LIP, the boundaries for different provinces may vary  
80 between 350 and 600 based on the gaps in data in Figure 2. Thus, we  
81 assumed that samples with Ti/Y of more than 600 were HT end-members,  
82 samples with Ti/Y of less than 350 were LT end-members, and samples  
83 with Ti/Y from 350 to 600 were the intermediate Ti group (IT).  
84 We determined the quality of olivine dataset, which comprised 2898 major  
85 element compositions of olivine from picritic samples of CFBs (Table 1s  
86 in appendix), by calculating the cardinality, minimum, mean, median,  
87 maximum and standard deviation of each element's concentration (Table  
88 1). Note, that in this study we assume all the collected data could represent  
89 the true composition of whole olivine by measuring composition of the  
90 core of olivine without the effect of diffusion (e.g. Cheng et al., 2020;  
91 Costa, 2020; Costa et al., 2020) and the random cut effect in thin sections  
92 (e.g. Cheng et al., 2017; Cheng and Costa, 2019). The cardinality measures

93 the number of distinct values. The cardinalities of  $\text{TiO}_2$  were much lower  
94 than 1000, and the minimum value and mean value were lower than 0.01,  
95 meaning that many  $\text{TiO}_2$  values were 0. The difference between the mean  
96 and median of each composition showed the outliers. Most of the elements  
97 differed only a little (0-1 wt%), which showed that there were not too many  
98 outliers. The standard deviations of the FeO and MgO values (3-4 wt%)  
99 were much larger than the standard deviations of the other elements (less  
100 than 1 wt%), showing the large FeO and MgO variation. However, the  
101 maximum values of several elements were much larger than the normal  
102 values of olivine. For example, the maximum of  $\text{SiO}_2$  was 63 wt% and that  
103 of  $\text{Al}_2\text{O}_3$  was 5 wt%. This indicated existence of several low-quality data  
104 points to be filtered out—those with analytical totals out of the range 98-  
105 101 and with stoichiometric ratios of  $(\text{Mg}+\text{Fe})/\text{Si}$  out of the range of 1.95-  
106 2.05). Furthermore, low-quality training data to filter out were ones with  
107  $\text{SiO}_2$  values out of the range of 38-42 wt%,  $\text{Al}_2\text{O}_3$  values out of the range  
108 of 0-0.15 wt%,  $\text{Cr}_2\text{O}_3$  values out of the range 0-0.2 wt%, and NiO values  
109 out of the range of 0.1-0.6 wt%. The remaining total of 1002 training data  
110 points were high-quality ([Table 1s in the appendix](#)). The same approach  
111 was taken to obtain high-quality data for IT samples.

112 To avoid the high linear relationship between features, we also calculated  
113 the correlation coefficient between each two elements ([Fig. 3](#)). The  
114 correlation coefficients showed that MgO had a negative linear relationship

115 with  $\text{FeO}^{\text{T}}$  and  $\text{MnO}$ , whose correlation coefficients were -0.98 and -0.84,  
116 respectively. There was a positive linear relationship between  $\text{MgO}$  and  
117  $\text{SiO}_2$ , whose correlation coefficient was 0.86. It meant  $\text{MgO}$  could  
118 represent  $\text{SiO}_2$ ,  $\text{FeO}^{\text{T}}$  and  $\text{MnO}$ . There were no clear positive or negative  
119 linear relationships between  $\text{Al}_2\text{O}_3$ ,  $\text{MgO}$ ,  $\text{CaO}$ ,  $\text{NiO}$ , or  $\text{Cr}_2\text{O}_3$ .

120

## 121 **ARTIFICIAL NEURAL NETWORKS**

122 There are several models of machine learning such as Support Vector  
123 Machine (SVM), Random Forest (RF), Naïve-Bayes Classifier (NBC),  
124 Artificial Neural Networks (ANN), Convolution Neural Network (CNN)  
125 and Recurrent Neural Networks (RNN) ([Ardabili et al., 2020](#); [Bergen et al.,](#)  
126 [2019](#); [Bishop, 2006](#)). They all can convert experience into expertise or  
127 knowledge during learning ([Ardabili et al., 2020](#); [Bergen et al., 2019](#)).  
128 Several ML models have been used in earth science studies (e.g. [Hazen,](#)  
129 [2014](#); [Morrison et al., 2017](#); [Petrelli and Perugini, 2016](#)).

130 In this study, the ANN model was selected, since our data (major elements  
131 compositions of olivine) are tabular and ANN is powerful. But, we also  
132 compared the performance of our ANN with other traditional ML methods  
133 including SVM and NBC (see Discussion). We built a supervised ANN  
134 according to the types of picrites. The first goal of our ANN was to produce  
135 good prediction results by learning the chemical characteristics of the  
136 training data. The second goal was to use the ANN to classify the olivine

137 data from IT samples which was a much more difficult task than  
138 predictions from training data. We used only Al<sub>2</sub>O<sub>3</sub>, MgO, CaO, NiO, or  
139 Cr<sub>2</sub>O<sub>3</sub> as features as they had no clear linear relationship between each  
140 other, as we mentioned above (Fig. 4). Our ANN used one hidden layer  
141 with 10 nodes. We chose ‘Levenberg-Marquardt backpropagation’  
142 (‘trainlm’ function in Matlab) as the training algorithm as it is often the  
143 fastest back propagation algorithm and gives us the most accurate results,  
144 although it does require more memory than other algorithms.

145 To train the ANN, we selected the olivine composition of an HT end-  
146 member to represent the HT group, and the composition of an LT end-  
147 member to represent the LT group. We had about 1000 high-quality olivine  
148 compositions from all the global CFBs. To avoid overfitting, we randomly  
149 split our data into three groups: the training set, the validation set and the  
150 test set, using the ratios of 70:15:15. Thus, we had about 700 training  
151 samples, about 150 validation samples, and about 150 test samples.

152

## 153 RESULTS

154 The results show that our ANN has achieved high accuracy (>95%) for all  
155 three sets (Fig. 5). For the training data, the ANN determined 233 data  
156 points as belonging to LT, out of which 229 predictions were correct and  
157 473 data points as HT, out of which 468 predictions were correct. The  
158 accuracy was thus 99 % (Fig. 5a). For the validation set, our ANN have

159 determined that 38 data points belonged to LT, out of which 36 predictions  
160 were correct and 112 points as HT, out of which 109 predictions were  
161 correct. The accuracy achieved was 96.7% (Fig. 5b). For the test set, the  
162 ANN labelled 57 data points as LT with 54 predictions correct, and 93 data  
163 points were labelled as HT with 89 predictions correct. Thus, the accuracy  
164 was 95.3 % (Fig. 5c). The high and close accuracy values of the three sets  
165 means there are no overfitting problems. In total, the ANN's accuracy is  
166 98.1 % for all of the data (Fig. 5d).

167 After training the ANN, we input all of the olivine data from olivine  
168 crystals contained in the IT samples. The olivine from the IT samples were  
169 determined by the ANN to belong to LT was labelled as IT-L, and the  
170 olivines determined to belong to HT were labelled as IT-H (Fig. 6). We  
171 find that most of LT and HT olivine are located in different part of NiO-  
172 MgO plot, but there are still many overlapping data points when MgO  
173 ranges from 40 to 45 wt% (Fig. 6a). The overlaps suggest that a simple  
174 relation such as NiO-MgO cannot accurately classify olivine crystals.  
175 However, the ANN model can classify them highly accurately (>95%),  
176 although several IT-L points whose MgO is about 40 wt% are located in  
177 the area of HT and IT-H, which suggests they are probably classified  
178 incorrectly (Fig. 6a). The LT and IT-L olivine show mostly higher CaO  
179 (Fig. 6b), higher Al<sub>2</sub>O<sub>3</sub> (Fig. 6c) compared to HT and IT-H. Most LT and  
180 IT-L data points range from 0.3 to 0.6 wt% CaO, while HT and IT-H vary



181 from 0.1 to 0.4 wt%. However, LT and HT olivine overlap more in their  
182 relationships between  $\text{Al}_2\text{O}_3$ , CaO vs. MgO compared to NiO vs. MgO.  
183 There are also many overlapping points around 0.3 wt% CaO and 0.04 wt%  
184  $\text{Al}_2\text{O}_3$  (Fig. 6c & 6d). The HT and LT samples overlap mostly in the  
185 relationship between  $\text{Cr}_2\text{O}_3$  and MgO compared to the rest (Fig.6d). Both  
186 HT and LT samples range from 0 to 0.16 wt%. Thus, we emphasize again  
187 that it is almost impossible to classify these overlapping data using simple  
188 relations. Overall, the ANN has correctly classified the olivine from the IT  
189 sample into the right group: most of IT-L points overlap the IT samples  
190 and most of IT-H points overlap the HT samples (Fig. 6). Moreover, ANN  
191 has performed well on the overlapping data points which could not be  
192 classified by the simple relations.

193

## 194 DISCUSSION

### 195 Comparison with other machine learning methods

196 In the previous section, we demonstrated the good performance of our  
197 ANN on IT olivine and on the overlapping data points where olivine  
198 crystals cannot be accurately classified by simple relations such as NiO-  
199 MgO. Although more complex relations such as NiO-MgO- $\text{Al}_2\text{O}_3$  could be  
200 used for overlapping data points, much longer time would be required, and  
201 distinguishing differences in three-dimensional space would be more  
202 difficult. In comparison, our ANN was able to directly predict olivine

203 populations with high accuracy for such cases within several minutes.  
204 Moreover, we compared the performance of the ANN to other traditional  
205 machine learning methods such as the Support Vector Machine (SVM) and  
206 Naïve Bayes Classifier (NBC). The SVM is a non-parametric classifier  
207 that finds a linear vector (if a linear kernel is used) to separate classes. It  
208 has been used in Earth science research. For example, [Petrelli and Perugini](#)  
209 [\(2016\)](#) outlined an SVM with a Gaussian kernel function for tectonic  
210 discrimination based on geochemical and isotopic data. We used the ‘linear’  
211 function in Matlab as the kernel function. The NBC is a simple  
212 ‘probabilistic classifier’ based on Bayes’ theorem, with strong  
213 independence assumptions between features (e.g., [Ren et al., 2019](#)). The  
214 NBC can be trained efficiently in a supervised learning setting, such as the  
215 one required in this study. We used the ‘kernel’ function in Matlab with a  
216 mean kernel smoothing density estimate. The SVM and NBC are highly  
217 accurate (96.5% and 94.5%, respectively), and capable of distinguishing  
218 between the two types of samples ([Fig.7](#)). However, since our ANN’s  
219 accuracy remains the highest, we suggest using ANN model ([Figs. 5 and](#)  
220 [7](#)).

221

## 222 **The sources of olivine populations**

223 We have shown that different machine learning models such as ANN and  
224 SVM are able to classify the olivine populations accurately. It indicates

225 that these results show that the olivine from two end-members are different.  
226 To investigate the link between olivine population and source lithology,  
227 we compare NiO concentrations of two olivine populations. We find that  
228 NiO of HT is much higher than that of LT at the given MgO value (Fig.  
229 8a). High NiO in olivine has, for example, been suggested to indicate a  
230 pyroxenitic source and thus determine the mafic sources for Hawaiian  
231 magma (Sobolev et al. 2005). It has been widely used to argue for an  
232 olivine-free pyroxenite source for both continental and oceanic basalts  
233 (Herzberg, 2011, 2006; Sobolev et al., 2007; Xu et al., 2012). However,  
234 high-Ni olivine could crystallize under low-temperature conditions from  
235 high-temperature peridotite melts without contributions from a pyroxenite  
236 source as shown in Fig. 8a (Matzen et al., 2017). Minor and trace element  
237 characteristics in olivine strongly depend on pressure, temperature and  
238 melt composition, as suggested by experimental petrology (Matzen et al.,  
239 2013). Examples such as high-Ni and low-Mn olivine in Karoo was  
240 suggested as the result of temperature and pressure variations (Heinonen  
241 and Fusswinkel, 2017). However, we found a relatively narrow range of  
242 LT olivine and there is a linear trend between Fo and NiO for the global  
243 data, while that of HT is quite large and the Fo-NiO relationship not easily  
244 determined. These HT olivine points are further divided into two groups.  
245 For example, the olivine from Ethiopian CFB has higher NiO content than  
246 that of LT, but a bit lower NiO than that of olivine from other CFBs. Note,

247 that olivine from other CFBs is located in the Ethiopian area (Fig. 8a). If  
248 the two populations are both from peridotite, we would expect similar  
249 trends even under different pressures or temperatures, and thus we suggest  
250 the two types of olivine are from different sources. However, we need to  
251 emphasize that the link between an olivine population and a source  
252 depends on the choice of markers of source lithology, and many markers  
253 have their own limitations (e.g. Yang et al., 2019, 2016). Thus, we also  
254 applied the last chemical marker suggested by Yang et al. (2019). This  
255 marker, combines FCKANTMS  $= \ln(\text{FeO}/\text{CaO}) - 0.08 * \ln(\text{K}_2\text{O}/\text{Al}_2\text{O}_3)$   
256  $- 0.052 * \ln(\text{TiO}_2/\text{Na}_2\text{O}) - 0.036 * \ln(\text{Na}_2\text{O}/\text{K}_2\text{O}) * \ln(\text{Na}_2\text{O}/\text{TiO}_2) -$   
257  $0.062 * (\ln(\text{MgO}/\text{SiO}_2))^3 - 0.641 * (\ln(\text{MgO}/\text{SiO}_2))^2 - 1.871 * \ln$   
258  $(\text{MgO}/\text{SiO}_2) - 1.473$ ; all major elements in wt%) with  $\ln$   
259  $(\text{SiO}_2/(\text{CaO}+\text{Na}_2\text{O}+\text{TiO}_2))$  and was able to distinguish approximately 80%  
260 and 50% low to moderate degree ( $\text{Fo}<60\%$ ) partial melts of mafic sources  
261 from those of peridotite and transitional lithologies. We calculated the  
262 FCKANTMS values for the picrites in this study and the global melts  
263 compiled from Yang et al. (2019). We found that most of LT samples are  
264 much closer to area of peridotite source compared to HT samples (Fig. 8b).  
265 Data points of HT samples are located in two quite different areas: many  
266 data points have much lower  $\ln(\text{SiO}_2/(\text{CaO}+\text{Na}_2\text{O}+\text{TiO}_2))$  which are all  
267 from Ethiopian CFB, while many have much higher FCKANTMS and  
268 middle  $\ln(\text{SiO}_2/(\text{CaO}+\text{Na}_2\text{O}+\text{TiO}_2))$  that are from North, Karoo LIPs. The

269 former is close to the carbonated mafic source and the latter is close to the  
270 mafic source. Two main areas of HT samples are consistent with the two  
271 main trends of HT olivines in [Fig. 8a](#). Samples from Emeishan LIP are  
272 located in both areas, which shows the complexity of their source lithology.  
273 We propose that these HT olivines and picrites represent mafic sources and  
274 LT indicate peridotite sources. Further, the source of HT olivine could be  
275 divided into mafic (HT1) and carbonated mafic source (HT2). Our ANN  
276 has further determined the three groups linked to three sources by training  
277 the ANN on data with three labels using the same five features ([Fig. 9](#)). We  
278 have found that the accuracy for all of the data is 95%, which is lower than  
279 the accuracy of the ANN model with two outputs ([Fig. 5](#)). Clearly,  
280 classifying samples from HT1 and HT2 is more challenging due to their  
281 similarity.

282

### 283 **Olivine populations in a single picritic sample**

284 We selected olivine from a single IT sample of each CFB and input them  
285 into our ANN model. Here, we used the ANN model with three outputs to  
286 determine whether LT, HT1 and HT2 olivine populations mix. Note, that  
287 we did not have IT olivine data from Karoo and Ethiopian CFBs. The  
288 results show that no single sample has all three olivine populations: some  
289 samples have both LT and HT1, and some samples only have LT or HT1.  
290 For example, for the Siberian flood basalt province, the ANN determined

291 that all the olivine from sample SU33 with  $Ti/Y=350$  belongs to the LT  
292 group, and all the olivine from SU50 whose  $Ti/Y$  is 474 belongs to the HT1  
293 group (Fig.10). However, the results show that: (1)  $3\pm 10\%$  and  $4\pm 8\%$   
294 of the olivine are HT1 from two IT samples from Etendeka province  
295 (97SB41 and 97SB62); (2)  $11\pm 5\%$ ,  $10\pm 3\%$  and  $20\pm 5\%$  of the olivine  
296 from three IT samples of Emeishan LIP are HT1 (13-EJH08, 7-EJH08, and  
297 1a-EJH06); and (3)  $10\pm 11\%$ ,  $11\pm 9\%$ ,  $7\pm 4\%$  of olivine are HT1 from  
298 three samples from North Atlantic province (400457, 400230, and 340740).  
299 We found that mixing of two olivine types was found in IT samples from  
300 Etendeka, Emeishan LIP, and North Atlantic provinces. The possible  
301 reasons are: (1) In some provinces, both types of picrite are found in the  
302 same location (e.g., in Binchuan succession in Emeishan LIP, Xu et al.,  
303 2001). The two types of olivine are relatively easier to mix when they both  
304 occur in the same location in these CFBs compare to different locations.  
305 (2) The proportion of HT1 olivine in these IT samples is low, which means  
306 a significant amount of olivine data is required to find HT1 olivine. But  
307 enough olivine data of intermediate samples whose  $Ti/Y$  is between 300  
308 and 500 in other CFBs are not available now. If more olivine data of  
309 samples with  $Ti/Y$  of about 300-400 are available, olivine population  
310 mixing could probably be found in other CFBs.  
311 With our crystal-scale classification, we are able to explain why two types  
312 of picrites are common in all the CFBs, yet, in some CFBs, the spatial and

313 temporal variations of different picrite types become unclear. Although the  
314 two or three types of olivine are produced by different sources at the  
315 beginning of flood basalt eruptions, during magma ascent, these olivine  
316 types may mix. Thus, if we consider only the classification of rocks, the  
317 two types of olivine (LT and HT) in the samples will be classified into one  
318 group. However, with the powerful machine learning tool, olivine from IT  
319 samples of CFBs such as Etendeka, Emeishan, and North Atlantic  
320 provinces can still be classified into different groups. Overall, the existence  
321 of different types of picrites may be better explained by variations in  
322 sources rather than crystallization processes. Their existence in different  
323 CFBs may indicate that the origin in the global CFBs is linked to the  
324 different lithologies: peridotitic or mafic sources (e.g. [Heinonen et al.,](#)  
325 [2013](#); [Heinonen and Luttinen, 2008](#); [Kamenetsky et al., 2012](#); [Li et al.,](#)  
326 [2014](#); [Sobolev et al., 2005](#)). The plume in these CFBs may start from the  
327 one source such as peridotite, but with the huge volume of magma, as the  
328 plume rises another source, such as mafic, starts melting and is mixed into  
329 the magma. Thus, our results show both peridotitic and mafic sources are  
330 involved in CFB provinces and olivine populations from two sources may  
331 mix during ascent.

332

333

## IMPLICATIONS

334 Our study shows a clear link between olivine populations and two types of  
335 picrites, with the olivine from different types of picrites showing varying  
336 chemical characteristics. Using the source markers including NiO-Fo and  
337 FCKANTMS, we propose HT and LT olivines represent mafic and  
338 peridotite sources, respectively. The source of HT olivine could be further  
339 divided into mafic and carbonated mafic sources. We have also built an  
340 ANN model with three outputs which are linked to three different sources.  
341 Using the ANN model, we are able to find olivine populations within a  
342 single sample, which indicates that olivine populations mixed in CFB.  
343 The ANN model we have built enables grouping the olivine from the  
344 picrites found in these CFBs without knowing the whole-rock composition  
345 of the picrites. Thus, our ANN for global CFB provinces could help  
346 classify the multitude of data on olivine published without the rocks'  
347 compositions, which could provide the information about source lithology.  
348 Another application is the recognition of multiple olivine populations in a  
349 single sample. As we mentioned above, the picritic samples are commonly  
350 used to constrain the source compositions which requires that the samples  
351 provide direct source information without any effect from crystal  
352 populations mixing. Thus, it is necessary to check the populations using  
353 our ANN model. Moreover, the application of ANN is much more simple  
354 and efficient compare to human judgment as we mentioned above. It only  
355 requires users to prepare the olivine composition with the five features and



356 input them into the ANN models we provided ([Matlab scripts and training](#)  
357 [data in appendix](#)). The ANN model will determine the olivine type  
358 correctly within several minutes.

359 Last but not least, there are many whole-rocks or mineral major elements,  
360 trace elements, or radiogenic isotope compositions, it is difficult for people  
361 to distinguish the hidden patterns of massive data. ML methods can exam  
362 these large and varied data sets to uncover information including hidden  
363 patterns, unknown correlations. Our study shows that ML models offer the  
364 potential to make more data-driven decisions such as classification at more  
365 high accuracy rates for these data sets.

366

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380

381

382 **Figures**

383 Figure 1 A map showing the location of the main Continental Flood Basalts  
384 (CFBs) around the world. The CFBs highlighted in the rectangle provide  
385 many olivine data points from picrites for this study. This map is adapted  
386 from ([Bryan and Ernst, 2008](#)).

387

388 Figure 2 Ti/Y of samples ranging from 200 to 1400 from the six CFBs. The  
389 gray area represents intermediate Ti/Y (IT) samples.

390

391 Figure 3 The correlations between major elements compositions of olivine.  
392 The diagonal shows the elements, the lower triangle is the diagram of two  
393 related elements, and the upper triangle shows the correlation coefficient  
394 of the two related elements. For example, 0.25 in the second column of the  
395 first row is the correlation coefficient of SiO<sub>2</sub> and Al<sub>2</sub>O<sub>3</sub>, and their plots are  
396 shown in the first column of the second row.

397

398 Figure 4 The general structure of the ANN. It has five features including  
399  $\text{Al}_2\text{O}_3$ ,  $\text{MgO}$ ,  $\text{CaO}$ ,  $\text{NiO}$  and  $\text{Cr}_2\text{O}_3$ . There are 10 nodes in a hidden layer.  
400 The output of the ANN is LT and HT.

401

402 Figure 5 A confusion matrix showing the classification accuracy of the  
403 ANN. (a) In the confusion matrix of the training data, the blue color  
404 represents a correct prediction and the red a wrong prediction. The number  
405 inside is the total number of samples. (b) The confusion matrix of the  
406 validation data. (c) The confusion matrix of test data. (d) The confusion  
407 matrix of all the data.

408

409 Figure 6 Variation of  $\text{NiO}$ ,  $\text{CaO}$ ,  $\text{Al}_2\text{O}_3$ , and  $\text{Cr}_2\text{O}_3$  versus  $\text{MgO}$  for olivine  
410 from global CFBs. It shows that a portion of IT samples whose major  
411 element content is similar to that of LT samples is determined as IT-L, and  
412 others similar to HT samples are determined as IT-H by our ANN. The  
413 grey triangle and circles represent olivines from HT and LT samples,  
414 respectively. The dark-yellow triangle and light-blue circles represent  
415 olivine from IT samples, which are classified as HT and LT by our ANN,  
416 respectively. The dashed line represents the area with most HT and IT-H  
417 olivines, and the solid line represents the area with most LT and IT-L  
418 olivine. Note, that many contents of  $\text{Al}_2\text{O}_3$  and  $\text{Cr}_2\text{O}_3$  in 6c and 6d are zero  
419 which may mean they were below the detection threshold.

420

421 Figure 7 A confusion matrix of all the data using an SVM and an NBC. It  
422 shows that the accuracy of the ANN shown in Fig.5 is better than the  
423 accuracy achieved by either an SVM or an NBC. The blue color represents  
424 a correct prediction and the red a wrong prediction. The number inside is  
425 the total number of samples which are same as in Fig.5.

426

427 Figure 8 (a) NiO-Fo relationship of olivine populations in picrites from the  
428 six CFBs. The pink field is for phenocrystals from mid-ocean-ridge basalts  
429 (after [Sobolev et al., 2005](#)). The light-green field is the NiO<sub>89</sub> content range  
430 produced by peridotite primary melts ([Matzen et al. 2017](#)). The white  
431 dashed circle is the data from Ethiopian CFB. (b) FCKANTMS vs.  
432  $\ln(\text{SiO}_2/(\text{CaO}+\text{Na}_2\text{O}+\text{TiO}_2))$  of whole-rock compositions of picrites which  
433 we collected in this study. Mafic, peridotite, and carbonatite mafic melts  
434 data were compiled by Yang et al. (2019). EM43 is one LT sample from  
435 Emeishan LIP. The black dashed circle are samples from Ethiopian LIP.

436

437 Figure 9 A confusion matrix showing the classification accuracy of the  
438 ANN with three outputs for all the data. HT1 and HT2 represent for mafic  
439 and carbonatite mafic source, respectively. The blue color represents a  
440 correct prediction and the red a wrong prediction. The numbers inside are

441 the total numbers of samples, and the percentage numbers inside are the  
442 ratios.

443

444 Figure 10 The classification results of a single IT sample for each CFB  
445 (except Karoo and Ethiopian CFBs, which do not have any IT samples).

446 Both HT1 and LT olivine are found in the same samples from Etendeka,

447 North Atlantic, and Emeishan CFBs.

448

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Table 1 Data description of olivine used in this study

	Count	Card.	Min	1st Qrt	Mean	Median
SiO <sub>2</sub> (wt%)	2898	2466	35.62	39.44	39.86	39.90
TiO <sub>2</sub> (wt%)	2898	749	0.00	0.00	0.01	0.00
Al <sub>2</sub> O <sub>3</sub> (wt%)	2898	1042	0.00	0.02	0.04	0.04
Cr <sub>2</sub> O <sub>3</sub> (wt%)	2898	1121	0.00	0.04	0.06	0.06
FeO(T)(wt%)	2898	2690	0.00	11.62	14.14	13.56
CaO(wt%)	2898	1644	0.00	0.26	0.31	0.32
MgO(wt%)	2898	2685	26.60	43.78	45.29	45.67
MnO(wt%)	2898	2048	0.00	0.17	0.20	0.20
NiO(wt%)	2898	1982	0.00	0.31	0.35	0.34

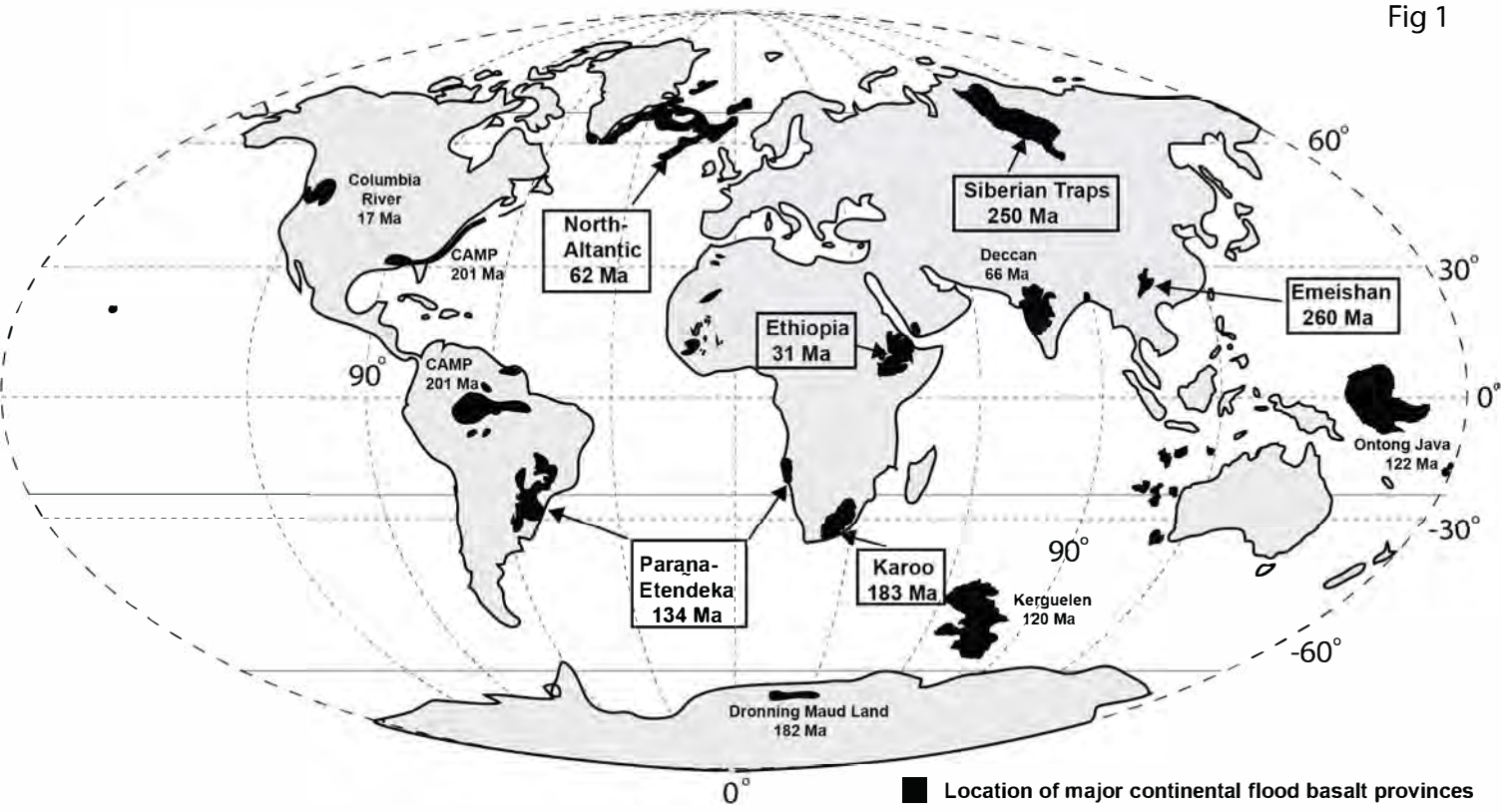
Card. Cardinality of each element, which measure the number of distinct values present

---

3rd Qrt.	Max	Std Dev.
40.29	62.52	1.02
0.01	0.36	0.01
0.06	5.00	0.11
0.08	0.49	0.04
16.16	31.37	4.08
0.36	4.51	0.12
47.51	52.88	3.32
0.23	0.48	0.06
0.40	0.63	0.09

---

Fig 1



■ Location of major continental flood basalt provinces

Fig 2

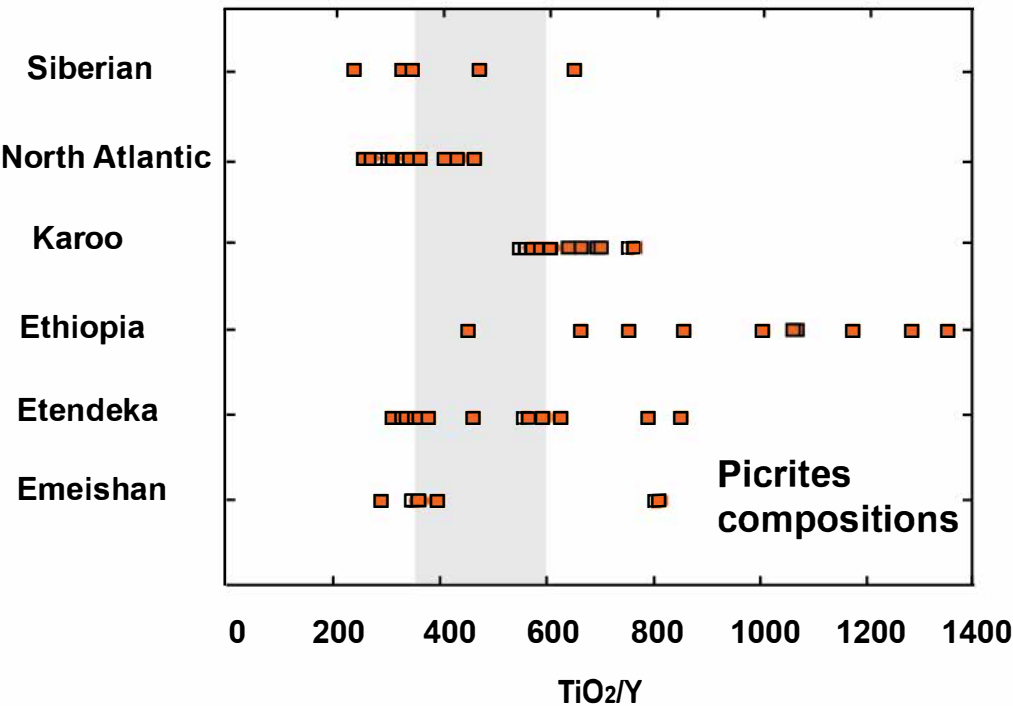
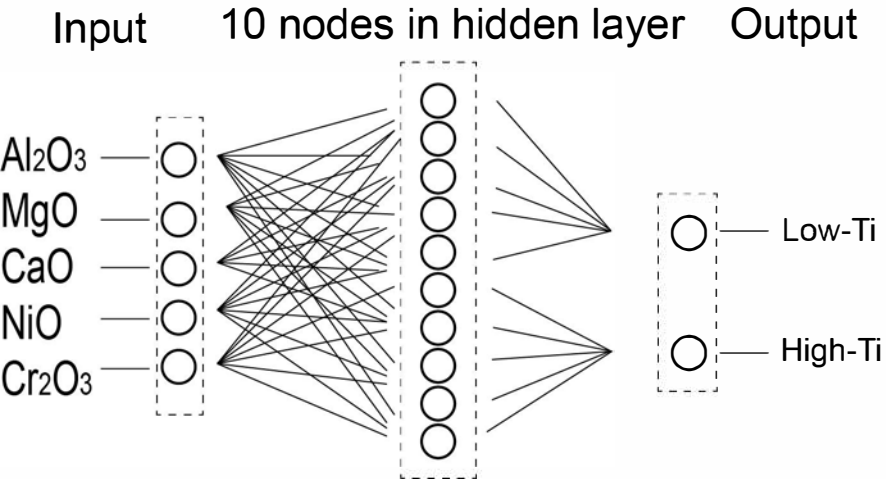




Fig 4



(a) Training Confusion Matrix

Output Class	LT	227 32.3%	2 0.7%	99.1% 0.9%
	HT	5 0.6%	468 66.6%	98.9% 1.1%
		97.8% 2.2%	99.6% 0.4%	99% 1%
		LT	HT	

(b) Validation Confusion Matrix

Output Class	LT	36 24.0%	2 1.3%	94.7% 5.3%
	HT	3 2.0%	109 72.7%	97.3% 2.7%
		92.3% 7.7%	98.2% 1.9%	96.7% 3.3%
		LT	HT	

(c) Test Confusion Matrix

Output Class	LT	54 36.0%	3 2.0%	94.7% 5.3%
	HT	4 2.7%	89 59.3%	95.7% 4.3%
		93.1% 6.9%	96.7% 3.3%	95.3% 4.7%
		LT	HT	
		Target Class		

(d) All Confusion Matrix

Output Class	LT	317 31.6%	7 0.7%	97.8% 2.2%
	HT	12 1.2%	666 66.5%	98.2% 1.8%
		96.4% 3.6%	99.0% 1.0%	98.1% 1.9%
		LT	HT	
		Target Class		

Fig 6

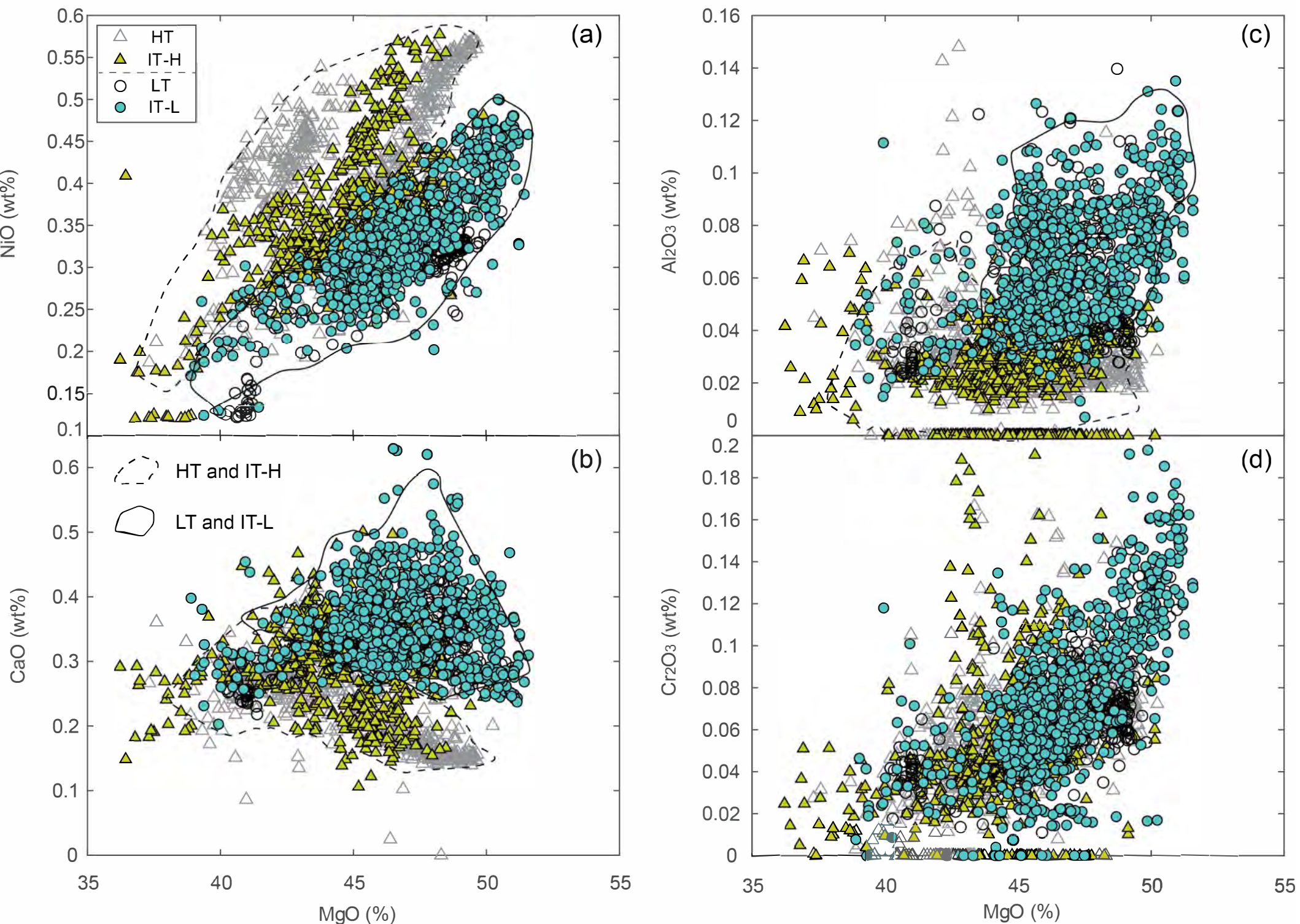




Fig 7

SVM

(a)

Output Class

LT	<b>316</b> 31.5%	<b>22</b> 2.2%	<b>93.5%</b> 6.5%
HT	<b>13</b> 1.3%	<b>651</b> 65.0%	<b>98.0%</b> 2.0%
	<b>96.0%</b> 4.0%	<b>96.7%</b> 3.3%	<b>96.5%</b> 3.5%

LT

HT

(b)

NBC

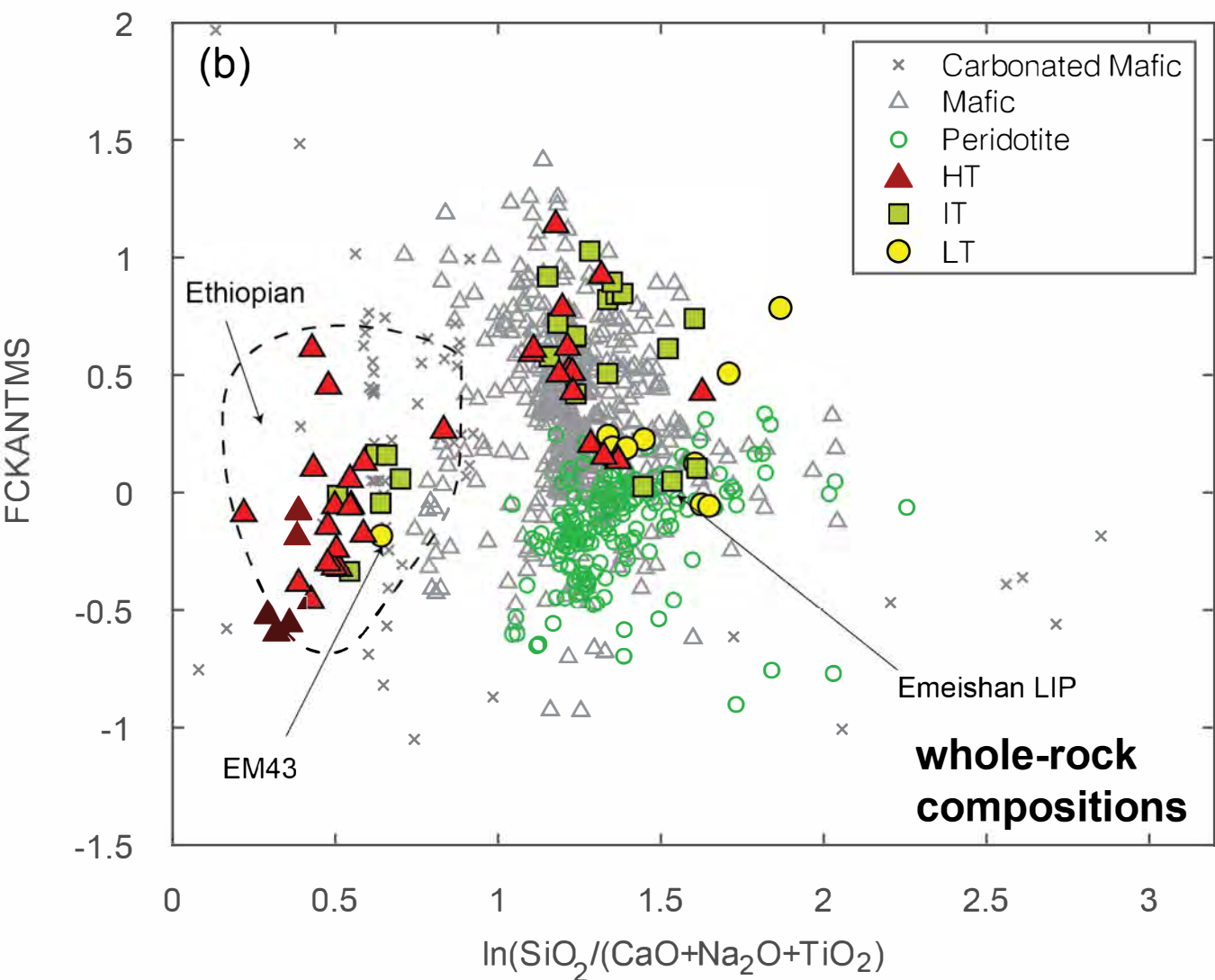
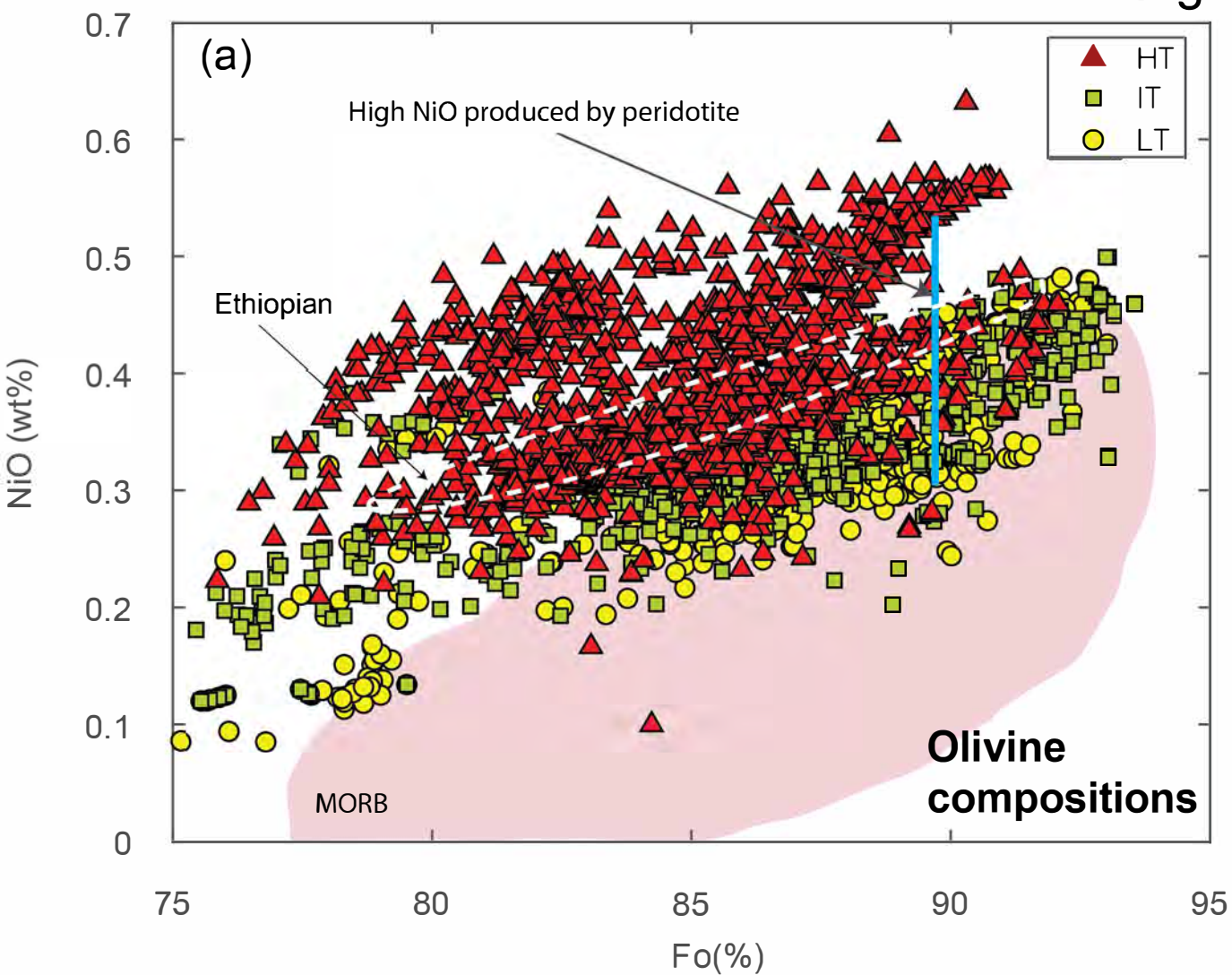
Output Class

LT	<b>300</b> 29.9%	<b>26</b> 2.6%	<b>92.0%</b> 8.0%
HT	<b>29</b> 2.9%	<b>647</b> 64.6%	<b>95.7%</b> 4.3%
	<b>91.2%</b> 8.8%	<b>96.1%</b> 3.9%	<b>94.5%</b> 5.5%

LT

HT

Target Class



All Confusion Matrix

Fig 9

Output Class

HT1

LT

HT2

<b>614</b> 61.3%	<b>9</b> 0.9%	<b>21</b> 2.1%	<b>95.3%</b> 4.7%
<b>13</b> 1.3%	<b>320</b> 31.9%	<b>4</b> 0.4%	<b>95.0%</b> 5.0%
<b>5</b> 0.5%	<b>0</b> 0.0%	<b>16</b> 1.6%	<b>76.2%</b> 23.8%
<b>97.2%</b> 2.8%	<b>97.3%</b> 2.7%	<b>39.0%</b> 61.0%	<b>94.8%</b> 5.2%

HT1

LT

HT2

Target Class

Fig 10

