

Statistics and segmentation:

Using Big Data to assess Cascades Arc compositional variability

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Abstract

Primitive lavas erupted in the Cascades arc of western North America demonstrate significant patterns of along-arc heterogeneity. Such compositional diversity may be the result of differences in mantle melting processes, subduction geometry, regional tectonics, or compositions of the slab, mantle or overlying lithosphere. Previous authors have partitioned the arc into four geochemically distinct segments in order to assess the importance and relative roles of these potential causes (Schmidt et al., 2008). However, despite the immense amount of data available from the Cascade arc, no previous study has utilized a statistical approach on a comprehensive dataset to address such a fundamental petrologic question. To better characterize the heterogeneity of the entire arc, we compiled >250,000 isotopic, major, and trace element analyses (glass and whole rock) from nearly 13,000 samples. To minimize inherent sampling bias – the effect where well-studied volcanoes heavily weight conclusions – we use a weighted bootstrap Monte Carlo approach in which the probability of a sample being selected to the posterior distribution was inversely proportional to the number of samples within its 0.25° latitude bin. This methodology produces a more uniform and unbiased distribution from which we can assess regional, rather than local, compositional variability in the Cascades arc. Using a multivariate statistical approach, we demonstrate that the four segments designated by Schmidt et al. (2008) are, in fact, statistically distinct. However, using a modified hierarchical clustering mechanism, we objectively divide the arc into six regions which have geochemical differences that are up to 6.3 times more statistically significant than in the previous scheme. Our new, more robust segmentation scheme includes the Garibaldi (49.75-51°N), Baker (48.5-49.75°N), Glacier Peak (47.75-48.5°N), Washington (45.75-47.75°N), Graben (44.25-45.75°N), and South (41.25-44.25°N) Segments. By partitioning the arc into the most statistically distinct segments and calculating unbiased mean compositions for each, we explore the petrogenetic causes for the regional-scale differences in primitive lava compositions. These bootstrapped mean data indicate significant inter-segment differences in fluid-flux signature, mantle fertility, and depth and degree of melting. We suggest that differences in subduction geometry, regional tectonics and mantle heterogeneity are the primary causes for these intra-arc differences. This study demonstrates the value of rigorous statistics and the use of big data in the field of petrology.

40 **1 Introduction**

41 The composition of magmas erupted at arc volcanoes bear evidence of the complex
42 interplay between geochemical contributions from subducted oceanic crust, sediment, and
43 liberated fluids, and from the mantle wedge and overlying lithosphere. The composition and
44 mass contributed from each of these varies worldwide and even within a single arc (Hildreth and
45 Moorbath, 1988; Elliott, 2003; Carr et al., 2004; Schmidt et al., 2008). This diversity is made
46 even more complex by the fact that other parameters such as the rate and angle of subduction,
47 slab age, mantle flow patterns, and thickness and tectonics of the overlying lithosphere may also
48 greatly affect the composition of arc magmas (Patino et al., 2000; Syracuse and Abers, 2006; Till
49 et al., 2013). Comparing along-arc compositional changes to variability in these parameters
50 provides an excellent means by which to identify those that may be most responsible for
51 production of heterogenous magmas within a single arc system. This, in turn, provides a more
52 comprehensive understanding of the complex magmatic processes that occur within arcs
53 worldwide.

54 Systematic intra-arc changes in volcanic rock compositions have been demonstrated for
55 many systems around the world, and numerous causes have been proposed for each. For
56 example, in the Central American Volcanic Arc (CAVA), systematic trends towards lower
57 La/Yb and higher U/Th and Ba/La in mafic lavas from the Nicaragua portion of the arc may
58 indicate higher degree partial melting and greater contribution from the slab (Carr et al., 2004).
59 This trend may be the result of a steeper slab angle in the central arc which could act to
60 concentrated fluid-flux (Patino et al., 2000; Shaw et al., 2003). Wörner *et al.* (1994) explore
61 geochemical variations in volcanoes from the Central Andes (17.5-22°S) and suggest that crustal
62 age is the predominant factor producing heterogeneity since crustal thickness, sediment supply,
63 slab depth, and distance from trench are invariant over this portion of the arc. Along-arc changes
64 in the Indonesian Sunda arc have been attributed to mantle heterogeneity and slab depth
65 (Whitford et al., 1979) or differing sediment compositions and degree of melting (Turner and
66 Foden, 2001). Thus, along-strike trends in geochemistry are a common feature in arcs worldwide
67 and provide a window into the effects that each factor has on arc geochemistry.

68 Numerous authors have also demonstrated along-arc compositional variability of the
69 Cascades volcanic arc (Leeman et al., 1990; Bacon et al., 1997; Schmidt et al., 2008; Mullen et
70 al., 2017), as well as differences in the spacing between volcanoes, volumetric production, and

71 eruptive style (Guffanti and Weaver, 1988; Sherrod and Smith, 1990; Hildreth, 2007). Schmidt et
72 al. (2008) suggest that the Cascades arc can be partitioned into four segments based on
73 abundance trace element and isotopic data, as well as relative abundance of several primitive
74 lava types (i.e. calc-alkaline, tholeiitic, intraplate, and absorokite). The four segments are: The
75 North (Mt. Meager to Glacier Peak), Columbia (Mt. Rainier to Mt. Jefferson), Central (Three
76 Sisters to Medicine Lake), and the South Segments (Mt. Shasta to Lassen Peak). These
77 boundaries were defined such that the geochemical composition of primitive lavas is visually
78 similar within a segment but are relatively distinct between segments. The definition of these
79 segments has been adopted by numerous subsequent authors working on Cascades volcanoes.
80 However, although this work made great strides in understanding the geochemical variability of
81 the arc, it is based on a relatively small data set (n=390) that is strongly spatially biased towards
82 just 14 of the over 3,400 Quaternary volcanic vents (Hildreth, 2007) of the Cascades arc (Fig. 1,
83 red columns) and did not use a statistically rigorous scheme to identify different segments.

84 To infer more robust conclusions about the causes of large-scale variability within an arc
85 requires that there is adequate geochemical data to fully characterize the compositional range
86 within each region and provide comprehensive spatial coverage of the entire arc. The Cascades is
87 one of the most highly studied arcs in the world, and the tremendous volume of geochemical data
88 that exists for this arc has not been utilized in its entirety by previous studies. This provides a
89 unique opportunity to apply more advanced statistical methods that were developed for larger
90 datasets to address Cascades arc variability in a novel way.

91 However, while a large dataset mitigates problems of incomplete sampling, this sampling
92 is inherently uneven; certain volcanoes within an arc tend to be oversampled, while other less
93 popular edifices remain poorly studied. This is a problem for studies that seek to address large
94 scale questions such as variability over an entire arc, since the oversampled volcanoes
95 overwhelm the overall trends, while compositions erupted at the rest of the volcanoes may not be
96 adequately represented. For example, in the Cascades arc, two volcanoes, Mount Adams and
97 Mount St. Helens, account for approximately 20% of all mafic data from Cascades arc literature.
98 Thus, simple calculations involving a comprehensive arc-wide dataset are highly skewed towards
99 the compositions of these two volcanoes and the local, rather than regional, processes that
100 produce them. In this case statistical treatment of these data can help avoid the ill-effects of
101 sampling bias and allow for more robust interpretations of larger, more representative datasets.

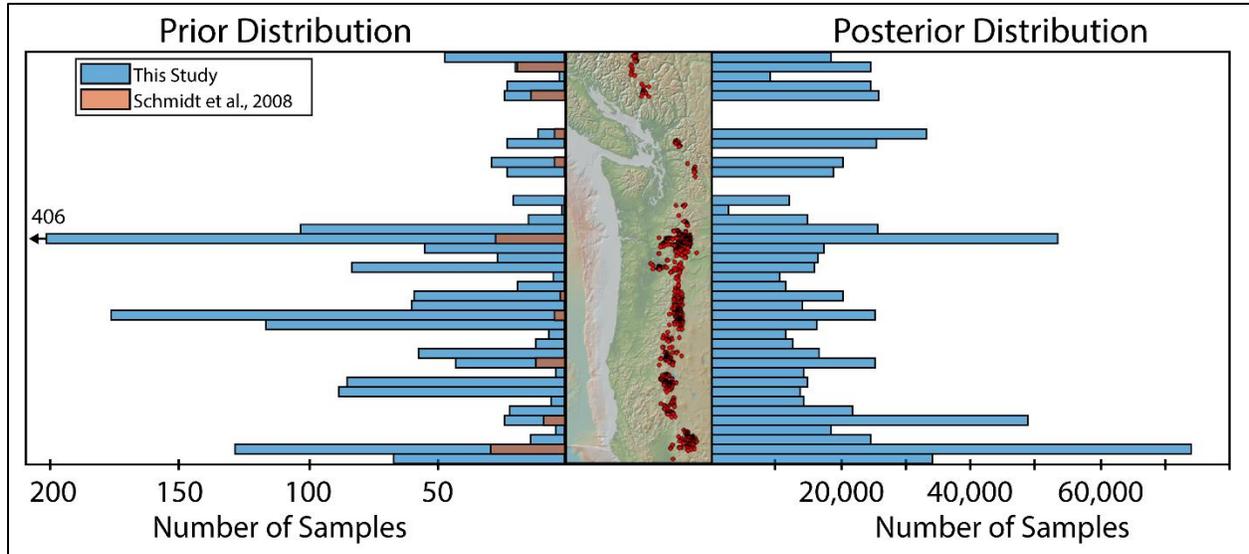


Figure 1: The histogram on the left shows the distribution of mafic samples used by Schmidt et al., 2008 (red) compared to the mafic arc-front dataset used in this study (blue). Bins are 0.25° latitude. The map in the middle shows the locations of samples used in our study. Only arc-front samples are shown. The histogram on the right shows the posterior distribution after the Monte Carlo simulation with bootstrap resampling. Note that the posterior distribution is much more evenly distributed than the prior distribution, thereby reducing the inherent sampling bias of the comprehensive dataset.

102 For our study, we compile major and trace element and isotopic data on 13,000 samples
103 from nearly 250 different publications and use multivariate statistical techniques to more
104 thoroughly assess geochemical variability along the Cascades arc. Our study consists of two
105 parts. We first re-examine the segments proposed by Schmidt et al. (2008) with this more
106 representative dataset, utilizing a Monte Carlo bootstrapping approach to reduce sampling bias.
107 We then use multivariate statistics to quantify differences among the segments, and to test
108 whether they are statistically distinct from each other. In the second part of our study, we
109 develop a multivariate clustering technique to objectively establish a more statistically robust
110 segmentation scheme.

111 To our knowledge, this study is the first of its kind to use rigorous multivariate statistics
112 to address geochemical variability within a single arc. By compiling and utilizing a more
113 representative dataset, reducing the influence of oversampled volcanoes, and partitioning the arc
114 into regions that are most geochemically distinct from each other, we can better assess the
115 petrogenetic causes of geochemical variability along the Cascades arc.

116 **2 Background**

117 Along-arc compositional variability in the erupted volcanic rocks of the Cascades arc
118 may be the result of observed differences in subduction geometry or the composition of slab,

119 mantle or overlying lithosphere that occur over the 1200 km arc (Guffanti and Weaver, 1988;
120 Leeman et al., 1990; Hildreth, 2007; Mullen et al., 2017). These along-arc changes are briefly
121 summarized below:

122

123 ***2.1 Subduction geometry***

124 Subduction transitions from nearly orthogonal in the north to highly oblique in the south.
125 The age of the slab that is subducted ranges from 3-5 Ma in the northernmost and southernmost
126 regions of the arc, to 10 Ma near the California-Oregon border (Wilson, 2002). The slab itself
127 may also be highly segmented, with differing angles, and slab gaps and tears that may allow
128 enriched sub-slab mantle into the overlying wedge (Porritt et al., 2011; Gao and Shen, 2014).
129 Finally, the depth of the slab beneath the arc volcanoes range from <70 km under Mt. St. Helens,
130 to >90 km for Glacier Peak, Lassen Peak, and rear-arc volcanoes (McCrorey et al., 2012).

131

132 ***2.2 Subducted slab composition***

133 The Gorda plate, which is subducted beneath the California portion of the arc, has a more
134 depleted MORB composition than that of the Juan de Fuca plate (Davis et al., 2008; Gill et al.,
135 2016). The Gorda plate and the northernmost portion of the Juan de Fuca plate are more
136 intensely fractured, which may introduce more subduction fluid to the mantle wedge beneath the
137 northern and southern portions of the arc than the central arc (Schmidt et al., 2008). Furthermore,
138 sediment abundance and composition also vary significantly from north to south on both the Juan
139 de Fuca and Gorda plates (Carpentier et al., 2014).

140

141 ***2.3 Mantle Heterogeneity***

142 Some authors suggest that the mantle beneath the arc is heterogeneous and contains many
143 isotopically distinct domains, which are sampled throughout the arc (Bacon et al., 1997).
144 However, Mullen et al. (2017) hold that there are only three isotopically distinct mantle
145 compositions which are sampled by the northernmost Garibaldi segment, the High Cascades, and
146 the rear-arc Simcoe Volcanic Field. In addition, mantle flow patterns may be toroidal around slab
147 edges, and the degree of melting may be highly dependent on position relative to slab edges or
148 gaps (Long, 2016, and references therein).

149

150 **2.4 Lithospheric heterogeneity**

151 Lithology changes from 50-km thick Paleozoic accreted terranes and old cratonic
152 lithosphere in the north, to 50-55 Ma accreted oceanic plateau in the central part of the arc
153 (Phillips et al., 2017), and the Paleozoic Klamath Terrain in the south (Schmidt et al., 2008).
154 Regional tectonics also change along arc from compressional in the north to extensional in the
155 south (Wells and McCaffrey, 2013; Brocher et al., 2017).

156

157 **3 Methods**

158 **3.1 Data compilation, filtering, and categorization**

159 To fully characterize the geochemical heterogeneity of the Quaternary Cascades arc, we
160 carefully compiled a comprehensive dataset from the literature (Appendix 1). To do this, we used
161 three online data repositories: EarthChem, GeoRoc, and the U.S. Geological Survey (USGS)
162 National Geochemical database. Data from these databases were carefully concatenated such that
163 no repeat analyses were included. We manually added data from 98 other sources, including
164 many theses and dissertations, that were not found by the aforementioned databases. Only whole
165 rock or glass analyses of Quaternary volcanic rocks were used. The study was limited to the
166 Quaternary since significant changes have occurred in some portions of the arc since the
167 initiation of the current High Cascades arc axis in the late Neogene (e.g. Pitcher *et al.*, 2017). We
168 compiled all analyses for a given sample into one line of data; for each element, priority was
169 given to the most recent data from the most precise analytical method (e.g. decreasing priority
170 methods for major elements are X-ray fluorescence, wet chemistry, electron microprobe, and
171 then atomic emission and absorption spectrometry). We removed analyses that were collected
172 before 1970 (n=245 samples) to increase the likelihood of retaining only higher quality data. We
173 converted all iron data to FeO*, removed all samples with analytical totals <90%, as suggested
174 by WoldeGabriel et al. (2005), and normalized all major element data to totals of 100%.

175 Because the processes of magma generation and differentiation within the rear-arc may
176 differ from those of the volcanic front (e.g. Pearce and Stern, 2006), we created a separate
177 dataset for the rear-arc volcanic centers (i.e. Simcoe Volcanic field, Newberry Volcano, and
178 Medicine Lake). USGS geological maps were used to constrain the longitudinal boundary for
179 these three rear-arc provinces. In total, our dataset includes 4,035 samples from the rear-arc,
180 which accounts 31% of all Cascades samples (Table 1).

181 In addition, since compositional differences in felsic rocks may indicate the influence of
182 very different processes than along-arc variability in mafic rocks, we separated the dataset into
183 three compositional groups: mafic (<52 wt.% SiO₂), intermediate (52-62.99 wt.%), and felsic
184 (≥63 wt.%). For the samples that did not have SiO₂ data, we used the rock names given by the
185 author. In addition, a separate dataset was created for more primitive samples (MgO >7wt.%,
186 Mg# >57.5) (ca. Schmidt *et al.*, 2008).

187 Although a major goal of this study is to fully characterize the compositional range of the
188 Cascades, outliers greatly affect the results of multivariate statistical techniques such as those
189 implemented in this study (Tryon *et al.*, 2011). Thus, we utilized a two-stage Chauvenet's
190 criterion for rejection to remove outliers. Unlike more traditional methods, such as removing
191 values beyond 2σ from the mean or 1.5 times the interquartile range from the median, the cutoff
192 point for Chauvenet's criterion is also dependent on the number of analyses used. After the
193 removal of outliers, our data compilation includes over 250,000 analyses on nearly 13,000
194 different samples. Of these, 35% are mafic samples, 48% are intermediate, and 17% are felsic
195 (Table 1). However, this study is based only on the 4,610 mafic samples within the data
196 compendium.

Table 1: Number of samples and analyses in our Cascades data compilation.

	Arc-front	Rear-arc	All data	Analyses
Primitive	1,064	853	1,917	37,756
Mafic	2,037	2,573	4,610	88,309
Intermediate	5,178	1,020	6,198	122,523
Felsic	1,714	442	2,156	40,678
Total	8,929	4,035	12,964	251,510

197 **3.2 Reducing Sampling bias: Weighted bootstrap resampling**

198 To better characterize along-arc variability, and to reduce sampling bias associated with
199 well-studied locations we used a Monte Carlo method with a weighted bootstrap resampling.
200 Bootstrap resampling, or bootstrapping, refers to any statistical technique that involves iterative
201 random sampling from a population, with replacement after each sample is drawn. Repeating this
202 sampling many times (n>10,000), referred to as a Monte Carlo technique, increases the
203 likelihood that the mean and standard deviation of the sample set accurately represent that of the
204 entire population. This technique is especially powerful in reducing sampling bias when an

205 inverse weighting scheme is used, such that each analysis from under-sampled regions are given
206 a much higher probability of being selected during bootstrapping, compared to those from
207 oversampled regions. Thus, analyses from under-sampled regions are “pulled up by their
208 bootstraps” to create a new “posterior distribution” that is much more uniform than the original
209 “prior distribution” (Fig. 1).

210 For our study, we first separated the data into bins of 0.25° latitude (“latbins”). Then, we
211 assigned each sample a weight, or probability of selection ($0.05 \leq W \leq 1$), that is inversely
212 proportional to the number of analyses within its latbin. The weight given to each element within
213 each latbin (W_i) was calculated by dividing number of analyses of a given element within that
214 latbin (N_i) into that of the bin that contains the least samples for a given segment (N_{min}),
215 ($W_i = \frac{N_{min}}{N_i}$). This was done separately for each compositional group (e.g. mafic and primitive).
216 Since samples often did not contain the full suite of major and trace elements, the final weight
217 given to all samples within a latbin (W_{latbin}) was calculated by taking the median of the weights
218 of all elements within that latbin: $W_{latbin} = median\left(\frac{\min(N_{SiO_2})}{N_{SiO_2}}, \frac{\min(N_{TiO_2})}{N_{TiO_2}}, \dots, \frac{\min(N_{Yb})}{N_{Yb}}\right)$. We
219 used a minimum weight of 0.05, such that the locations that are most highly sampled (i.e. Mt. St.
220 Helens) are not completely disregarded (Keller and Schoene, 2012). Thus, the improvement in
221 the posterior distribution was limited to 20 times (Fig. 1).

222 Bootstrap sampling was implemented via a MATLAB code. Our procedure was as
223 follows:

- 224 1) For each bootstrap iteration, a random number, r , between 0 and 1 is assigned to each
225 sample in the dataset. MATLAB uses a Mersenne Twister pseudorandom number
226 generator, which has been shown to be sufficiently close to true randomness (Matsumoto
227 and Nishimura, 1998). New r values are generated for each iteration
- 228 2) Each sample for which $W > r$, was “chosen” for that round.
- 229 3) For each element of the chosen sample, a random value is drawn from a Gaussian
230 distribution formed by μ =reported value, σ = analytical error, and all these values for a
231 chosen sample are added to the bootstrap subset.
- 232 4) Step (3) is completed for each chosen sample ($W > r$) of that bootstrap iteration.
- 233 5) The bootstrap subset from this iteration is concatenated to the subsets from all previous
234 iterations into a single Monte Carlo results set

235 6) Steps 1-5 are repeated until the number of samples within the Monte Carlo re-sampled
236 dataset >1 million.

237 Step 3 is necessary because the bootstrap subset must have a continuous distribution. We
238 used an analytical uncertainty of 2%, as suggested by Keller and Schoene (2012). To test the
239 effect of this choice of analytical uncertainty, we did two additional test runs, one in which all
240 elements had a 4% uncertainty, and one where major elements had 2% uncertainty and trace
241 elements had 4%. We found that this made almost no difference in the final bootstrapped
242 averages of all elements, and the effect on the bootstrapped confidence intervals was small
243 enough that it could not be visually observed on most bivariate plots.

244 ***3.3 Calculating Confidence intervals for bootstrapped means***

245 For each bootstrapped mean, we also calculated a 95% confidence interval (CI), using the
246 following: $\bar{x} \pm t \frac{\sigma}{\sqrt{n}}$, where \bar{x} and σ are the bootstrapped mean and standard deviation, and t is
247 the right-tail critical value for a student t distribution at the 0.05 level. We use the original
248 number of samples for n , not the number of samples in the Monte Carlo set (Keller et al., 2015).
249 These CI calculations rely on the assumption of normality. However, even if the original data
250 was not normally distributed, by the Central Limit Theorem, means of the Monte Carlo set will
251 always be normally distributed due to the large number of samples selected.

252 ***3.4 Testing the robustness of segmentation schemes***

253 Partitioning the arc should be done in a way that the segments are most geochemically
254 dissimilar to one another, so that the compositions can be compared, and inferences can be made
255 as to the causes for the differences. If two segments are relatively similar, then they should be
256 combined. Thus, to test whether segments are geochemically distinct, we use a multivariate
257 technique called the Hotelling's T^2 test. This test is the multivariate equivalent of the Student's t
258 test and is a "post-hoc test" that follows a multivariate analysis of variance (MANOVA).
259 Hotelling's T^2 test essentially evaluates whether the multivariate means ("mean vector") of two
260 segments, are different enough in n -dimensional space to reject the null hypothesis that the two
261 are the same. Before testing this, the variables (elements) are transformed by the MANOVA
262 technique, such that the new transformed variables minimize the within-segment variation and
263 maximize the between-segment variation. Thus, instead of just simply comparing the
264 multivariate distances between mean values of each segment, the Hotelling's T^2 compares the

265 means of each element, variance of each element, and multivariate covariance between elements
266 (i.e. multivariate trends) of the data in each segment.

267 For large populations ($N > 30$), such as the dataset in our study, the Hotelling's T^2 statistic
268 follows a X^2 distribution with k degrees of freedom, where k is the number of geochemical
269 elements, allowing us to calculate a p value. Small p values indicate that two segments are more
270 different than would be expected for two samples drawn from a single population. Specifically, if
271 the $p < 0.05$, then we reject the null hypothesis, and the two segments are considered statistically
272 distinct. The Mahalanobis distance, which is closely related to the Hotelling's T^2 , provides the
273 multivariate distance between the mean vectors of the two groups. We used the Hotelling's T^2
274 test on both the segmentation scheme of Schmidt et al. (2008) and our new statistically-based
275 scheme and compared the Mahalanobis distances between segments to assess which created
276 more distinct groups.

277 ***3.5 Establishing new segments: modified Hierarchical clustering mechanism***

278 To determine a statistics-based segmentation scheme that best separates the Cascades arc
279 into geochemically distinct regions, we developed a new, modified hierarchical clustering
280 technique. For each step in a classic hierarchical clustering analysis, the two individuals or
281 groups that are most similar (e.g. have the shortest distance between their mean values) are
282 combined into a new group and this process is repeated until the desired number of groups are
283 reached or all individuals are combined. Thus, the process clusters data such that the within-
284 group similarity is maximized. This process can be represented by a dendrogram, in which all
285 individuals start out as separate branches on the y axis, and as two individuals are merged
286 together, the distance between their means (distance of fusion) are shown on the x axis (Fig. 4).
287 We had to modify this traditional hierarchical clustering technique to reduce sampling bias, deal
288 with problems associated with missing data, ensure that clusters consisted of regions that were
289 proximally close to one another, and account for correlation between elements (i.e.
290 differentiation trends). These modifications will be discussed in further detail below.
291 To account for the significant covariation expected between many elements in geochemical data
292 (e.g. correlation with SiO_2) we chose to use the Mahalanobis distance (MD) as the measure of
293 dissimilarity between groups in our hierarchical clustering method. In contrast to the more
294 common centroid linkage approach, which uses Euclidian distance to measure the distance
295 between clusters and assumes a spherical distribution for all elements around these centroids,

296 MD measures the distance between the centroids of two groups while also considering the
297 dispersion around the centroids. This dispersion is measured by a dataset's covariance matrix.

298 The MD between groups i and j is given by: $MD_{ij} = \sqrt{(\bar{x}_i - \bar{x}_j)^T S^{-1}(\bar{x}_i - \bar{x}_j)}$ where S is the
299 covariance matrix and \bar{x}_i is the mean vector for sample i that contains the means of each element.
300 To calculate the covariance matrix, we used the Monte Carlo bootstrapped dataset for each
301 latbin. Because most samples had data for only a subset of elements, missing data was common.
302 The covariance matrix of a dataset can become singular if it has excessive missing values. Thus,
303 in order to calculate the covariance matrix for our dataset, we used the Expectation Conditional
304 Maximization (ECM) algorithm of Meng and Rubin (1993) to calculate a non-singular
305 covariance matrix. This algorithm imputes values for these missing data, based on the mean and
306 variance of that element, and then iteratively changes these imputed values until the log-
307 likelihood function is maximized. Further explanation of the theory can be found in Little and
308 Rubin (2014).

309 We wanted to reduce the effects of sampling bias when creating our new segments. Thus,
310 every time two groups of latbins were combined, we performed a new Monte Carlo analysis with
311 bootstrap re-sampling to find that new group's bootstrapped mean elemental concentrations. This
312 portion of our procedure was almost identical to the one described above in section 3.2.

313 To create the clusters (segments), we used mafic data because primitive data are
314 relatively sparse in some parts of the arc (Schmidt et al., 2008). We also chose to exclude rear-
315 arc data, because this allows us to focus on the processes that may be responsible for along-strike
316 variability, without adding complications from the additional processes involved in rear-arc
317 magma generation.

318 We completed the clustering process in two stages. The initial stage was used to combine
319 the seven latbins with little to no data for some elements ($n < 4$) with the neighboring latbin that
320 was more similar. Since Mahalanobis distances are highly skewed by data with few observations,
321 we used only the 15 elements for which all latbins had at least 4 analyses, for this initial stage.
322 After merging those sparsely-sampled latbins with a neighbor, there were 25 elements for which
323 there were at least 4 analyses in all latbins of data. Thus, we completed the second stage of

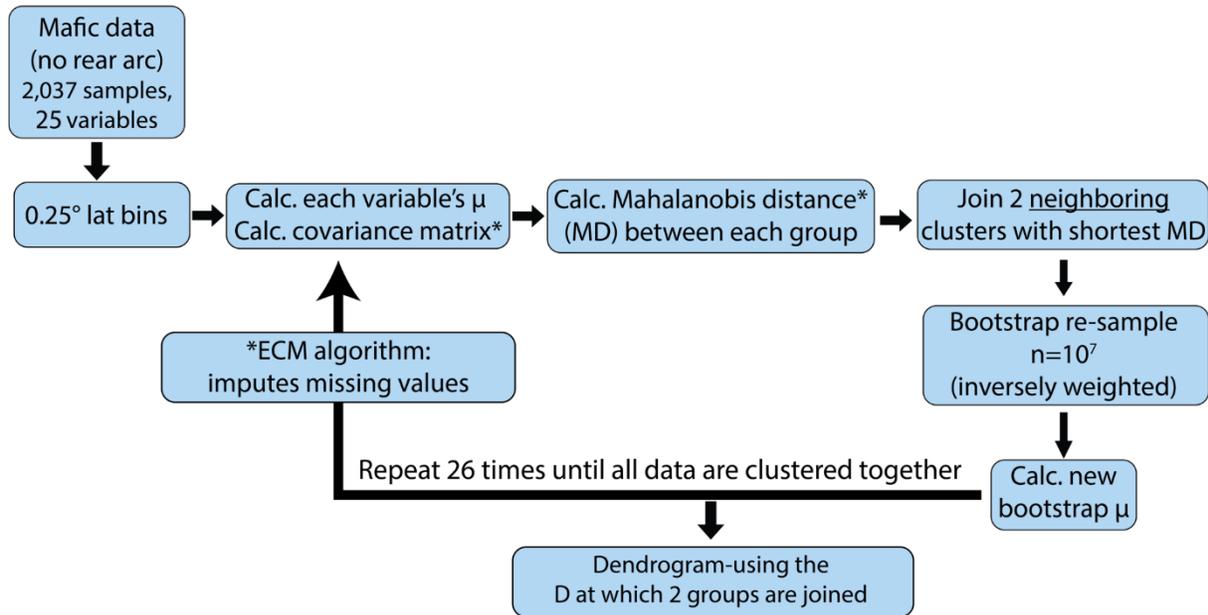


Figure 2: Flowchart of the new modified hierarchical clustering methodology developed in this study. Note that this methodology was completed in two stages, one with 15 elements to combine the sparsely sampled latbins, and the second with 25 elements.

324 clustering using these 25 elements. We wrote a MATLAB script for our modified hierarchical
 325 clustering technique, which is summarized in Figure 2.

326 To objectively determine the step at which to end the clustering, we use the upper-tail
 327 stopping rule of Mojena (1977). This rule states that the clustering should be cut when, for the
 328 first time, $\alpha_{j+1} > \bar{\alpha} + k(s_{\alpha})$, where $\bar{\alpha}$ and s_{α} are the mean and standard deviation of all the j
 329 previous distances of fusion. The k value is the upper-tail critical value for a t distribution that is
 330 defined by the number of original separate groups, and a choice in confidence level. Since we
 331 start with 25 separate latbins in the second round of clustering (after combining the ones with
 332 little to no data), the critical t value at the 97.5% confidence level is 2.064. In other words, we
 333 stopped the hierarchical clustering once the “closest” segments are separated by a MD that is
 334 $(2.064 * s_{\alpha})$ higher than the average of all previous steps’ distance of fusion.

335

336 4 Results

337 Bootstrapped means and standard errors of the new segmentation scheme are given in
 338 Appendix 2.

339 **4.1 Statistical test of the previous segmentation scheme**

340 Our Hotelling's T^2 tests indicate that all four of the segments defined by Schmidt et al.
341 (2008) are statistically distinct for mafic and primitive compositions (Table 2); for all neighboring
342 segments, $p \ll 0.05$. Bootstrapped MD values range from 2.5 to 3.1 for mafic compositions and
343 2.3 to 4.4 for primitive compositions. These MDs indicate that for mafic and primitive
344 compositions, the Central and South Segments are less distinct than the other pairs (MD=2.5 and
345 2.31, respectively). The North and Columbia Segments are most dissimilar with MD values of
346 3.1 and 4.4 for mafic and primitive compositions, respectively.
347

348 **4.2 The new statistically-derived segmentation scheme**

349 Using our modified
350 hierarchical clustering
351 technique, we establish a new
352 statistically-based segmentation
353 scheme for the Cascades arc
354 (Fig. 4). Based on the upper tail
355 stopping rule of Mojena
356 (1977), we terminate the
357 second stage of clustering after
358 12 steps (Fig. 3), at which point
359 the Mahalanobis distance of
360 fusion (4.9) exceeded the
361 critical value (4.8). At this
362 step, we have six clusters of
363 data, with MD values that range
364 between 3.3 and 15.9. Cutting the clustering process at this step leaves one solitary latbin, the
365 region that includes the Columbia River (45.5-45.75°N), without a cluster. To avoid an unusual
366 segment that spans only a quarter degree latitude and includes only 25 samples, we chose to add
367 it to the cluster to the south, as it produces larger MD between the two neighboring segments
368 (MD=3.6) than if we had added it to the north (MD=3.1).

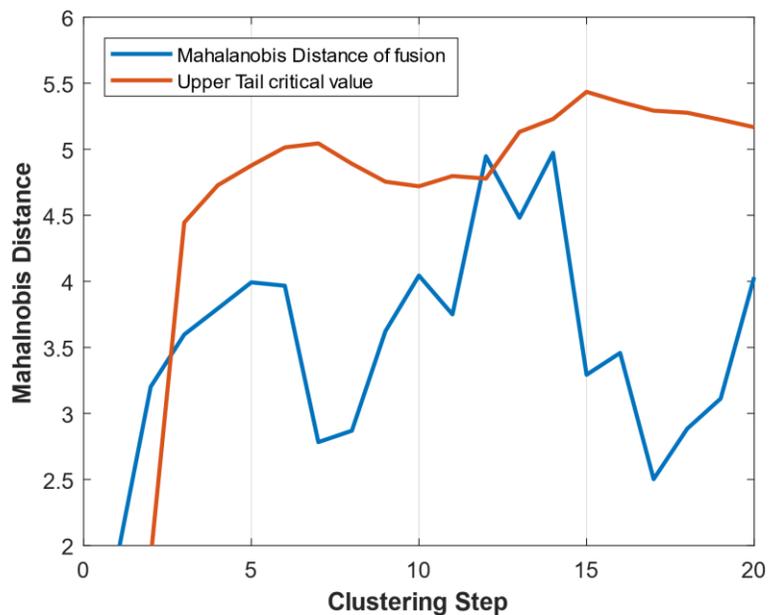


Figure 3: Methodology used to determine the step at which to end the hierarchical clustering. The Upper-tail stopping rule of Mojena (1977) states that we should end the clustering after the 12th step, as that is the first time that the MD of fusion (blue line) is greater than the critical value (red line).

369 Thus, we propose a new scheme for the Cascades arc with seven segments, hereafter
 370 referred to as the Garibaldi (49.75-51°N), Baker (48.5-49.75°N), Glacier Peak (47.75-48.5°N),
 371 Washington (45.75-47.75°N), Graben (44.25-45.75°N), and South (41.25-44.25°N) Segments
 372 (Fig 4). Hotelling's T² tests indicate that for all compositions, p<<0.05, and thus, these new
 373 segments are all statistically distinct from each other (Table 2). MD values for mafic
 374 compositions range between 3.6 and 16.0, with the largest difference between the Baker and
 375 Glacier Peak Segments (MD=16.0) and Garibaldi and Baker Segments (MD=10.0). The smallest
 376 distinction is between Washington and Graben Segments, with a MD of 3.6.

Table 2: Hotelling's T² test results for neighboring segments of our new segmentations scheme (left) compared to those of Schmidt et al., 2008. We used the same data for each scheme and used the same Monte Carlo bootstrap methods. All neighboring segments have p<<0.01, indicating that both schemes create statistically distinct segments. However, T² values, F-values, and Mahalanobis distances (MD) between segments are much higher in the new scheme indicating that it creates more statistically distinct segments.

	New Segments					Schmidt et al., 2008		
	Garibaldi vs. Baker	Baker vs. GP	GP vs. WA	WA vs. Graben	Graben vs. South	North vs. Columbia	Columbia vs. Central	Central vs. South
n	157	98	686	887	1,191	1,035	1,565	999
MD	10.0	16.0	7.3	3.6	4.5	3.1	2.6	2.5
T ²	3,142	6,229	2,671	2,392	4,124	1,651	2,678	1,244
T ² critical	40	40	40	40	40	40	40	40
F	97	169	95	86	149	60	98	45
F critical	1.6	1.6	1.5	1.5	1.5	1.5	1.5	1.5
p-value	<<0.01	<<0.01	<<0.01	<<0.01	<<0.01	<<0.01	<<0.01	<<0.01

377

378 5 Discussion

379 5.1 Comparison of segmentation schemes

380 The primary objective of partitioning the arc into segments is to explore the causes for
 381 the geochemical differences between them. Thus, it is most useful if the partitioning is done such
 382 that the geochemical differences between segments is maximized. Although the segments
 383 defined by Schmidt et al. (2008) are statistically different from each other, our new statistically-
 384 derived segments are up to 6.3 times more geochemically distinct than the previous version.
 385 Thus, our new objective scheme better maximizes the differences between neighboring segments
 386 and is therefore better suited for partitioning the arc for compositional comparisons.

387 The new segmentation also provides new insight into longstanding issues related to
 388 Cascades arc volcanism and magma sources. For example, the marked change in the strike of the

389 arc near Mount Baker and Glacier Peak are typically used to colloquially subdivide the arc into
 390 the Garibaldi Volcanic Belt to the north and the High Cascades to the south (Mullen and Weis,
 391 2015), however, the border between these portions of the arc is point of contention that may be
 392 resolved by our objective statistical approach. Recent high precision Sr, Nd, Pb, and Hf isotopic

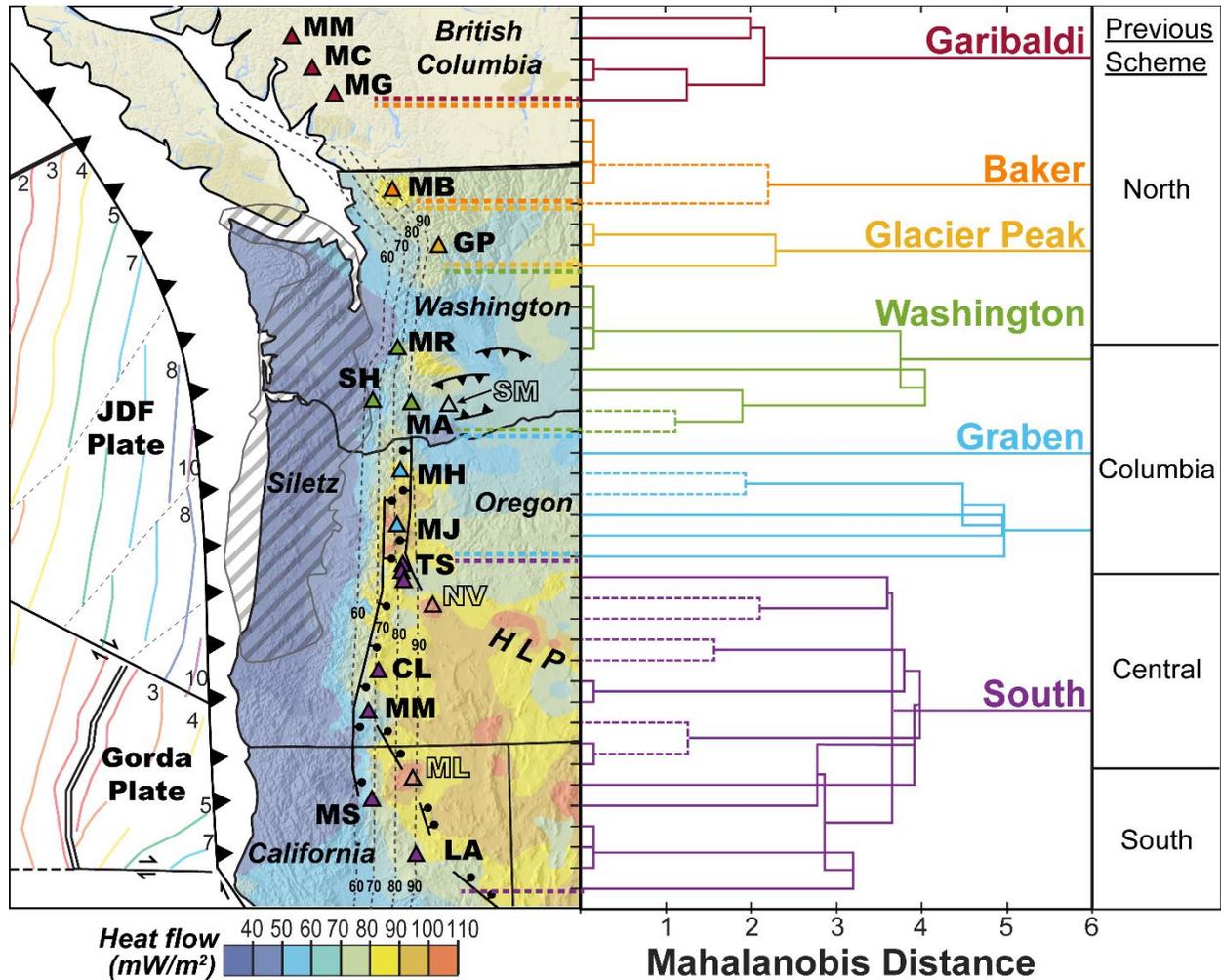


Figure 4: Dendrogram (right) showing the MD at which each latbin was clustered during the modified hierarchical clustering. Latbins that were combined in the first round of clustering (15 elements) are designated by dashed lines. In some cases, after a new cluster was formed at a higher MD, the resulting cluster became more similar to another and was then combined at a lower MD than the prior step. This leads to crossing dendrogram branches. Final segments are designated by color and can be compared to the previous scheme of Schmidt et al. (2008) on the far right. The map (left) summarizes various along-strike differences that may lead to compositional variability of the Cascades arc. Approximate age of Juan de Fuca (JDF) and Gorda plates, shown as colored lines, are from Wilson (2002). Estimated extent of the Siletz Terrain is from Phillips et al. (2017). Heat flow data is from Ingebritson and Mariner (2010). Depth of the subducting slab is estimated by McCrory et al. (2012). General locations of major faults are from Schmidt et al. (2008). General location of the High Lava Plains (HLP) is also shown. Major stratovolcanoes are shown with triangles, colored by the new segmentation scheme. From north to south: Mount Meager (MM), Mount Cayley (MC), Mount Garibaldi (MG), Mount Rainier (MR), Mount St. Helens (SH), Mount Adams (MA), Mount Hood (MH), Mount Jefferson (MJ), Three Sisters (TS), Crater Lake/Mazama (CL), Mount McLoughlin (MM), Mount Shasta (MS), and Lassen Peak (LA). Rear-arc volcanoes, including Simcoe volcanic field (SM), Newberry (NV), and Medicine Lake (ML), which were not used to create the new scheme, are shown as empty triangles.

393 work finds significant differences between the Garibaldi and Cascades arcs and suggests that
394 they are fed by isotopically distinct mantle sources and should thus be considered separate arc
395 segments (Mullen et al., 2017). Our study, which utilizes a much larger major and trace element
396 dataset agrees with this distinction, showing statistically significant differences between the
397 Garibaldi volcanic belt (north of the US-Canada border) and the High Cascades to the south.
398 While multiple studies consider Glacier Peak to be part of the Garibaldi belt (Hildreth, 2007;
399 Schmidt et al., 2008; Mullen and Weis, 2015), Mullen et al. (2017) choose to reclassify it to be
400 part of the High Cascades based on isotopic data. However, our results indicate that Glacier Peak
401 and Mount Baker are compositionally distinct from both the Garibaldi Segment and the
402 Washington Segment of the High Cascades to the south, as well as from each other. In fact, these
403 are the most statistically distinct portions of the arc (MD=16 and MD=10). This distinction is
404 important as it implies that these two transition volcanoes result from different processes or
405 source conditions than those to both the north and the south; this will be explored further in the
406 following section.

407 In addition to considering Mount Baker and Glacier Peak to be disparate segments, our
408 scheme differs from that of Schmidt et al. (2008) by several other key features. Our results
409 indicate that volcanic rocks north of the Columbia river (Washington Segment) and those south
410 of the river are statistically distinct from one another (MD=3.6), despite having been grouped
411 together within the Columbia Segment of the previous study (Fig. 4). Furthermore, because we
412 used a comprehensive dataset that includes data from the many smaller mafic vents between the
413 major stratovolcanoes, we can better define the boundaries between all segments. For example,
414 while mafic rocks in the vicinity of Mount Rainier were not included within any segment by the
415 previous study, our results indicate that they are statistically more similar to those to the south
416 and can therefore be considered part of the Washington Segment. Finally, although Schmidt et
417 al. (2008) drew a boundary near the Oregon-California border based on data from rear-arc
418 Medicine Lake, there was no data from the over 70 vents (Hildreth, 2007) located within the 140
419 km region between Crater Lake and Medicine Lake. Our study, which utilizes nearly 200
420 samples from that region, finds that they are statistically similar to those that surround Crater
421 Lake. In fact, we find that bootstrapped mean compositions of all latbins from Lassen Peak to the
422 Three Sisters Region are similar enough to warrant placing them within the same segment (Fig.
423 4).

424 We also note that whereas Schmidt et al. (2008) used data from rear-arc volcanoes to
425 partition the arc, our study chose to exclude these data. This continues a longstanding pattern in
426 the Cascades where many authors consider Simcoe, Newberry, and Medicine Lake to be rear-arc
427 or back-arc volcanoes that should be distinguished from those the arc-front (Hildreth, 2007;
428 Donnelly-Nolan et al., 2008; Long et al., 2012), but others treat these as part of the arc-front
429 (Guffanti and Weaver, 1988; Blakely et al., 1997; Schmidt et al., 2008; Mullen et al., 2017). Our
430 Hotelling's T^2 tests indicate that all three are statistically dissimilar than the adjacent arc-front
431 segments that lie to the west, with bootstrapped MD values of 4.2, 3.6, and 4.0 for Simcoe,
432 Newberry and Medicine Lake, respectively. Thus, we suggest that future regional studies treat
433 these as rear-arc volcanic centers that have significantly different compositions, and thus
434 processes of magma generation, compared to the adjacent arc-front volcanoes.

435

436 ***5.2 Compositional differences between segments***

437 By calculating the bootstrapped means of our comprehensive dataset, we have removed
438 significant sampling bias and therefore established mean compositions that best represent each of
439 our new arc segments as a whole. From this we can explore the bulk compositional differences
440 between each arc segment and infer better the regional processes affecting them, rather than local
441 processes at individual volcanoes. Although previous studies have explored the causes of
442 compositional variability within the Cascades arc (e.g. Bacon *et al.*, 1997; Green and Harry,
443 1999; Leeman *et al.*, 1990, 2005; Mullen and Weis, 2015; Schmidt *et al.*, 2008), our study differs
444 in that we are examining differences between the unbiased mean compositions of statistically
445 distinct segments to elucidate causes for these differences.

446

447 ***5.2.1 Distribution of primitive Cascades arc endmembers***

448 Several end-member primitive basalt compositions have been proposed for the Cascades
449 including arc-typical calc-alkaline basalts (CABs), low-K tholeiites (LKTs) (sometimes referred
450 to as high alumina olivine tholeiite; e.g. Bacon *et al.*, 1997; HART *et al.*, 1984), and intraplate-
451 type basalts (IPBs) (sometimes called ocean island, within-plate, or HFSE-type basalts; e.g.
452 Conrey *et al.*, 1997; Schmidt *et al.*, 2008). A detailed description of each of these Cascades arc
453 end-members is given in Mullen et al. (2017). The differing major and trace element
454 compositions of these endmembers are suggested to be the result of different mantle processes or

455 compositions (Leeman et al., 1990; Bacon et al., 1997; Conrey et al., 1997; Leeman et al., 2005;
456 Schmidt et al., 2008; Rowe et al., 2009; Mullen et al., 2017; Carlson et al., 2018). Although these
457 studies have demonstrated that all endmember compositions exist within each portion of the arc,
458 no previous study has ascertained the relative proportion of these compositions using a
459 comprehensive dataset that is statistically treated to mitigate sampling bias.

460 We classified 628 of the 1,064 primitive samples in our dataset based on the
461 compositional definitions (Table 3) given in Schmidt et al. (2008) and Leeman et al. (2005).
462 Many samples were mixtures of the endmembers and could not be definitively classified as a
463 single endmember type. One common mixture were basalts that had LKT-like low K_2O (<0.4
464 wt.%) and K_2O/TiO_2 (<0.4) but were enriched in subduction fluid-mobile elements such as Ba
465 and Sr similar to CABs. Due to their abundance, we chose to create a separate category of
466 “High-Ba LKTs” when calculating proportions.

Table 3: Criteria used to classify primitive samples into Cascades endmembers. Similar criteria were used by Leeman et al. (2005) and Schmidt et al. (2008).

Primitive Type	K_2O	K_2O/TiO_2	Ba/Nb	Sr/Y	Nb/Zr	$(K/Nb)_N$
CAB	> 0.5 wt.%	> 0.4	> 20	> 15	< 0.09	> 0.2
High-Ba LKT	< 0.5 wt.%	< 0.4	> 20		< 0.09	> 0.2
LKT	< 0.5 wt.%	< 0.4	< 20	< 20	< 0.09	> 0.2
IPB	> 0.25 wt.%	> 0.4	< 20		> 0.08	< 0.25

467 Utilizing the Monto Carlo bootstrap methodology to remove sampling bias, we observe
468 significant inter-segment differences in the distribution of primitive lava types (Fig. 5). The
469 Garibaldi Segment consists almost entirely (86%) of IPB-type basalts, while these are
470 completely absent in the Baker and Glacier Peak Segments. In these latter two, more arc-typical
471 CAB-types are most common (75% and 62%, respectively). IPB-type basalts are also relatively
472 common in the Washington (37%) and Graben Segments (33%). True LKT basalts are entirely
473 absent in the northern portion of the Cascades and Garibaldi Segment and become quite common
474 in the southern half of the arc, which is undergoing overall extension (Wells et al., 1998;
475 McCaffrey et al., 2007). This extension, which is likely also responsible for higher heat flow in
476 the southern arc (Fig. 4) may also allow more decompression-driven LKT-type melts form and
477 erupt (Schmidt et al., 2008; Ingebritsen and Mariner, 2010; Mullen et al., 2017).

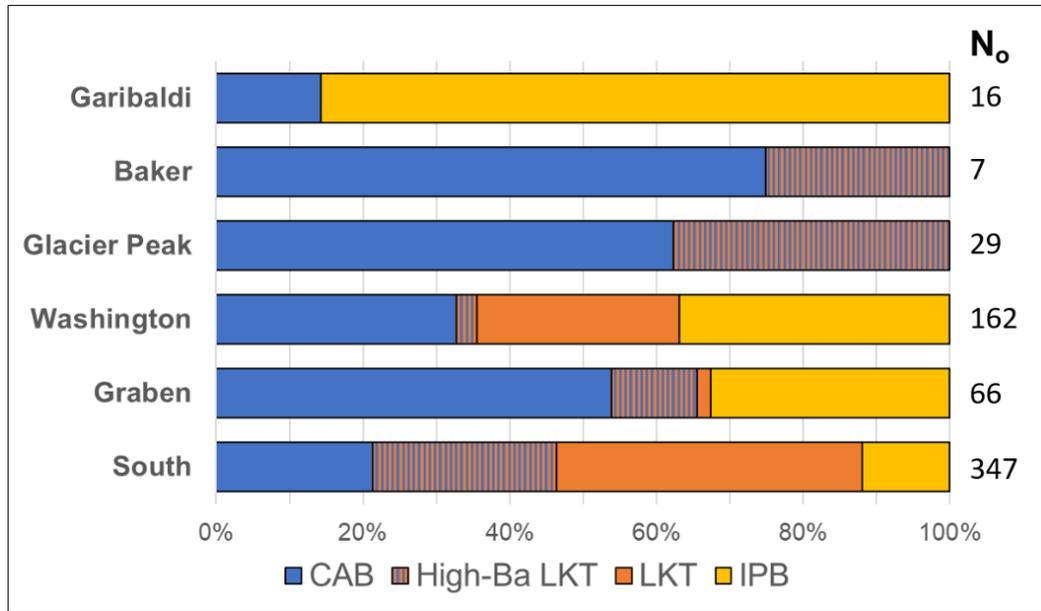


Figure 5: Posterior distribution of primitive lava types for the new segments. The total number of samples in the prior dataset (N_o), are shown on the right.

478 While some authors suggest that the mantle beneath the Cascades may be inherently
479 heterogenous (e.g. Bacon et al., 1997), Mullen et al. (2017) find that there are no isotopic
480 differences between these endmembers and suggest an isotopically homogeneous mantle source
481 for all endmember types. Reiners et al. (2000) and Rowe et al. (2009) demonstrate that Cascades
482 CABs and LKTs can both be produced from the same initial composition, simply by varying the
483 flux of fluids and degree of melting. Thus, compositional differences between Cascades arc
484 endmembers are likely to be primarily the result of differing processes of mantle melting and
485 variable degrees of modification by the subduction components (Mullen et al., 2017).

486 In addition to comparing the relative proportions of these endmembers, our study allows
487 us to compare the bootstrapped mean compositions, which can be thought of as a representation
488 of the unbiased bulk mixture of various primitive lava types, and thus, the relative contributions
489 of the process that lead to their formation. In addition, our Monte Carlo approach allows us to
490 calculate confidence intervals of these mean compositions which provides the unique
491 opportunity to examine both the inter-segment differences in mean compositions and the
492 unbiased variance in compositions within each segment. In the following sections we will
493 explore these differences with respect to subduction fluid contribution, depth and processes of
494 mantle melting, and mantle fertility.

495

496 5.2.1 Subduction fluid signature

497 The Glacier Peak, Mount Baker and South Segments demonstrate the largest influence of
498 fluid-flux melting. These are each characterized by an arc-typical negative Nb and Ta anomaly
499 (Fig. 6), as well as a relative enrichment in LILE, such as high Sr/P, Ba/Nb (Fig. 7) and Ba/Ce,
500 which have been shown to be good indicators of the influence of slab fluids (Pearce, 1982; Borg
501 et al., 1997; Pearce and Stern, 2006; Ruscitto et al., 2010). Intense fracturing and internal
502 deformation of the subducting Gorda Plate due to motion along the Mendocino Fracture Zone
503 (Wilson, 2002) may lead to increased fluid penetration and higher delivery of subduction fluids
504 into the South Segment (Grove et al., 2003; Schmidt et al., 2008). Other studies have previously
505 demonstrated the more hydrous nature of lavas and melt inclusions near Lassen Peak (Borg et
506 al., 1997) and Mount Shasta (Sisson and Layne, 1993; Grove et al., 2002). It has also been
507 suggested, based on radiogenic Sr, Nd, and Pb isotopes in these primitive lavas, that some of the
508 fluid-flux signature could be from prior metasomatism of the mantle by much older subduction
509 fluids (Borg et al., 1997; Borg et al., 2002; Carlson et al., 2018). Subduction rates were much

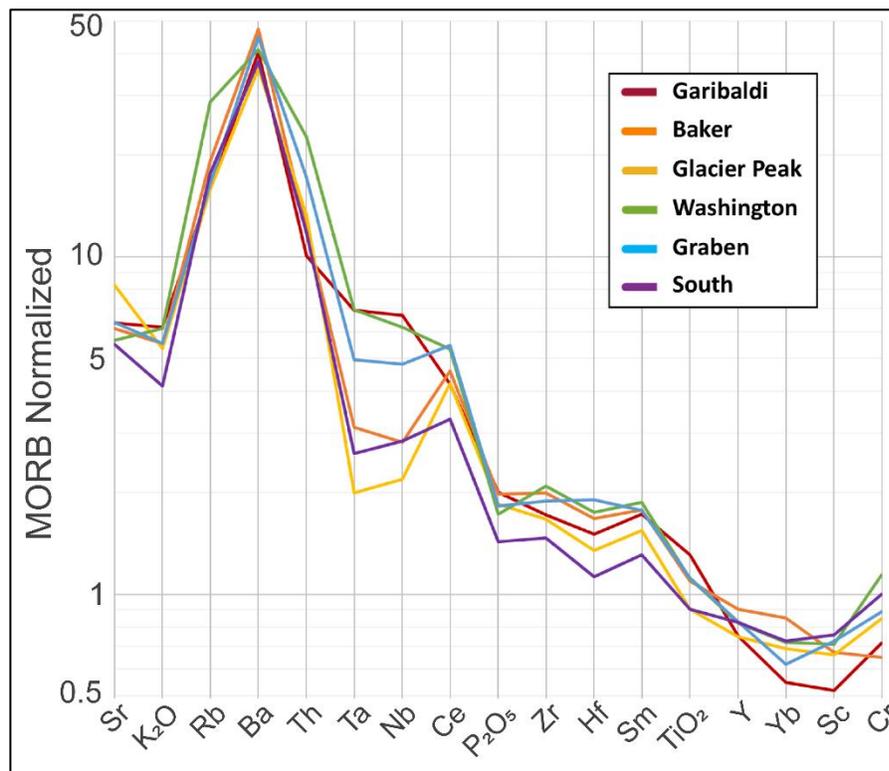


Figure 6: "Spider diagram" showing the MORB-normalized (Pearce, 1983) bootstrapped mean concentrations of minor and trace elements. For clarity, confidence intervals are not shown. However, trace element differences discussed in the text are statistically significant. Segment color scheme is the same as in Fig. 4.

510 faster in the past (Verplanck and Duncan, 1987), which would have caused sufficient heating and
511 dehydration of the slab to take place further inboard of the subduction zone (Leeman et al.,
512 2005).

513 In addition, the South Segment may record the largest degree of mantle melting, as it has
514 the flattest REE and thus lowest Ce/Yb (Fig. 7), which is in stark contrast to the neighboring
515 Graben Segment, that has the steepest REE pattern (Fig. 8). This is consistent with
516 thermobarometry results of Ruscitto et al. (2010) that indicate higher degrees of partial melting
517 (>20 %) of a more hydrous source (>0.7 wt. % H₂O) in the Mount Shasta region compared to
518 volcanoes of the Graben Segment (9-11 % melting, 0.4-0.56 wt. % H₂O). The relatively flat
519 REE patterns of the South Segment are not likely to be simply the result of shallower melting, as
520 HREE and Y abundances are similar to Graben segment, and previous studies have shown

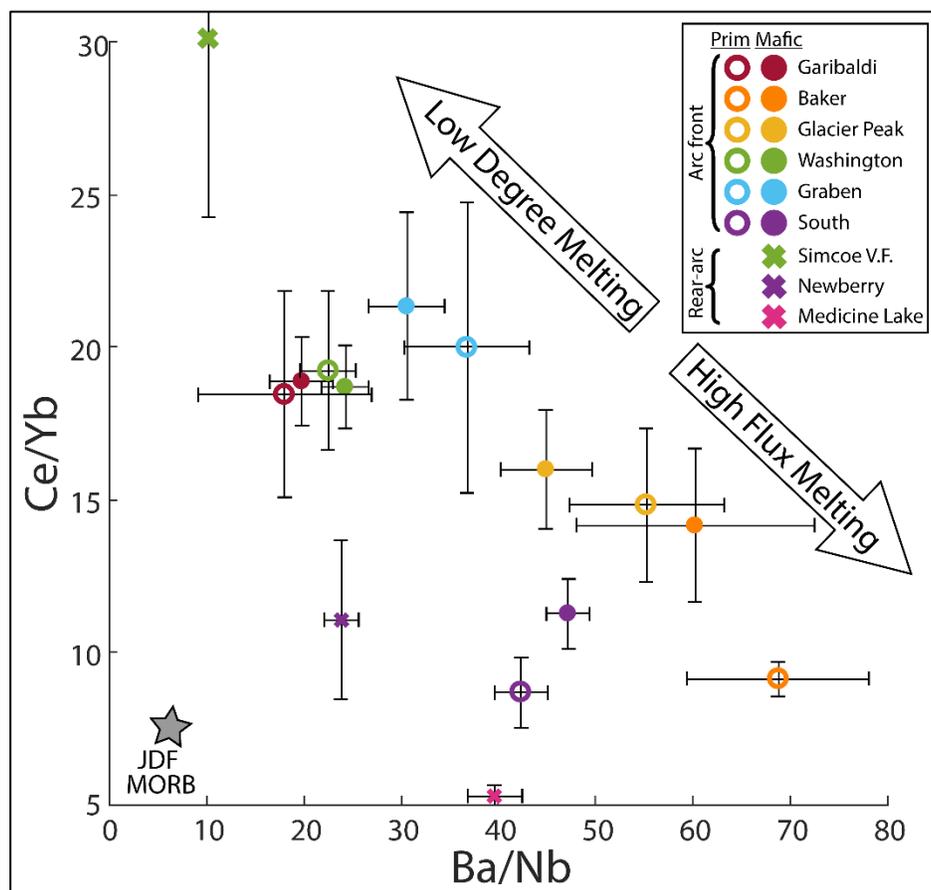


Figure 7: Ba/Nb vs. Ce/Yb diagram of bootstrapped mean values and 95% confidence intervals for primitive (open circles) and mafic (closed) compositions of the new segments. Mafic compositions for rear-arc volcanoes are also shown by the x symbol. The mean value for Juan de Fuca MORB (Gill et al., 2016) is also shown. Gorda MORB has Ce/Yb value (3.5) that could not be shown on this scale.

521 similar melt segregation depths for volcanoes from these two segments (Elkins Tanton et al.,
522 2001; Leeman et al., 2005; Ruscitto et al., 2010; Till et al., 2013). Furthermore, magnetotelluric
523 (MT) studies indicate that the southern portion of the arc exhibits the highest supra-slab MT
524 resistivity, interpreted to be the highest degree of flux melting in the Cascades arc (Wannamaker
525 et al., 2014).

526 Primitive lavas from the Glacier Peak region are the most enriched in Sr, Th, U, and Pb,
527 both in terms of the elemental concentration, as well as in ratios where a high field strength
528 element such as Nb or Ta is the denominator. These particular elements have been demonstrated
529 to have fluid-rock partition coefficients that are highly temperature dependent, such that Sr, Th,
530 and U are fluid-immobile ($D=0.3, 0.1, 0.1$ respectively) at lower temperatures (i.e. 700°C at 4

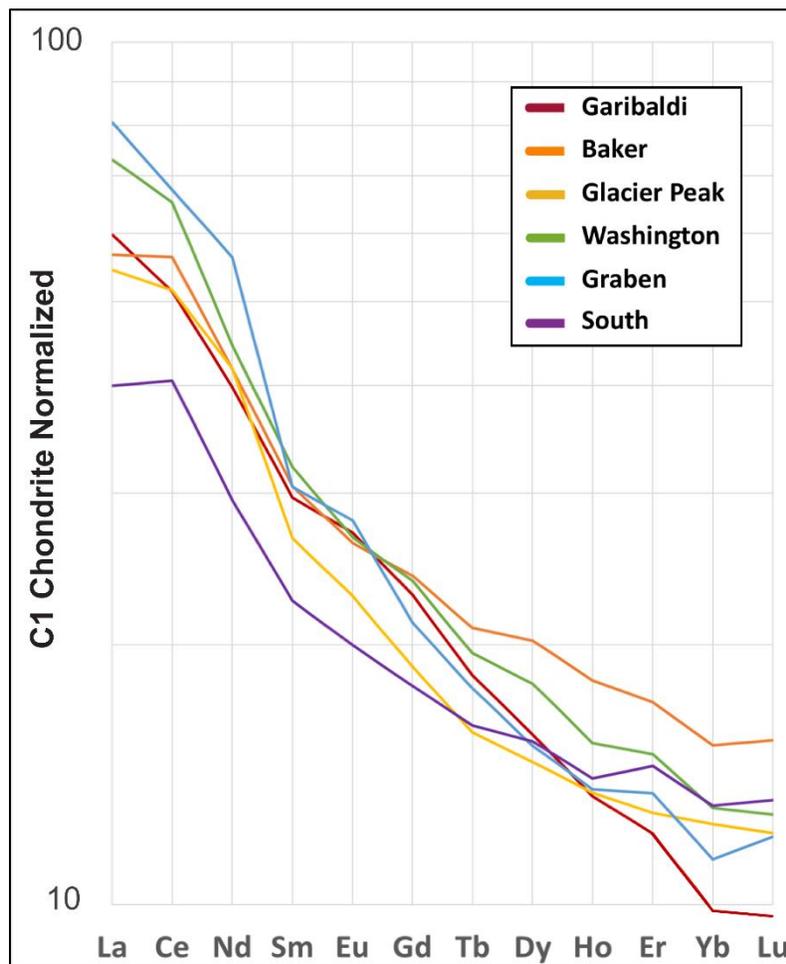


Figure 8: REE plot of the C1-Chondrite normalized (Sun and McDonough, 1989) bootstrapped mean values for the new segments. For clarity, confidence intervals are not shown. However, differences in REE discussed in the text are statistically significant.

531 GPa) but then become highly fluid-compatible ($D=22,23,17$, resp.) at higher temperatures
532 (1100°C) (Kessel et al., 2005). Thus, the enrichment of these elements in Glacier Peak, which
533 lies further east than any other Cascades volcano, may be the result of the input of deeper and
534 hotter supercritical subduction fluids. In fact, McCrory et al. (McCrory et al., 2012) estimate that
535 the volcano is situated approximately 95 km above the Juan de Fuca slab, whereas the
536 neighboring volcanoes, Mount Baker and Mount Rainier are 80 and 70 km above the slab,
537 respectively. This composition-depth relationship can also be seen at Medicine Lake, a southern
538 rear-arc volcano that lies approximately 85 km above the slab (McCrory et al., 2012) and has
539 higher Th, U, Th/Nb and Th/Ta than the arc-front South segment.

540 The Garibaldi Segment exemplifies the lowest fluid-flux signal in the arc (lowest Ba/Nb,
541 Th/Nb, and high HFSE), which may result from the slab being young and hot (Wilson, 2002)
542 which would cause dehydration of the slab significantly trench-ward of the arc (Schmidt et al.,
543 2008). The Washington Segment also has a reduced fluid signature, lacking the arc-typical Nb-
544 Ta anomaly (Fig. 6) and the second lowest Sr/P, Ba/Nb, Pb/Ce, and Th/Ta ratios.

545 Although the Graben Segment has a reduced fluid component compared to that of the
546 Glacier Peak, Mount Baker, and South Segments, it does have a small Nb-Ta anomaly and
547 significantly higher Ba/Zr and Sr/P than the neighboring Washington Segment. In addition, the
548 Graben Segment has the highest primitive Cs/Rb, $\text{K}_2\text{O}/\text{Rb}$, and La/Sm, indicating that there may
549 be a larger contribution from subducted sediment (Labanieh et al., 2012), as offshore drill cores
550 of Cascadia sediment have elevated values for these ratios (Carpentier et al., 2014). Furthermore,
551 low Pb/Ce indicates that the sediment contribution is likely as melt rather than aqueous fluid
552 (Brenan et al., 1995; Kelemen et al., 2003), as Pb would be more strongly partitioned into the
553 fluid. However, Ce does become more compatible than Pb in supercritical fluid at pressure >6
554 GPa and temperature above $1,000^{\circ}\text{C}$ (Kessel et al., 2005). Our segmentation scheme places the
555 boundary between the Graben and Washington Segments at the approximate latitude of the pole
556 of rotation of the Cascades fore-arc block which causes overall compression in the Washington
557 Segment and extension in the Graben Segment (Wells et al., 1998; McCaffrey et al., 2007;
558 Labanieh et al., 2012). A marked increase in hydrothermal heat discharge and crustal heat flow
559 (Fig. 4) south of 44.75°N latitude (near Mount Jefferson) is consistent with extensional stresses
560 (Ingebritsen and Mariner, 2010) or increased flux of basalt and magmatic heat from the mantle.
561 Extension in the Graben Segment has been suggested to induce decompression mantle melting

562 (Conrey et al., 2002; Conrey, 2004) or focus upwelling mantle that is already undergoing
563 decompression melting directly into the arc (Till et al., 2013). We propose that the increased
564 fluid-flux signature in the Graben Segment could be the result of regional extension-driven
565 decompression melting of lithospheric or asthenospheric mantle which was previously
566 metasomatized by ancient subduction fluids and sediment melt. A similar process for the genesis
567 of CAB-like signatures has been proposed elsewhere in the arc (Borg et al., 1997; Borg et al.,
568 2002; Leeman et al., 2005), in the back-arc (Carlson et al., 2018), and in the Great Basin (Harry
569 and Leeman, 1995). This provides a mechanism for increasing the fluid signature in the Graben
570 Segment relative to the Washington Segment despite being a similar distance from major slab
571 termini and similar subducted slab age and depth (Wilson, 2002; McCrory et al., 2012). This
572 ancient metasomatism would also help explain the radiogenic Pb and Sr isotope signature of the
573 primitive lavas in the region, although it should be noted that the Washington Segment has a
574 slightly more radiogenic Pb isotopic signature, and isotopic data for the Graben Segment are
575 scarce (n=4).

576

577 *5.2.2 Depth of mantle melting and slab melting*

578 Differences in REE abundances between segments also suggest there are differences in
579 the depth of melting and the degree to which slab melts contribute. The Garibaldi Segment of the
580 arc has a bootstrapped mean composition that suggests greater involvement of garnet as a
581 residual phase, thereby indicating deeper mantle melting than elsewhere in the arc. The segment
582 has the lowest concentration of Y, Yb, Sc, Cr (Fig. 6), and has the steepest HREE depletion (Fig.
583 8). Furthermore, the bootstrapped mean occupies a unique position on a plot of Dy/Yb vs.
584 Dy/Dy* that is separate from the rest of the arc (Fig. 9). Mantle melting with amphibole (or
585 clinopyroxene) residual would lead to a more concave MREE pattern (decrease in Dy/Dy*) with
586 only a minor decrease in Dy/Yb. A garnet residuum leads to HREE depletion relative to MREE
587 (large increase in Dy/Yb), with little change to the concavity of the REE (Dy/Dy*) (Davidson et
588 al., 2013). While the rest of the arc lies within the variably enriched MORB-like field, the
589 Garibaldi Segment lies at much higher Dy/Yb, indicating that it alone is characterized by deeper
590 melting.

591 In addition, the Garibaldi Segment has the highest Nb/Zr and Nb/Yb (Fig. 10) of any
592 segment, which may indicate a more enriched, IPB-like source (Pearce and Stern, 2006). In

593 stark contrast, the neighboring segments to the south seem to lack the deep and enriched mantle
594 melting signature. The Mount Baker and Glacier Peak regions have the highest Y, Yb, and Y/Zr
595 values and relatively low Dy/Dy*, Nb/Yb and Nb/Zr (Figs. 9 and 10) indicating a more depleted
596 source in which garnet is not likely a residual phase. Deep melting of an enriched mantle source
597 seen in the Garibaldi Segment may be the result of toroidal flow of enriched sub-slab mantle
598 around the northern edge of the Juan de Fuca plate, which becomes progressively diluted
599 southwards, as suggested by Mullen and Weis (2015). Our results indicate that the magnitude of
600 southward depletion is statistically significant over the one-degree latitude that separates Mount
601 Garibaldi and Mount Baker, thus leading to a segment boundary between them.

602 Slab melting could also contribute to the geochemical signature of the Garibaldi
603 Segment. In addition to having the highest Dy/Yb, the segment has the second highest Sr/Y ratio
604 of any portion of the arc, a signature which has been used by many authors to suggest slab
605 melting in arcs worldwide (Pearce and Peate, 1995; Stern and Kilian, 1996; Kelemen et al.,

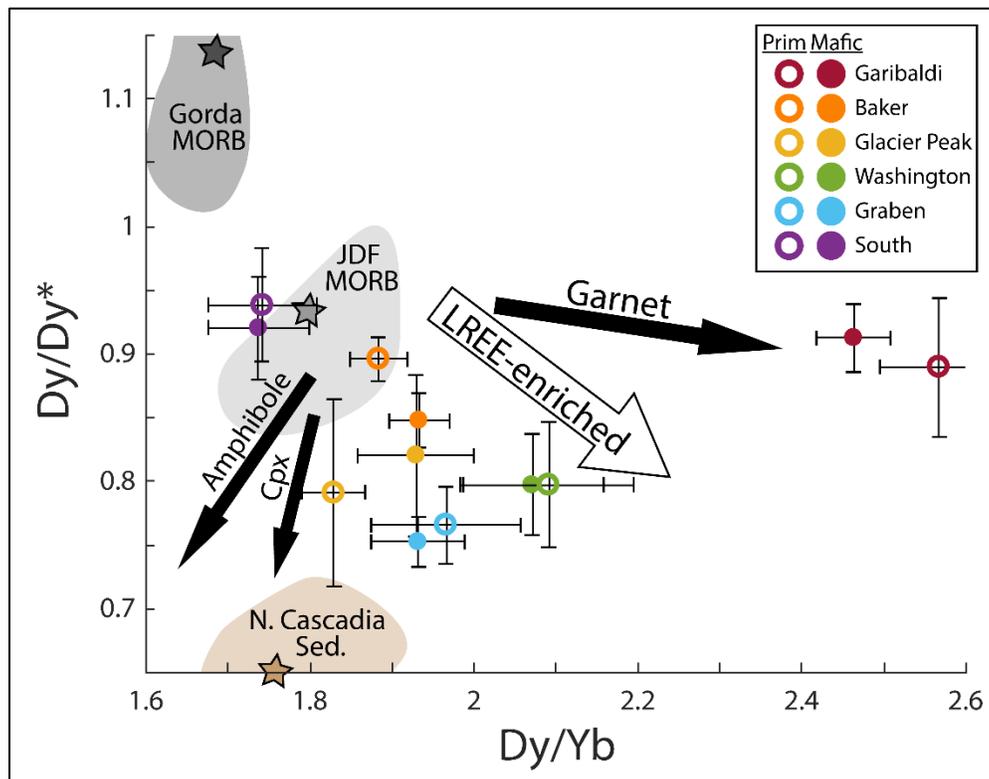


Figure 9: Dy/Yb vs. Dy/Dy* as defined by Davidson et al. (2012). Bootstrapped means of primitive and mafic compositions are shown. Fields of data from Gorda MORB (Davis et al., 2008), Juan de Fuca MORB (Gill et al., 2016), and offshore North Cascadia sediment (Carpentier et al., 2014) are also shown, along with the mean value (stars). Effect of enrichment of LREE is shown. Arrows indicate the effect of amphibole, clinopyroxene or garnet as residual phases during melting (Davidson et al., 2013).

606 2003). Slab melting would be a reasonable process in this portion of the arc, since the slab is
607 much deeper (McCroory et al., 2012), and younger (3-5 Ma, Wilson, 2002). Additionally, toroidal
608 flow of hot mantle has been suggested to cause thermal erosion of the edges of slabs (Thorkelson
609 and Breitsprecher, 2005). However, we may expect slab melting to produce higher SiO₂ as well
610 as larger enrichments in Zr and Hf than we see in the Garibaldi Segment (Pearce and Peate,
611 1995).

612 Although Walowski et al. (2015) demonstrated that slab melting likely occurs in the
613 southernmost Cascades beneath Lassen Peak, our bootstrapped data indicate that this may not be
614 a dominant process throughout the entire South Segment, since the bootstrapped mean has high
615 HREE, Y, Cr, and Sc, and the lowest Dy/Yb and Sr/Y of any segment. This is true even if we
616 calculate bootstrapped mean of only the California portion of the Cascades. Thus, it is possible
617 that slab melting in the South Segment is only localized to the region beneath Lassen Peak,
618 where larger slab depths and hot toroidal flow may allow for more slab melting.

619

620 *5.2.3 Mantle fertility beneath the arc-front and rear-arc*

621 Although the enrichment of the Garibaldi Segment may be attributed to toroidal flow of
622 sub-slab enriched mantle around the northern slab edge, a similar mechanism cannot explain the
623 IPB-like enriched signature of both the Washington and Graben Segments which are not
624 similarly situated near the terminal edge of a slab. These segments have the second or third
625 highest concentrations of Nb, Zr, Ta (Fig. 6) and Nb/Yb, Nb/Zr (Fig. 10), as well as the steepest
626 REE patterns (Fig. 8) and thus highest Ce/Yb (Fig. 7) of the arc-front. However, the Simcoe
627 Volcanic Field, which lies in the rear-arc behind the Washington Segment, is more enriched than
628 anywhere in the arc-front (Fig. 10). The enriched signature of the rear-arc compared to that of the
629 Washington Segment, may indicate westward flow of enriched mantle (Leeman et al.,
630 2005) which is first slightly depleted by the rear-arc volcanic field before being melted beneath
631 the arc-front. A similar pattern of depletion from the back arc to the arc-front is seen in the Izu-
632 Bonin, Scotia, and Marianas arcs (Pearce and Stern, 2006). Further evidence of the relationship
633 between the enriched rear-arc mantle and the Washington Segment is provided by Mullen et al.
634 (2017) who demonstrate that primitive lavas from Mt Adams deviate from the normal Cascades
635 arc trend in terms of Sr Nd, and Pb isotopes and instead lie on a separate “Adams array” that
636 trends toward a different Simcoe endmember. Slab-induced corner flow could provide the arc

637 with enriched mantle material from the back arc (Long et al., 2012). Alternatively, a slab gap
638 such the one suggested by Gao and Shen (2014) to underlie the latitude of Mount Hood, could
639 provide both of the arc-front segments and the back-arc region with enriched sub-slab mantle
640 material. Either mechanism of upwelling deeper fertile mantle could also help to explain the
641 relatively deep melting signature (low HREE and Y/Zr) of the Graben and Washington Segments
642 (Figs 9, 10).

643 Our results also suggest that the IPB-like composition of the Washington and Graben
644 Segments is not likely due to interaction with the accreted Siletz terrain lithosphere as previous
645 authors have suggested (Church et al., 1986; Schmidt et al., 2008). Both segments lie within the
646 Columbia Embayment, a region of accreted oceanic crust (Trehu et al., 1994), that includes the
647 Late Paleocene-Eocene Siletz Terrain, interpreted to be an oceanic large igneous province (LIP)

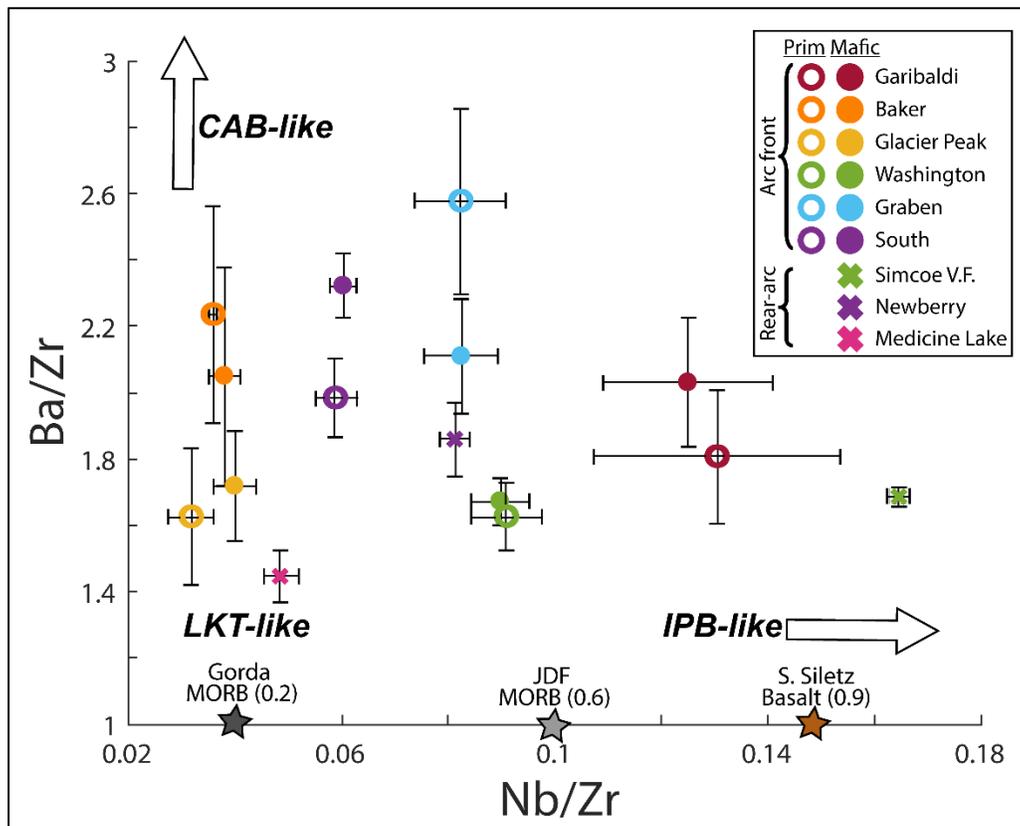


Figure 10: Nb/Zr vs. Ba/Zr of bootstrapped means of new segments and rear-arc volcanoes. Mean Nb/Zr values for Gorda MORB, JDF MORB, and Siletz basalt (south of 47°N) are depicted, and Ba/Zr values are in parentheses (Davis et al., 2008; Gill, et al., 2016; Phillips et al., 2017). Approximate locations of the three most common Cascades endmembers are shown.

648 with a plume-origin (Wells et al., 2014; Phillips et al., 2017). While some authors suggest based
649 on geophysical data that the Siletz Terrane may terminate west of the modern High Cascades

650 boundary (Finn, 1990; McCrory and Wilson, 2013; Bedrosian and Feucht, 2014), others hold
651 that Siletzia lithosphere could extend well east of the arc, near the Idaho border (Gao et al.,
652 2011). Assimilation of enriched Siletzia crust is unlikely since we would expect such
653 assimilation to cause compositional differences between the primitive and mafic composition of
654 a given segment, yet these bootstrapped means are indistinguishable for the Washington and
655 Graben segments. Furthermore, although Siletz basalts (south of 47°N) are slightly more
656 enriched Nb/Yb and Nb/Zr (Phillips et al., 2017) than the primitive compositions of either
657 Washington or Graben Segments, they are much less enriched than the Simcoe Volcanic Field
658 (Fig. 10), indicating that Siletz mantle cannot be the source of the rear arc enrichment. Thus, we
659 suggest that a westward flow of fertile mantle from the back arc is a more reasonable explanation
660 for enrichment trends of these two segments and the rear arc Simcoe Volcanic Field.

661 A similar, albeit more reduced, depletion in Nb/Zr is seen from the rear-arc Newberry
662 volcano to the arc-front South Segment (Fig. 10), indicating that such mantle flow may be
663 common in the middle portions of the arc. This mantle flow is further evidenced by trench
664 perpendicular (east-west) mantle anisotropy observed by various studies (Long et al., 2009;
665 Wannamaker et al., 2014; Long, 2016). It is possible that continuous depletion of westward-
666 flowing mantle by the High Lava Plains volcanics of eastern Oregon (Long et al., 2012; Till et
667 al., 2013) prior to being melted beneath Newberry has led it to have a more depleted signature
668 than the Simcoe rear-arc volcanics to the north.

669

670 **6. Conclusions**

671 The Cascades arc exhibits significant along-strike variability in major and trace element
672 compositions of mafic lavas, and numerous studies have proposed mechanisms such as mantle
673 heterogeneity, regional tectonics and/or geochemical differences in the overlying lithosphere or
674 subducting slab to be responsible for these compositional differences. Although considerable
675 heterogeneity exists even at a single location, partitioning the arc into compositionally distinct
676 groups allows one to explore the regional-scale causes for such differences. Schmidt et al.
677 (2008) proposed a segmentation scheme for the Cascades that provides an excellent initial
678 framework for such regional-scale studies. However, the study does not quantify differences
679 between proposed segments, and is based on a limited dataset (390 samples) which is spatially
680 biased toward only 11 arc-front locations.

681 We improve on this study by compiling a dataset of major and trace element analyses of
682 over 2,000 mafic samples and utilizing a Monte Carlo approach with bootstrap resampling to
683 reduce the inherent bias that over-sampled volcanoes have on overall trends. In doing so, we can
684 assess regional, rather than local processes. Our study develops a novel approach to assess
685 geochemical variability by partitioning the arc using entirely objective and statistically-based
686 methodology. Using this new approach, we separate the Cascades arc into 6 segments such that
687 the geochemical differences between each is maximized. Although we demonstrate that those
688 proposed by Schmidt et al. (2008) are statistically dissimilar from one another, we propose a new
689 segmentation scheme, which includes the Garibaldi, Baker, Glacier Peak, Washington, Graben,
690 and South Segments, which are up to 6.3 times more statistically distinct than the previous
691 scheme. By separating the arc into the most statistically disparate regions, we can better assess
692 the different processes that lead to geochemical heterogeneity within a single arc.

693 Our results demonstrate significant differences in mantle fertility, degree of melting, and
694 input from the slab to each of the segment regions, which are briefly summarized below and in
695 Table 4. The Garibaldi Segment is characterized by overall deeper melting of enriched mantle
696 which may be the result of toroidal flow around the northern edge of the Juan de Fuca slab. The
697 segment has the lowest fluid-flux signature, which may be due to the young (3-5 Ma) (Wilson,
698 2002) and thus hot slab, which may be largely dehydrated before the arc-front, and may cause
699 the slab to undergo partial melting. In stark contrast, the neighboring Baker Segment to the south
700 has a strong contribution from subduction fluids and is the result of melting a much more
701 depleted mantle source. Because of these distinctions, the statistical difference between the
702 Baker and Garibaldi Segments is penultimate in the arc. Thus, we suggest that Mount Baker
703 should not be considered a part of the Garibaldi volcanic belt as numerous previous authors have
704 advocated (Hildreth, 2007; Schmidt et al., 2008; Mullen and Weis, 2015; Mullen et al., 2017).
705 Moving south, the Glacier Peak Segment is also characterized by significant fluid-flux melting of
706 a depleted mantle source. However, it has the signature of much deeper fluids, consistent with its
707 eastward position, where the slab is deeper (>95 km) than any other Cascades arc-front volcano
708 (McCroory et al., 2012). In contrast, the Washington and Graben Segments are more enriched
709 which may result from slab-induced corner flow or a slab gap. The relative enrichment of the
710 rear-arc Simcoe Volcanic Field indicates that the mantle source of such enrichment is not
711 associated with the accreted Siletz Terrain LIP. Although the fluid-flux signature of both

712 segments is relatively low, the Graben Segment is more enriched in fluid mobile elements as
713 well as potential sediment melt indicators. We suggest that this difference between the two is a
714 result of extension in the Graben Segment which allows for more melting of mantle which had
715 been previously metasomatized by ancient fluids and sediment melts. Finally, the South Segment
716 has the largest CAB-like fluid-flux melting signature, which could partially result from increased
717 fluid penetration into the highly fractured Gorda plate. Alternatively, higher extension rates in
718 the South could cause melting of previously-metasomatized mantle at a higher degree than we
719 propose for the Graben Segment. Such a mechanism, which has also been suggested by previous
720 authors (Borg et al., 1997; Borg et al., 2002; Carlson et al., 2018), would explain the higher fluid
721 signature, higher degree melts, more radiogenic Sr, Pb, and Nd isotopic compositions observed
722 in the South Segment. Slab melting, as proposed for the Lassen Peak area (Walowski et al.,
723 2015), does not appear to be common signature observed elsewhere in the segment, and may be
724 localized to the southernmost volcanic edifice, where the slab is deeper and toroidal flow around
725 the slab edge could bring hot decompression melts that could erode the slab edge (Thorkelson
726 and Breitsprecher, 2005).

727 In this study, we have demonstrated the advantage of approaching important petrologic
728 questions, such as along-arc variability, using statistically rigorous methodology. With the
729 continual growth of online data repositories, scientists now have access to massive datasets that
730 can allow for much more detailed studies of particular regions or at the global scale. While these
731 data can be quite powerful, great care must be taken in assessing the quality of data and reducing
732 sampling bias. More complete and evenly-distributed sampling of arcs worldwide can allow
733 future studies to use our new methodology to investigate other compositionally heterogeneous
734 arcs in statistically robust manner.

735

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