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First 15 probability-based multidimensional tectonic discrimination diagrams for intermediate magmas and their robustness against postemplacement compositional changes and petrogenetic processes

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Abstract: Although for ultrabasic and basic magmas a plethora of tectonomagmatic diagrams have been used, with the exception of one bivariate diagram for refined tectonic setting of orogenic andesites, none is available for highly abundant intermediate magma. We present 3 sets of discrimination diagrams obtained from the correct statistical methodology of log,-ratio transformation and linear discriminant analysis. All major element log -ratio variables in 3664 samples, only immobile major and trace element log -ratio variables in 1858 samples, and immobile trace element log-ratio variables in 1512 samples were used. These diagrams with probability-based tectonic field boundaries and high success rates (about 69%-96%, 63%-100%, and 64%-100%, respectively, for diagrams based on all major elements, immobile major and trace elements, and immobile trace elements) were first tested for fresh and highly altered rocks. The expected tectonic setting was indicated from our diagrams. The probability-based decisions and total percent probability estimates can fully replace the actual plotting of samples in the diagrams. The probability calculations were then used for tectonic discrimination of 7 case studies of Archean to Proterozoic rocks. An island arc setting was indicated for the Wawa greenstone belt (Canada), implying the existence of plate tectonic processes during the Late Archean, for western Tasmania (Australia) during the Cambrian, and for Chichijima Island (Bonin Islands, Japan) during the Eocene. Similarly, an arc setting (indecisive island or continental type) was obtained for south-central Sweden during the Paleoproterozoic and for Adola (southern Ethiopia) during the Neoproterozoic. A within-plate setting was inferred for the Neoproterozoic Malani igneous complex, Rajasthan, India. A collision setting was indicated for the Alps (France-Italy-Switzerland) during the Late Carboniferous. Modeling of likely as well as extreme processes indicates that these diagrams are robust against postemplacement compositional changes caused by analytical errors, element mobility, Fe-oxidation, alteration, and petrogenetic processes.

Key words: Arc, collision, natural logarithm transformation of element ratios, tectonomagmatic discrimination, within-plate tectonic setting

1. Introduction

Magmas, subdivided into 4 main categories on the basis of anhydrous 100% adjusted SiO₂ contents (Le Bas *et al.* 1986; ultrabasic with $(SiO_2)_{adj} = 35\%-45\%$, basic with 45%-52%, intermediate with 52%-63%, and acid with >63%), may originate in different tectonic settings (island arc [IA], continental arc [CA], continental rift [CR], ocean-island [OI], collision [Col], and mid-ocean ridge [MOR]). To reconstruct the geologic-tectonic history, especially in older or tectonically complex areas, it is mandatory to know the most likely tectonic setting that gave rise to magmas in a given region. One commonly used method

is the application of tectonomagmatic discrimination diagrams (e.g., Rollinson 1993). Numerous such diagrams (bivariate [x-y], ternary [x-y-z], and multidimensional [DF1-DF2]) are available for ultrabasic, basic, or acid magmas (e.g., Pearce & Cann 1971, 1973; Wood 1980; Shervais 1982; Pearce *et al.* 1984; Meschede 1986; Verma 2010; Verma & Agrawal 2011; Verma *et al.* 2012). Only 1 bivariate-type diagram (Bailey 1981) has been proposed for fine-scale discrimination of only 1 type of intermediate magma (orogenic or arc andesite). For its application to old terrains, the user will have to ensure that the samples actually come from an arc setting.

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Therefore, tectonic origin of intermediate magma (basaltic andesite, andesite, basaltic trachyandesite, trachyandesite, tephriphonolite, phonolite, and boninite) cannot be inferred from discrimination diagrams, and new ones are very much required to fill this important deficiency of the widely used geochemical technique. For intermediate magma, we propose a total of 15 multidimensional diagrams (in 3 sets of 5 diagrams each), evaluate their success rates, argue in favor of the refined procedure of probability calculations for individual samples, test their functioning for fresh and altered samples from known tectonic settings, and efficiently use the probability estimates for 7 case studies demonstrating the versatility of these diagrams. More importantly, we also demonstrate their robustness against extreme compositional changes related to analytical errors and postemplacement changes, bulk assimilation, and petrogenetic processes.

2. Database and the statistically correct procedure

For constructing the new diagrams, a representative 5-part database (IA, CA, CR, OI, and Col, in which MOR was not included due to the scarcity of intermediate magma from mid-ocean ridges) was established from Miocene to Recent rocks from different parts of the world (see Table S1 in the electronic supplement to this paper; the relevant references are, however, included in the main paper in order to give due credit to the authors whose data were used for constructing our database and proposing new diagrams), where the tectonic setting is clearly and unambiguously known. Although we have assigned IA to samples from Japan and New Zealand, it could have been CA. It could be checked in the future if this change in assignment would improve the success rates of IA and CA discrimination. Importantly, the character of intermediate magma for each sample included in the database was confirmed by SINCLAS software (Verma et al. 2002).

Natural logarithm (In or log,) transformation of element ratios (Aitchison 1986; Agrawal & Verma 2007) was used to provide the normal or Gaussian variable space, because compositional data represent a closed space with unit sum constraint and linear discriminant analysis (LDA) requires that the LDA variables be normally distributed. Before applying the LDA, the compiled data from each tectonic setting were processed using DODESSYS software (Verma & Díaz-González 2012) for identifying and separating discordant outliers (Barnett & Lewis 1994) in the 10 variables of logarithms of element ratios (natural logarithms of the ratio of all major elements, TiO₂ to P₂O₂, with SiO₂ as the common denominator). The choice of the element used as the common denominator is immaterial (Aitchison 1986) and does not actually affect the proposal and functioning of the multidimensional diagrams.

The samples with complete analyses and discordant outlier-free log_e-ratio data were used to propose the diagrams. The total number of samples from each tectonic

setting available for the different combination of elements is listed in Table S2. Commercial software Statistica was used to perform LDA. No attempt was made to randomly separate the database in training and testing sets, because in all previous studies when the diagrams were proposed from training-set data, the evaluation by testing-set data provided similarly high success rates (high values of correct classification expressed as percentages) as the original proposal (Verma *et al.* 2006; Agrawal *et al.* 2008; Verma & Agrawal 2011; Verma *et al.* 2012). Thus, the generally similar success rates for the training and testing sets made it unnecessary to split the data into training and testing sets.

Success rates were calculated from counting the correctly discriminated samples. The probability-based boundaries following the initial suggestion of Agrawal (1999) and the probabilities for individual samples were computed from the method recently outlined by Verma and Agrawal (2011). For applications, probabilities for individual samples of intermediate magma were used to infer the dominant tectonic setting. The concept recently proposed by Verma (2012) of total percent probability of samples from a given area corresponding to each tectonic setting was used to better illustrate the functioning and inferences from our diagrams.

Similar procedures were adopted for the other 2 sets of diagrams based on relatively immobile elements.

3. New multidimensional diagrams

We have proposed 3 sets of diagrams. Each set consists of 5 diagrams to discriminate 4 tectonic settings of island arc, continental arc, continental rift and ocean island together as within-plate, and collision. The very similar tectonic settings of island and continental arcs are separated for the first time from such complex diagrams for intermediate magma. We recall that it was not possible to do so from major elements in basic and ultrabasic rocks (Agrawal et al. 2004; Verma et al. 2006), nor was it attempted from immobile element-based diagrams (Agrawal et al. 2008; Verma & Agrawal 2011), although such a discrimination was successfully achieved from diagrams for acid magma (Verma et al. 2012). All diagrams were obtained from LDA of natural logarithms of element ratios. These 3 sets of diagrams are based, respectively, on the complete set of all major elements including the 2 Fe-oxidation varieties obtained from the Middlemost (1989) Fe subdivision with the SINCLAS computer program (Verma et al. 2002), relatively immobile selected major and trace elements easily determinable by conventional X-ray fluorescence spectrometry, and immobile elements involving a combination of trace and rare earth elements. Finally, no attempt was made to discriminate the within-plate setting in its 2 tectonic types (continental rift and ocean island). This is best achieved from basic and ultrabasic

magmas (Verma *et al.* 2006; Agrawal *et al.* 2008; Verma & Agrawal 2011), which are highly abundant in these 2 environments. Intermediate rock samples are much less abundant, especially in the ocean island setting (Table S2), and, therefore, it is not advisable at present to attempt their discrimination from the continental rift setting. Furthermore, 4 additional diagrams for each set of 5 diagrams would be required if we were to attempt it.

3.1. Major element-based diagrams

A total of 4023 intermediate rock samples with complete major-element analyses were available in our complete database. The results of LDA performed on these samples (success rates) can be summarized as follows: 84.56% for IA+CA together, 76.84% for CR+OI together, and 84.44% for Col. When the LDA was applied to the 3664 discordant outlier-free samples (remaining after the application of the DODESSYS software to 4023 analyses; Table S2), the success rates increased by about 2.05%, 3.39%, and 2.38%, respectively. Similar improvements were observed for all other combinations of 3 tectonic settings (average increase of about 0.98% to 5.90% in success rates). This increment of success rates clearly showed the advantage of fulfilling the basic requirement of LDA that this multivariate technique should be applied to data drawn from a normal distribution (Morrison 1990).

The geochemical characteristics of adjusted majorelement and log_e-ratios of discordant outlier-free 3664 complete major element analyses of intermediate rocks from the 5 tectonic settings are presented in Table S3. The statistical data for log_e-ratio variables (Table S3; note the data in this and other tables are reported as rounded values following the flexible rules put forth by Verma [2005]) showed that although IA and CA as well as CR and OI are somewhat similar, there are differences among them, which can be tested by Wilks' lambda and F-ratio statistics. Thus, the log_e-transformed ratios for these 5 tectonic groups or classes showed statistically significant differences inferred from both statistical tests (Wilks' lambda = 0.2002–0.2522, i.e. Wilks' lambda << 1, and F-ratio = 8.4–247.5, i.e. F-ratio >> 1) at an extremely low significance level approaching 0 (equivalently at a very high confidence level approaching 100%) for all variables (Table S4). These differences were enhanced by the multivariate technique of LDA practiced here.

The LDA was performed 5 times on 3664 samples of the training set, the first time being for all groups with IA+CA (arc samples were kept together), CR+OI (withinplate samples were maintained together), and Col settings (Figure 1a), and 4 times for all possible combinations of 3 groups at a time out of 4 groups, IA, CA, CR+OI, and Col (Figures 1b–1e). The equations for the DF1 and DF2 functions (x- and y-axes; Figures 1a–1e) obtained from the LDA (canonical analysis) are as follows.

For Figure 1a, Eqs. (1) and (2) are used to calculate the x- and y-axis variables, $DF1_{(IA+CA-CR+OI-Col)mint}$ and $DF2_{(IA+CA-CR+OI-Col)mint}$, respectively, where the subscript mint stands for the major element (_m)-based diagram for intermediate (_{int}) magmas. The multiplication factors and the constant are the raw coefficients from the canonical analysis (LDA; Root 1 and Root 2 values from Statistica).

$$DF1_{(IA + CA - CR + OI - Col)_{mint}} = (-2.45605 \times \ln(TiO_2/SiO_2)_{adj}) + (1.11985 \times \ln(Al_2O_3/SiO_2)_{adj}) + (-2.22475 \times \ln(Fe_2O_3/SiO_2)_{adj}) + (2.48861 \times \ln(FeO/SiO_2)_{adj}) + (-0.212024 \times \ln(MnO/SiO_2)_{adj}) + (-0.06661 \times \ln(MgO/SiO_2)_{adj}) + (-0.212024 \times \ln(MnO/SiO_2)_{adj}) + (-0.28377 \times \ln(Na_2O/SiO_2)_{adj}) + (-0.40211 \times \ln(K_2O/SiO_2)_{adj}) + (0.030635 \times \ln(P_2O_5/SiO_2)_{adj}) - 11.43097347 \quad (1)$$

$$DF2_{(IA + CA - CR + OI - Col)_{mint}} = (-0.57759 \times \ln(TiO_2/SiO_2)_{adj}) + (-0.01121 \times \ln(Al_2O_3/SiO_2)_{adj}) + (0.69125 \times \ln(Fe_2O_3/SiO_2)_{adj}) + (-1.99798 \times \ln(FeO/SiO_2)_{adj}) + (-1.72014 \times \ln(MnO/SiO_2)_{adj}) + (0.305275 \times \ln(MgO/SiO_2)_{adj}) + (0.816018 \times \ln(CaO/SiO_2)_{adj}) + (-1.791727 \times \ln(Na_2O/SiO_2)_{adj}) + (0.871298 \times \ln(K_2O/SiO_2)_{adj}) + (0.335479 \times \ln(P_2O_5/SiO_2)_{adj}) - 12.20158596 \quad (2)$$

For Figure 1b, Eqs. (3) and (4) give the x- and y-axis variables, respectively.

$$\begin{split} \mathrm{DF1}_{\mathrm{(IA-CA-CR+OI)}_{\mathrm{mint}}} &= (-2.51880 \times \ln(\mathrm{TiO}_2/\mathrm{SiO}_2)_{\mathrm{adj}}) + (0.54210 \times \ln(\mathrm{Al}_2\mathrm{O}_3/\mathrm{SiO}_2)_{\mathrm{adj}}) + \\ &\quad (-3.790190 \times \ln(\mathrm{Fe}_2\mathrm{O}_3/\mathrm{SiO}_2)_{\mathrm{adj}}) + (3.846277 \times \ln(\mathrm{FeO}/\mathrm{SiO}_2)_{\mathrm{adj}}) + \\ &\quad (-0.362718 \times \ln(\mathrm{MnO}/\mathrm{SiO}_2)_{\mathrm{adj}}) + (-0.176632 \times \ln(\mathrm{MgO}/\mathrm{SiO}_2)_{\mathrm{adj}}) + \\ &\quad (1.426496 \times \ln(\mathrm{CaO}/\mathrm{SiO}_2)_{\mathrm{adj}}) + (0.111801 \times \ln(\mathrm{Na}_2\mathrm{O}/\mathrm{SiO}_2)_{\mathrm{adj}}) + \\ &\quad (-0.219223 \times \ln(\mathrm{K}_2\mathrm{O}/\mathrm{SiO}_2)_{\mathrm{adj}}) + (-0.07248 \times \ln(\mathrm{P}_2\mathrm{O}_5/\mathrm{SiO}_2)_{\mathrm{adj}}) - 14.3151255 \quad (3) \end{split}$$

$$\begin{split} \mathrm{DF2}_{\mathrm{(IA-CA-CR+OI)_{mint}}} &= (-1.04907 \times \ln(\mathrm{TiO}_2/\mathrm{SiO}_2)_{\mathrm{adj}}) + (3.440438 \times \ln(\mathrm{Al}_2\mathrm{O}_3/\mathrm{SiO}_2)_{\mathrm{adj}}) + \\ &\quad (-3.43323 \times \ln(\mathrm{Fe}_2\mathrm{O}_3/\mathrm{SiO}_2)_{\mathrm{adj}}) + (4.807165 \times \ln(\mathrm{FeO}/\mathrm{SiO}_2)_{\mathrm{adj}}) + \\ &\quad (-3.499257 \times \ln(\mathrm{MnO}/\mathrm{SiO}_2)_{\mathrm{adj}}) + (0.373928 \times \ln(\mathrm{MgO}/\mathrm{SiO}_2)_{\mathrm{adj}}) + \\ &\quad (-2.147775 \times \ln(\mathrm{CaO}/\mathrm{SiO}_2)_{\mathrm{adj}}) + (3.00229 \times \ln(\mathrm{Na}_2\mathrm{O}/\mathrm{SiO}_2)_{\mathrm{adj}}) + \\ &\quad (-0.773719 \times \ln(\mathrm{K}_2\mathrm{O}/\mathrm{SiO}_2)_{\mathrm{adj}}) + (1.061808 \times \ln(\mathrm{P}_2\mathrm{O}_5/\mathrm{SiO}_2)_{\mathrm{adj}}) - 13.4885545 \quad (4) \end{split}$$

For Figure 1c, Eqs. (5) and (6) are as follows.

$$\begin{split} DF1_{(IA-CA-Col)_{mint}} &= (-0.88680 \times \ln(TiO_2/SiO_2)_{adj}) + (-0.781835 \times \ln(Al_2O_3/SiO_2)_{adj}) + \\ &\quad (-2.43157 \times \ln(Fe_2O_3/SiO_2)_{adj}) + (4.10644 \times \ln(FeO/SiO_2)_{adj}) + \\ &\quad (2.050295 \times \ln(MnO/SiO_2)_{adj}) + (-0.386860 \times \ln(MgO/SiO_2)_{adj}) + \\ &\quad (-0.74023 \times \ln(CaO/SiO_2)_{adj}) + (1.35997 \times \ln(Na_2O/SiO_2)_{adj}) + \\ &\quad (-0.816315 \times \ln(K_2O/SiO_2)_{adj}) + (-0.468418 \times \ln(P_2O_5/SiO_2)_{adj}) + 4.31214432 \end{split}$$

$$\begin{split} \mathrm{DF2}_{(\mathrm{IA-CA-Col})_{\mathrm{mint}}} &= (1.76033 \times \ln(\mathrm{TiO}_2/\mathrm{SiO}_2)_{\mathrm{adj}}) + (-4.32894 \times \ln(\mathrm{Al}_2\mathrm{O}_3/\mathrm{SiO}_2)_{\mathrm{adj}}) + \\ &\quad (2.60111 \times \ln(\mathrm{Fe}_2\mathrm{O}_3/\mathrm{SiO}_2)_{\mathrm{adj}}) + (-4.96088 \times \ln(\mathrm{FeO}/\mathrm{SiO}_2)_{\mathrm{adj}}) + \\ &\quad (2.89683 \times \ln(\mathrm{MnO}/\mathrm{SiO}_2)_{\mathrm{adj}}) + (-0.362075 \times \ln(\mathrm{MgO}/\mathrm{SiO}_2)_{\mathrm{adj}}) + \\ &\quad (2.23018 \times \ln(\mathrm{CaO}/\mathrm{SiO}_2)_{\mathrm{adj}}) + (-2.96677 \times \ln(\mathrm{Na}_2\mathrm{O}/\mathrm{SiO}_2)_{\mathrm{adj}}) + \\ &\quad (0.790236 \times \ln(\mathrm{K}_2\mathrm{O}/\mathrm{SiO}_2)_{\mathrm{adj}}) + (-1.326438 \times \ln(\mathrm{P}_2\mathrm{O}_5/\mathrm{SiO}_2)_{\mathrm{adj}}) + 7.58611734.8 \end{split}$$

For Figure 1d, Eqs. (7) and (8) provide the respective x- and y-axis variables.

$$DF1_{(IA-CR+OI-Col)_{mint}} = (-2.43565 \times \ln(TiO_2/SiO_2)_{adj}) + (1.53913 \times \ln(Al_2O_3/SiO_2)_{adj}) + (-1.51665 \times \ln(Fe_2O_3/SiO_2)_{adj}) + (1.45582 \times \ln(FeO/SiO_2)_{adj}) + (0.4961937 \times \ln(MnO/SiO_2)_{adj}) + (-0.050128 \times \ln(MgO/SiO_2)_{adj}) + (1.258138 \times \ln(CaO/SiO_2)_{adj}) + (-0.8274299 \times \ln(Na_2O/SiO_2)_{adj}) + (-0.4884699 \times \ln(K_2O/SiO_2)_{adj}) + (0.1123605 \times \ln(P_2O_5/SiO_2)_{adj}) - 7.894955173$$
(7)

$$DF2_{(IA-CR+OI-Col)_{mint}} = (-0.736658 \times \ln(TiO_2/SiO_2)_{adj}) + (-0.078809 \times \ln(Al_2O_3/SiO_2)_{adj}) + (0.065533 \times \ln(Fe_2O_3/SiO_2)_{adj}) + (-1.130176 \times \ln(FeO/SiO_2)_{adj}) + (-2.130889 \times \ln(MnO/SiO_2)_{adj}) + (0.245709 \times \ln(MgO/SiO_2)_{adj}) + (0.6816946 \times \ln(CaO/SiO_2)_{adj}) + (-1.3284307 \times \ln(Na_2O/SiO_2)_{adj}) + (0.7709408 \times \ln(K_2O/SiO_2)_{adj}) + (0.295664 \times \ln(P_2O_5/SiO_2)_{adj}) - 15.24062267$$
(8)

Finally, for Figure 1e, Eqs. (9) and (10) are used for calculating the respective x- and y-axis variables.

$$\begin{split} DF1_{(CA-CR+OI-Col)_{mint}} &= (-2.32173 \times \ln(TiO_2/SiO_2)_{adj}) + (1.97128 \times \ln(Al_2O_3/SiO_2)_{adj}) + \\ &\quad (-0.537435 \times \ln(Fe_2O_3/SiO_2)_{adj}) + (0.431388 \times \ln(FeO/SiO_2)_{adj}) + \\ &\quad (-1.139286 \times \ln(MnO/SiO_2)_{adj}) + (0.527984 \times \ln(MgO/SiO_2)_{adj}) + \\ &\quad (0.9884038 \times \ln(CaO/SiO_2)_{adj}) + (-0.894467 \times \ln(Na_2O/SiO_2)_{adj}) + \\ &\quad (0.16138688 \times \ln(K_2O/SiO_2)_{adj}) + (0.0778358 \times \ln(P_2O_5/SiO_2)_{adj}) - 12.34961873 \quad (9) \end{split}$$

$$\begin{split} \mathrm{DF2}_{(\mathrm{CA-CR+OI-Col})_{\mathrm{mint}}} &= (-0.40691 \times \ln(\mathrm{TiO}_2/\mathrm{SiO}_2)_{\mathrm{adj}}) + (2.60576 \times \ln(\mathrm{Al}_2\mathrm{O}_3/\mathrm{SiO}_2)_{\mathrm{adj}}) + \\ &\quad (0.1610669 \times \ln(\mathrm{Fe}_2\mathrm{O}_3/\mathrm{SiO}_2)_{\mathrm{adj}}) + (1.345967 \times \ln(\mathrm{FeO}/\mathrm{SiO}_2)_{\mathrm{adj}}) + \\ &\quad (0.4457959 \times \ln(\mathrm{MnO}/\mathrm{SiO}_2)_{\mathrm{adj}}) + (-0.260127 \times \ln(\mathrm{MgO}/\mathrm{SiO}_2)_{\mathrm{adj}}) + \\ &\quad (-0.464534 \times \ln(\mathrm{CaO}/\mathrm{SiO}_2)_{\mathrm{adj}}) + (0.9211739 \times \ln(\mathrm{Na}_2\mathrm{O}/\mathrm{SiO}_2)_{\mathrm{adj}}) + \\ &\quad (-1.2769499 \times \ln(\mathrm{K}_2\mathrm{O}/\mathrm{SiO}_2)_{\mathrm{adj}}) + (-0.142884 \times \ln(\mathrm{P}_2\mathrm{O}_5/\mathrm{SiO}_2)_{\mathrm{adj}}) + 3.501318155 \ (10) \end{split}$$

The 3 boundaries dividing the fields in each diagram (Figures 1a-1e) were based on probability calculations expressed in percentages, as explained by Verma and Agrawal (2011) and Verma et al. (2012). Training set group centroid DF1-DF2 values required for these calculations are included in Figures 1a-1e. Each boundary represents 50% probability for the 2 fields that it separates, and this probability decreases to 33.33% at the triple point (the intersection of 3 tectonic boundaries). For all fields (Figure 1a), we also calculated the probability-based curves for 70% (dotted curves) and 90% (dashed curves). The probability to belong to a certain group increases very rapidly for transects from the discrimination boundaries (thick solid lines) into a given field (dotted and dashed curves). To better show the data and the equal probability discrimination boundaries, we did not add these additional 70% and 90% probability curves to other diagrams (Figures 1b-1e). These curves are very similar to those in Figure 1a.

The correct and incorrect discriminations (Table S5) are reported separately for the 5 tectonic settings (Figures 1a-1e). For each tectonic setting, only 4 of the 5 diagrams (Figures 1a-1e) are applicable (the inapplicable diagram is indicated by an asterisk in Table S5). The success rates for IA and CA, discriminated as the combined IA+CA setting, were fairly high (90.1% and 79.3%, respectively). When these IA or CA samples were discriminated as either IA (see IA in Figure 1d) or CA (see CA in Figure 1e) in diagrams from which the CA or IA setting was missing, the success rates were about 89.1% and 80.0%, respectively. The similarity of these 2 arc settings is evident from those diagrams in which the same IA or CA samples were wrongly discriminated as CA and IA, respectively, because 84.5% of IA samples plotted in the CA field in Figure 1e, from which the IA field is absent, and 73.0% of CA samples did so for the IA field in Figure 1d where the CA field is missing. The similarity of these 2 tectonic settings is again clear from the other 2 diagrams (see Figures 1b and 1c), in which the IA and CA samples showed somewhat lower success rates of 69.1% to 72.5%, respectively, because most of the misdiscriminated arc samples are plotted in the other arc field. Nevertheless, these major element-based diagrams do show the feasibility of discriminating these 2 very similar subduction-related tectonic settings. The success rates for CR and OI were, respectively, 71.2%-

76.6% and 93.9%–96.4%. Finally, the success rates for the Col magmas were consistently high (85.3%–86.8%, Figures 1a and 1c–1e; Table S5). Thus, the first set of 5 multidimensional diagrams showed success rates of about 69.1% to 96.4% for the discrimination of IA, CA, CR+OI, and Col settings.

3.2. Immobile major and trace element-based diagrams In our database a total of 1868 samples (Table S2) were available with complete data for the selected immobile elements: 3 major elements $(TiO_2)_{adj}$, $(MgO)_{adj}$, and (P_2O_5) adi, and 5 trace elements Nb, Ni, V, Y, and Zr. The selection was based on the feasibility of determining all major and these trace elements by the commonly used analytical technique of X-ray fluorescence spectrometry, which will facilitate the use of these diagrams, as well as those based on only major elements in most applications. We note that for proposing these diagrams, all major element data were first processed by SINCLAS under the Middlemost (1989) option for Fe-oxidation adjustment. The output TiO₂ value from the SINCLAS program, (TiO₂)_{adi}, was declared as the common denominator, and the resulting log-transformed ratios were used for the LDA of 1868 discordant outlier-free samples. We also note that for all trace to major element log, ratios, trace element data were expressed in the same unit (wt.%) as the major element (TiO₂)_{adi}. The geochemical characteristics of these elements and log-ratios for intermediate rocks from the 5 tectonic settings (Table S2) are presented in Table S6. This statistical synthesis indicated that differences among the tectonic settings do exist. Wilks' lambda and F-ratio tests (Table S7) clearly showed that statistically significant differences (Wilks' lambda = 0.2119-0.2391, i.e. Wilks' lambda << 1, and F-ratio = 25.1–88.0, i.e. F-ratio >> 1) are present at an extremely low significance level approaching 0 for all variables. Therefore, all log, ratio variables (Table S7) can be used in the LDA, which was performed 5 times on 1868 samples as done for the earlier set of diagrams. The equations of the DF1(IA+CA-CR+OI-Col)mtint and DF2(IA+CACR+) functions (x- and y-axes; Figure 2a; similar nomenclature for other diagrams in Figures 2b-2e) were obtained from the LDA, where the subscript mtint stands for the major $\binom{1}{m}$ and trace $\binom{1}{t}$ element-based diagrams for intermediate (_{int}) magmas.



Figure 1. The first set of 5 new discriminant-function multidimensional diagrams based on \log_{e} -transformed ratios of major elements for the discrimination of intermediate rocks from island arc (IA), continental arc (CA), continental rift (CR) and ocean-island (OI) combined together, and collision (Col) tectonic settings, showing samples from the training set. The symbols are explained in the inset

in Figure 1a. In (a), 5 groups are represented as 3 groups by combining IA and CA as IA+CA and CR and OI as CR+OI. The other 4 diagrams (b-e) are for 3 groups at a time. The subscript right refers to the set of multidimensional diagrams based on natural logarithmtransformed major element (,,) ratios for intermediate (,,) magmas. Group centroids (filled circles) refer to the training set samples and are reported in each diagram. The percentages are correct discrimination for training set samples (see Table S5). The thick lines represent equal probability discrimination boundaries in all diagrams. (a) IA+CA-CR+OI-Col (1+2-3+4-5) diagram; the coordinates of the field boundaries are (0.42744, -8.0) and (-0.67554, 0.27663) for IA+CA-CR+OI, (8.0, 5.53331) and (-0.67554, 0.27663) for IA+CA-Col, and (-8.0, 4.73569) and (-0.67554, 0.27663) for CR+OI-Col; the group centroids are (0.8054338548, -0.2585540725) for IA+CA, (-1.964671917, -0.6277101314) for CR+OI, and (-0.4642378707, 1.836804090) for Col; the green dotted curves are for 70% probability and blue dashed curves represent 90% probability. (b) IA-CA-CR+OI (1-2-3+4) diagram; the coordinates of the field boundaries are (8.0, 0.76690) and (-0.63205, 0.08764) for IA-CA, (-1.50230, -8.0) and (-0.63205, 0.08764) for IA-CR+OI, and (-2.73408, 8.0) and (-0.63205, 0.08764) for CA-CR+OI; the group centroids are (0.7455503041, -0.3210198532) for IA, (0.6646759663, 0.7065892584) for CA, and (-2.065048896, -0.01859066688) for CR+OI. (c) IA-CA-Col (1-2-5) diagram; the coordinates of the field boundaries are (8.0, -3.06676) and (-0.71170, 0.24138) for IA-CA, (-1.18110, 8.0) and (-0.71170, 0.24138) for IA-Col, and (-3.55140, -8.0) and (-0.71170, 0.24138) for CA-Col; the group centroids are (0.6581080574, 0.2819229794) for IA, (0.2861131966, -0.6975830163) for CA, and (-2.0761856179, 0.1163864964) for Col. (d) IA-CR+OI-Col (1-3+4-5) diagram; the coordinates of the field boundaries are (0.66776, -8.0) and (-0.44102, 0.17933) for IA-CR+OI, (8.0, 6.27226) and (-0.44102, 0.17933) for IA-Col, and (-8.0, 4.24657) and (-0.44102, 0.17933) for CR+OI-Col; the group centroids are (1.069154781, -0.3163633417) for IA, (-1.764731542, -0.7005214343) for CR+OI, and (-0.4360327298, 1.7689356843) for Col. (e) CA-CR+OI-Col (2-3+4-5) diagram; the coordinates of the field boundaries are (-3.42497, 8.0) and (-0.033967, -0.10997) for CA-CR+OI, (8.0, -0.16286) and (-0.033967, -0.10997) for CA-Col, and (-4.17272, -8.0) and (-0.033967, -0.10997) for CR+OI-Col; the group centroids are (0.8905493277, 0.99156690835) for CA, (-1.4673931178, 0.005642657408) for CR+OI, and (0.8759650737, -1.223577442) for Col.

For Figure 2a, Eqs. (11) and (12) are as follows:

$$DF1_{(IA+CA-CR+OI-Col)_{mtint}} = (1.02293 \times \ln(MgO/TiO_2)_{adj}) + (0.63053 \times \ln(P_2O_5/TiO_2)_{adj}) + (-0.93889 \times \ln(Nb/TiO_2)_{adj}) + (-0.41538 \times \ln(Ni/TiO_2)_{adj}) + (1.676898 \times \ln(V/TiO_2)_{adj}) + (0.453813 \times \ln(Y/TiO_2)_{adj}) + (0.5831823 \times \ln(Zr/TiO_2)_{adj}) + 1.9007264 \ \ (11)$$

$$DF2_{(IA+CA-CR+OI-Col)_{mtint}} = (0.248529 \times \ln(MgO/TiO_2)_{adj}) + (-0.477177 \times \ln(P_2O_5/TiO_2)_{adj}) + (-0.33628 1 \times \ln(Nb/TiO_2)_{adj}) + (-0.131072 \times \ln(Ni/TiO_2)_{adj}) + (-1.712035 \times \ln(V/TiO_2)_{adj}) + (0.213840 \times \ln(Y/TiO_2)_{adj}) + (-2.008435 \times \ln(Zr/TiO_2)_{adj}) - 18.63750138$$
(12)

For Figure 2b, the functions are calculated from Eqs. (13) and (14).

$$DF1_{(IA-CA-CR+OI)_{mtint}} = (0.8750597 \times \ln(MgO/TiO_2)_{adj}) + (0.4279822 \times \ln(P_2O_5/TiO_2)_{adj}) + (-0.6864967 \times \ln(Nb/TiO_2)_{adj}) + (-0.372419 \times \ln(Ni/TiO_2)_{adj}) + (1.924254 \times \ln(V/TiO_2)_{adj}) + (0.835240 \times \ln(Y/TiO_2)_{adj}) + (0.8428416 \times \ln(Zr/TiO_2)_{adj}) + 8.228368089$$
(13)

$$DF2_{(IA-CA-CR+OI)_{mtint}} = (-1.171625 \times \ln(MgO/TiO_2)_{adj}) + (-2.650912 \times \ln(P_2O_5/TiO_2)_{adj}) + (0.176065 \times \ln(Nb/TiO_2)_{adj}) + (0.1183849 \times \ln(Ni/TiO_2)_{adj}) + (-0.18532798 \times \ln(V/TiO_2)_{adj}) + (1.9213464 \times \ln(Y/TiO_2)_{adj}) + (0.3868149 \times \ln(Zr/TiO_2)_{adj}) + 12.45160186$$
(14)

For Figure 2c, Eqs. (15) and (16) are as follows:

$$DF1_{(IA-CA-Col)_{mtint}} = (-0.801371 \times \ln(MgO/TiO_2)_{adj}) + (0.125028 \times \ln(P_2O_5/TiO_2)_{adj}) + (0.908386 \times \ln(Nb/TiO_2)_{adj}) + (0.320442 \times \ln(Ni/TiO_2)_{adj}) + (-0.3683636 \times \ln(V/TiO_2)_{adj}) + (-0.6405805 \times \ln(Y/TiO_2)_{adj}) + (0.72337227 \times \ln(Zr/TiO_2)_{adj}) + 8.1087217398$$
(15)

$$DF2_{(IA-CA-Col)_{mtint}} = (1.317201 \times \ln(MgO/TiO_2)_{adj}) + (2.199955 \times \ln(P_2O_5/TiO_2)_{adj}) + (-0.1235449 \times \ln(Nb/TiO_2)_{adj}) + (-0.1339018 \times \ln(Ni/TiO_2)_{adj}) + (-0.8720114 \times \ln(V/TiO_2)_{adj}) + (-1.7825807 \times \ln(Y/TiO_2)_{adj}) + (-1.36498299 \times \ln(Zr/TiO_2)_{adj}) - 20.63036447$$
(16)

For Figure 2d, Eqs. (17) and (18) are given as follows:

$$DF1_{(IA-CR+OI-Col)_{mtint}} = (-0.85601 \times \ln(MgO/TiO_2)_{adj}) + (-0.300589 \times \ln(P_2O_5/TiO_2)_{adj}) + (0.861909 \times \ln(Nb/TiO_2)_{adj}) + (0.384727 \times \ln(Ni/TiO_2)_{adj}) + (-1.5827037 \times \ln(V/TiO_2)_{adj}) + (-0.757282 \times \ln(Y/TiO_2)_{adj}) + (-0.692422 \times \ln(Zr/TiO_2)_{adj}) - 4.468550646$$
(17)

$$DF2_{(IA-CR+OI-Col)_{mtint}} = (0.21504 \times \ln(MgO/TiO_2)_{adj}) + (-0.503675 \times \ln(P_2O_5/TiO_2)_{adj}) + (-0.32252 \times \ln(Nb/TiO_2)_{adj}) + (-0.122383 \times \ln(Ni/TiO_2)_{adj}) + (-1.7097486 \times \ln(V/TiO_2)_{adj}) + (0.426039 \times \ln(Y/TiO_2)_{adj}) + (-1.980676 \times \ln(Zr/TiO_2)_{adj}) - 17.04082095$$
(18)

Finally, for Figure 2e, the respective equations are as follows:

$$DF1_{(CA-CR+OI-Col)_{mtint}} = (-1.25554 \times \ln(MgO/TiO_2)_{adj}) + (-1.082014 \times \ln(P_2O_5/TiO_2)_{adj}) + (1.437934 \times \ln(Nb/TiO_2)_{adj}) + (0.5454469 \times \ln(Ni/TiO_2)_{adj}) + (-1.6196297 \times \ln(V/TiO_2)_{adj}) + (0.3368725 \times \ln(Y/TiO_2)_{adj}) + (-0.71359906 \times \ln(Zr/TiO_2)_{adj}) + 5.752160917$$
(19)

$$DF2_{(CA-CR+OI-Col)_{mtint}} = (-0.02400 \times \ln(MgO/TiO_2)_{adj}) + (-0.054413 \times \ln(P_2O_5/TiO_2)_{adj}) + (-0.8608025 \times \ln(Nb/TiO_2)_{adj}) + (-0.174160 \times \ln(Ni/TiO_2)_{adj}) + (-1.6407186 \times \ln(V/TiO_2)_{adj}) + (0.068523 \times \ln(Y/TiO_2)_{adj}) + (-1.772088 \times \ln(Zr/TiO_2)_{adj}) - 21.02758313$$
(20)

The success rates (Table S8) are reported separately for the 5 tectonic settings (Figures 2a–2e). For each tectonic setting, only 4 of the 5 diagrams (Figures 2a–2e) are applicable (the inapplicable diagram is indicated by an asterisk in Table S8). The success rates for IA and CA, discriminated as the combined IA+CA setting, were high (86.3% and 88.5%, respectively), whereas IA and CA were discriminated as IA (Figures 2b–2d) and CA (Figures 2b, 2c, and 2e), respectively,

with success rates of 62.8%–85.5% and 76.2%–94.7%. The success rates for CR and OI were, respectively, 72.9%–79.2% and 98.7%–100%. The success rates for the Col magmas were very high (90.2%–92.7%; Table S8), even higher than for the major element-based diagrams (Table S5). Thus, the second set of 5 multidimensional diagrams showed success rates of about 62.8% to 100% for the discrimination of IA, CA, CR+OI, and Col settings.

significant differences (Wilks' lambda = 0.1466-0.1986,

i.e. Wilks' lambda << 1, and F-ratio = 5.0–140.0, i.e. F-ratio

>> 1) exist also for these log_-transformed ratios (Table

S10) at an extremely low significance level approaching

0 for all variables, except for ln(La/Yb); for the latter, the

differences are significant at the 95% confidence level. All variables were used in the LDA performed 5 times on 1512

samples. The equations of the $\mathrm{DF1}_{(\mathrm{IA}+\mathrm{CA}-\mathrm{CR}+\mathrm{OI-Col})_{tint}}$ and

DF2_{(IA+CA-CR+OI-Col)tint} functions (x- and y-axes; Figure

3a; similar nomenclature for other diagrams in Figures

3b-3e) obtained from the LDA are now presented where the subscript $_{tint}$ stands for the trace (,) element-based

diagrams for intermediate (_{int}) magmas.

3.3. Immobile trace element-based diagrams

In our database, a total of 1512 samples (Table S2) were available with discordant outlier-free complete data for the selected immobile trace elements (Yb used as the common denominator, La, Ce, Sm, Nb, Th, Y, and Zr; Table S9). Although, unlike the earlier 2 sets of diagrams, it is not mandatory to use SINCLAS (Verma *et al.* 2002) for these elements, this computer program is still considered useful even for this set of diagrams for ascertaining the intermediate nature of the igneous rock samples. The geochemical characteristics of these elements and log_e-ratios for intermediate rocks from the 5 tectonic settings (Table S2) are presented in Table S9. Statistically

For Figure 3a, Eqs. (21) and (22) are as follows:

$DF1_{(IA+CA-CR+OI-Col)_{tint}} = (-0.1672589 \times \ln(La/Yb) + (-1.2542899 \times \ln(Ce/Yb) + (-1.2542899 \times \ln(Ce/Yb)) + (-1.254289 \times \ln(Ce/Yb)) + (-1.25428 \times \ln(Ce/Yb)) + (-1.2548 \times \ln(Ce/Yb)) + (-1.2548 \times \ln(Ce/Yb)) + (-1.254$	
$(1.295171 \times \ln(Sm/Yb) + (1.3318361 \times \ln(Nb/Yb) +$	
$(0.2698636 \times \ln(Th/Yb) + (1.9286976 \times \ln(Y/Yb) +$	
(0.18097357×ln(Zr/Yb)-3.815745639	(21)
$DF2_{(IA+CA-CR+OI-Col)_{tint}} = (-0.2426713 \times \ln(La/Yb) + (1.7265475 \times \ln(Ce/Yb) + (1.7265475 \times \ln(Ce/Yb)) + (1.726575 \times \ln(Ce/Yb)) + (1.7265575 \times \ln(Ce/Yb)) + (1.726575 \times \ln(Ce/Yb)) + (1.726575 \times \ln(Ce/Yb))) + (1.726575 \times \ln(Ce/Yb)) + (1.726575 \times \ln(Ce/Yb))) + (1.726575 \times \ln(Ce/Yb)) + (1.726575 \times \ln(Ce/Yb))) + (1.726575 \times \ln(Ce/Yb)) + (1.7265755 \times \ln(Ce/Yb))) + (1.7265755 \times \ln(C$	
$(0.4902224 \times \ln(Sm/Yb) + (-1.2755648 \times \ln(Nb/Yb) +$	
$(0.9602491 \times \ln(Th/Yb) + (0.8511852 \times \ln(Y/Yb) +$	
(-0.4894082×ln(Zr/Yb) - 3.305510646	(22)
For Figure 3b, the functions are calculated from Eqs. (23) and (24).	
$DF1_{(IA-CA-CR+OI)_{tint}} = (0.0178001 \times \ln(La/Yb) + (-1.2689712 \times \ln(Ce/Yb) + (-1.2689712 \times \ln(Ce/Yb)) + (-1.2689712 \times \ln($	
$(1.7407108 \times \ln(Sm/Yb) + (1.324421438 \times \ln(Nb/Yb) +$	
$(0.0288819 \times \ln(Th/Yb) + (1.580888497 \times \ln(Y/Yb) +$	
$(0.17161461 \times \ln(Zr/Yb) - 3.3845534709)$	(23)
$DF2_{(IA-CA-CR+OI)_{tint}} = (-2.099551 \times \ln(La/Yb) + (-2.044178 \times \ln(Ce/Yb) + (-2.044178 \times \ln(Ce/Yb)) + (-2.044178 \times \ln(Ce$	
$(-0.41179008 \times \ln(Sm/Yb) + (1.022466699 \times \ln(Nb/Yb) + (1.022466699 \times \ln(Nb/Yb)) + (1.02246669 \times \ln(Nb/Yb)) + (1.0226669 \times \ln$	
$(1.24448424 \times \ln(Th/Yb) + (1.87700276 \times \ln(Y/Yb) +$	
(1.07017399797×ln(Zr/Yb)-0.2920468400	(24)
For Figure 3c, Eqs. (25) and (26) are used:	
$DF1_{(IA-CA-Col)_{tint}} = (0.092724 \times \ln(La/Yb) + (0.752143 \times \ln(Ce/Yb) + (0.752143 \times \ln(Ce/Yb)) + (0.$	
$(0.9296053 \times \ln(Sm/Yb) + (0.12351021 \times \ln(Nb/Yb) +$	
$(0.3479451 \times \ln(Th/Yb) + (1.472513 \times \ln(Y/Yb) +$	
$(-0.0339674 \times \ln(Zr/Yb) - 5.801482381)$	(25)
$DF2_{(IA-CA-CR+OI)_{tint}} = (-2.038286 \times \ln(La/Yb) + (-0.073322 \times \ln(Ce/Yb) + (-0.073322 \times \ln(Ce/Yb)) + (-0.07322 \times \ln(Ce/Yb)) + (-0.0722 \times \ln(C$	
$(-1.360432 \times \ln(\text{Sm/Yb}) + (-0.0782899 \times \ln(\text{Nb/Yb}) +$	
$(1.8248761 \times \ln(Th/Yb) + (2.7738488 \times \ln(Y/Yb) +$	
(0.44440139×ln(Zr/Yb) - 3.684349292	(26)



Figure 2. The second set of 5 new discriminant-function multidimensional discrimination diagrams based on \log_{e} -transformed ratios of immobile major and trace elements, showing samples from the training set. The symbols are explained in the inset in Figure 2a. More details are given in Figure 1. The subscript _{mtint} in axis names refers to major and trace element ratios. The percentages in each figure are

correct discriminations for training set samples (see Table S8). (a) IA+CA-CR+OI-Col (1+2-3+4-5) diagram; the coordinates of the field boundaries are (0.92190, 8.0) and (-0.82858, 0.29965) for IA+CA-CR+OI, (6.39297, -8.0) and (-0.82858, -8.0) and (-0.8 Col, and (-8.0, -4.20284) and (-0.82858, 0.29965) for CR+OI-Col; the group centroids are (0.8717919136, 0.1836538565) for IA+CA, (-2.4119835116, 0.9301323744) for CR+OI, and (-0.9487745230, -1.4004245813) for Col. (b) IA-CA-CR+OI (1-2-3+4) diagram; the coordinates of the field boundaries are (8.0, -3.76290) and (-0.95018, 0.45941) for IA-CA, (-1.24490, 8.0) and (-0.95018, 0.45941) for IA-CR+OI, and (-3.41007, -8.0) and (-0.95018, 0.45941) for CA-CR+OI; the group centroids are (0.7875504506, 0.2520734663) for IA, (0.3148863535, -0.7498501616) for CA, and (-2.666419140, 0.1170769090) for CR+OI. (c) IA-CA-Col (1-2-5) diagram; the coordinates of the field boundaries are (-8.0, 3.71126) and (0.60491, -0.23211) for IA-CA, (0.95093, -8.0) and (0.60491, -0.23211) for IA-Col, and (4.00195, 8.0) and (0.60491, -0.23211) for CA-Col; the group centroids are (-0.6826446433, -0.2400902940) for IA, (-0.2296800482, 0.7483231874) for CA, and (1.8880671989, -0.1255771906) for Col. (d) IA-CR+OI-Col (1-3+4-5) diagram; the coordinates of the field boundaries are (-0.87616, 8.0) and (0.62149, 0.34939) for IA-CR+OI, (-6.61289, -8.0) and (0.62149, 0.34939) for IA-Col, and (8.0, -4.51524) and (0.62149, 0.34939) for CR+OI-Col; the group centroids are (-1.0703369201, 0.2441771424) for IA, (2.2277092202, 0.8896913710) for CR+OI, and 0.7578341279, -1.3397609987) for Col. (e) CA-CR+OI-Col (2-3+4-5) diagram; the coordinates of the field boundaries are (-1.16430, 8.0) and (-0.028516, 0.35743) for CA-CR+OI, (-7.33632, -8.0) and (-0.028516, 0.35743) for CA-Col, and (8.0, -3.84452) and (-0.028516, 0.35743) for CR+OI-Col; the group centroids are (-1.7443803369, 0.5101687902) for CA, (1.5687968044, 1.0025551371) for CR+OI, and (0.3517867418, -1.3227417914) for Col.

For Figure 3d, Eqs. (27) and (28) are given as follows:

$$DF1_{(IA-CR+OI-Col)_{tint}} = (0.720851 \times \ln(La/Yb) + (-1.352147 \times \ln(Ce/Yb) + (1.378563 \times \ln(Sm/Yb) + (1.1641465 \times \ln(Nb/Yb) + (-0.0423769 \times \ln(Th/Yb) + (1.5584709 \times \ln(Y/Yb) + (-0.1644980 \times \ln(Zr/Yb) - 2.9336489118)$$
(27)
$$DF2_{(IA-CR+OI-Col)_{tint}} = (0.2378909 \times \ln(La/Yb) + (-2.03548886 \times \ln(Ce/Yb) + (-2.0354886 \times \ln(Ce/Yb) + (-2.03548886 \times \ln(Ce/Yb) + (-2.03548886 \times \ln(Ce/Yb) + (-2.0354886 \times \ln(Ce$$

$$(-0.2501036699 \times \ln(Sm/Yb) + (1.34733326 \times \ln(Nb/Yb) + (-0.760673982 \times \ln(Th/Yb) + (-0.786605747 \times \ln(Y/Yb) + (0.37736968328 \times \ln(Zr/Yb) + 4.154732286)$$
(28)

Finally, for Figure 3e, the respective equations are as follows:

$$DF1_{(CA-CR+OI-Col)_{tint}} = (-0.977026 \times \ln(La/Yb) + (-1.3886489 \times \ln(Ce/Yb) + (1.36560 \times \ln(Sm/Yb) + (1.8999127 \times \ln(Nb/Yb) + (0.5690460 \times \ln(Th/Yb) + (1.65772638 \times \ln(Y/Yb) + (-0.30523813 \times \ln(Zr/Yb) - 0.87680549008)$$
(29)

$$DF2_{(CA-CR+OI-Col)_{tint}} = (-0.086967 \times \ln(La/Yb) + (1.1636159 \times \ln(Ce/Yb) + (0.3635930 \times \ln(Sm/Yb) + (-0.90127239 \times \ln(Nb/Yb) + (1.1257989 \times \ln(Th/Yb) + (1.19149068 \times \ln(Y/Yb) + (-0.39964298 \times \ln(Zr/Yb) - 3.915383182)$$
(30)

As for the earlier 2 sets of diagrams, only 4 of the 5 diagrams (Figures 3a–3e) are applicable for each tectonic setting (the inapplicable diagram is indicated by an asterisk in Table S11). The success rates for IA and CA (Table S11), discriminated as the combined IA+CA setting, were very high (91.4% and 90.4%, respectively), whereas IA and CA were discriminated as IA (Figures 3b–3d) and CA (Figures

3b, 3c, and 3e), respectively, with success rates of 72.7%– 90.3% and 64.5%–95.7%. The success rates for CR and OI were, respectively, 74.3%–80.5% and 94.1%–100%. The success rates for the Col magmas were also high (81.0%– 84.7%; Table S11). Thus, the third set of 5 multidimensional diagrams showed success rates of about 64.5% to 100% for the discrimination of IA, CA, CR+OI, and Col settings.



Figure 3. The third set of 5 new discriminant-function multidimensional diagrams based on \log_{e} -transformed ratios of immobile trace elements for the discrimination of intermediate rocks, showing samples from the training set. The symbols are explained in the inset in Figure 3a. More details are given in Figure 1. The subscript _{tint} in axis names refers to the set of multidimensional diagrams based on

log_-transformed trace element ratios. The percentages in each figure refer to correct discrimination for training set samples (see Table S11). (a) IA+CA-CR+OI-Col (1+2-3+4-5) diagram; the coordinates of the field boundaries are (-0.69292, -8.0) and (0.64148, 0.34301) for IA+CA-CR+OI, (-6.91145, 8.0) and (0.64148, 0.34301) for IA+CA-Col, and (8.0, 3.04640) and (0.64148, 0.34301) for CR+OI-Col; the group centroids are (-0.9774289603, -0.1013788344) for IA+CA, (2.0410269070, -0.5841593120) for CR+OI, and (1.1079374566, 1.9556336665) for Col. (b) IA-CA-CR+OI (1-2-3+4) diagram; the coordinates of the field boundaries are (-8.0, -5.45793) and (0.58959, 0.68699) for IA-CA, (0.87619, 8.0) and (0.58959, 0.68699) for IA-CR+OI, and (3.67939, -8.0) and (0.58959, 0.68699) for CA-CR+OI; the group centroids are (-1.1051018735, 0.2721190917) for IA, (-0.3503347313, -0.7829225361) for CA, and (2.2466156797, 0.1407633232) for CR+OI. (c) IA-CA-Col (1-2-5) diagram; the coordinates of the field boundaries are (-8.0, -7.28196) and (0.90473, 0.82230) for IA-CA, (0.64537, 8.0) and (0.90473, 0.82230) for IA-Col, and (4.86730, -8.0) and (0.90473, 0.82230) for CA-Col: the group centroids are (-0.6933875947, 0.2346902936) for IA, (0.1696340466, -0.7135732664) for CA, and 2.5411240984, 0.3515850688) for Col. (d) IA-CR+OI-Col (1-3+4-5) diagram; the coordinates of the field boundaries are (-0.87235, 8.0) and (0.37157, -0.26385) for IA-CR+OI, (-6.10890, -8.0) and (0.37157, -0.26385) for IA-Col, and (8.0, -2.82217) and (0.37157, -0.26385) for CR+OI-Col; the group centroids are (-1.2898249628, 0.1152106837) for IA, (1.8477651525, 0.5874997038) for CR+OI, and (1.0359821323, -1.8330905346) for Col. (e) CA-CR+OI-Col (2-3+4-5) diagram; the coordinates of the field boundaries are (-0.10284, -8.0) and (-0.15459, 0.29462) for CA-CR+OI, (-8.0, 5.41425) and (-0.15459, 0.29462) for CA-Col, and (8.0, 4.74335) and (-0.15459, 0.29462) for CR+OI-Col; the group centroids are (-1.5332986559, -0.4569150582) for CA, (1.2333855428, -0.4396529035) for CR+OI, and (-0.02124818532, 1.8606170376) for Col.

4. Applications

4.1. Probability estimates for individual samples

As recently suggested by Verma (2012), we can use the probability calculations (modified from Verma & Agrawal 2011; a few nomenclatural errors are corrected in this work) to fully replace the discrimination diagrams (Figure 1). Therefore, we outline the procedure to calculate the probabilities of individual samples to belong to the 3 tectonic settings discriminated in a given diagram. The subscripts, such as $(IA+CA-CR+OI-Col)_{mint}$, $DF1_{(IA+CA-CR+OI-Col)_{mint}}$, and $DF1_{(IA+CA-CR+OI-Col)_{tint}}$, are purposely eliminated from Eqs. (31) through (39) to keep them relatively simple. Otherwise, we would have had to list 126 more equations (9 for each diagram).

The distances $(d_{g1}, d_{g2}, and d_{g3})$ of a sample under evaluation from the 3 group centroids $(mdf1_{g1}, mdf2_{g1})$, $(mdf1_{g2}, mdf2_{g2})$, and $(mdf1_{g3}, mdf2_{g3})$ of the tectonic groups g1, g2, and g3, respectively, in a given diagram are as follows:

$$d_{g1} = \sqrt{(df1_s - mdf1_{g1})^2 + (df2_s - mdf2_{g1})^2}$$
(31)

$$d_{g2} = \sqrt{(df1_s - mdf1_{g2})^2 + (df2_s - mdf2_{g2})^2}$$
(32)

$$d_{g3} = \sqrt{(df1_s - mdf1_{g3})^2 + (df2_s - mdf2_{g3})^2}$$
(33)

where dfl_s and $df2_s$ are the coordinates or scores of the sample under evaluation in a given diagram.

New functions sg1, sg2, and sg3 based on distances d_{g1} , d_{g2} , and d_{g3} of Eqs. (31) through (33) for that particular sample are then computed from Eqs. (34) through (36) as follows:

$sg1=e^{\{(d_{g1})^2/2\}}$	(34)
$sg2=e^{\{(d_{g2})^2/2\}}$	(35)
$sg3=e^{\{(d_{g3})^2/2\}}$	(36)

Finally, the probabilities for belonging to each of 3 groups (P1_s, P2_s, and P3_s; if desired, they could be expressed in percentages) are then calculated from the above parameters (sg1, sg2, and sg3) as follows:

$$P1_{s} = \frac{sg1}{sg1 + sg2 + sg3}$$
(37)

$$P2_{s} = \frac{sg2}{sg1 + sg2 + sg3}$$
 (38)

$$P3_s = \frac{sg3}{sg1 + sg2 + sg3}$$
(39)

These probability estimates (P1_s, P2_s, and P3_s) directly provide the inferred tectonic setting for the sample under consideration. The inferred setting is the one for which the corresponding probability (P1_s, P2_s, or P3_s) is the highest. The actual value of the highest probability also indicates how far away from the tectonic field boundary the sample will actually plot in the field of the inferred tectonic setting. Thus, a simple comparison of the 3 probabilities will provide the inferred tectonic setting for a given sample or a set of samples, without any special need to plot the data in a discrimination diagram.

Nevertheless, these calculations must be carried out 5 times to obtain probabilities for all 5 discrimination diagrams of each set (Figures 1–3). Thus, probability estimates can be obtained for a given set of samples analyzed from the area under study. Mean and standard deviation values, as well as total probabilities and the resulting total percent probabilities for the different tectonic settings, can be calculated and inferences made without the need of actually plotting the samples in diagrams. A similar procedure is valid for the other 2 sets of diagrams.

For actual applications, it is mandatory to use the highly precise centroid values (i.e. with many significant digits; Figures 1–3) in the probability calculations. Otherwise, the probability-based decisions of sample assignment to a group or class may not fully agree with the actual plotting of samples in the diagrams, particularly for samples that plot very close to the field boundaries.

To avoid excessive complication, we did not apply discordancy tests to the probability data and, therefore, we report only the initial mean probability values along with the respective standard deviation values; after all, these central tendency and dispersion estimates are for indication purposes only. The total probability and the respective total percent probability values are more important for the interpretation and inferences from these 15 diagrams, as recently documented by Verma (2012).

4.2. Evaluation of discrimination diagrams from samples of known tectonic settings

Independently of the database used for proposing new diagrams (Table S1), we compiled geochemical data for Neogene rock samples from known tectonic settings and separated those for the intermediate rocks to be used in our diagrams. More importantly, we present an innovative way to infer tectonic setting from probability calculations, particularly the total percent probability concept explained below in Section 4.2.1.

We did not process the log_e-transformed data of the evaluation and application samples using the DODESSYS computer program (Verma & Díaz-González 2012), because such statistically censored data have generally increased the success rates and strengthened the inferences of the tectonic setting (see, e.g., Verma & Agrawal 2011; Verma *et al.* 2012). As seen below, the inferences from the 3 sets of diagrams are mutually consistent in most instances, and so there is no special need to identify discordant outliers in our applications. Furthermore, the concept of total probability values for the different tectonic settings is better applied to all samples without the identification and separation of samples representing discordant outlying observations.

Due to space limitations, we do not comment on the results of published sets of multidimensional diagrams for basic and ultrabasic (Verma *et al.* 2006; Agrawal *et al.* 2008; Verma & Agrawal 2011) or for acid magmas (Verma *et al.* 2012); such an application generally provided consistent results with those of the present work. Besides, only one

set of plots is shown (Figures 4a-4e), but the results of all applicable diagrams (Figures 1-3) are summarized in Tables S12–S17. To familiarize the reader with this relatively new concept of using a set of 5 diagrams instead of just 1 diagram, especially the inferences based on probability calculations alone without the actual plotting of samples, the first example is described in greater detail than the remaining ones.

4.2.1. Samples from an island arc setting

Thirty rock samples of Pleistocene age from the Ijen volcanic complex, eastern Java, Indonesia (Handley *et al.* 2007) proved to be of intermediate magma types (Figure 4; Table S12). An island arc setting is known for this area (Handley *et al.* 2007).

For total probability estimates for a given tectonic setting in any diagram, we summed up the probability of only those samples that plotted in that particular tectonic setting. The smaller values of probability of these samples for the remaining 2 tectonic settings were not considered. For example, our first diagram (Figure 4a) discriminates 3 tectonic settings of IA+CA, CR+OI, and Col. Now, suppose that a sample plots in the IA+CA field and has the probability of 0.5010. Its remaining probability of 0.4990 (= 1 - 0.5010) will be divided for 2 other settings of CR+OI and Col. These 2 smaller probability values, which will add up to 0.4990, will actually depend on where exactly this sample plots in the combined arc (IA+CA) field. In the calculation of the total probability, we will assign the value of 0.5010 to the IA+CA field, but we will ignore the remaining 2 minor probability values corresponding to the other 2 fields, i.e. only the highest probability values are taken into account.

We could, of course, have used the other procedure to sum up all probabilities, irrespective of in which field the samples actually plot, but then the number of samples plotting in a given field and the total or mean probability values would have to be interpreted differently. As presented now, the mean probability values for a given field give us an idea of how far away from the boundaries the samples might be plotting in a tectonic field, without actually preparing and visually examining the plots.

Twenty-two samples (out of 30, with a success rate of about 73%) plotted in the combined arc (IA+CA) field, whereas the remaining 3 samples belonged to the within-plate and 5 to the collision field (Figure 4a). The probabilities for belonging to the field in which the samples plotted varied from 0.5010 to 0.9925 (p_{IA+CA} ; n = 22 samples, with the mean \overline{x} and standard deviation *s* values of 0.732 and 0.181, respectively, i.e. 0.732 ± 0.181) for the combined arc field, from 0.6157 to 0.8597 (p_{CR+OI} ; n = 3, 0.743 ± 0.122) for the within-plate, and from 0.4832 to 0.8280 (p_{CoI} ; n = 5, 0.622 ± 0.131) for the collision setting. The 22 samples plotted more inside the combined arc



Figure 4. Evaluation of the first set of 5 discriminant-function multidimensional diagrams based on \log_{e} -transformed ratios of major elements for the discrimination of intermediate rocks from areas of known tectonic setting. The symbols are explained in the inset in Figure 4a. For more information, see Figure 1. (a) IA+CA-CR+OI-Col (1+2-3+4-5) diagram; (b) IA-CA-CR+OI (1-2-3+4) diagram; (c) IA-CA-Col (1-2-5) diagram; (d) IA-CR+OI-Col (1-3+4-5) diagram; and (e) CA-CR+OI-Col (2-3+4-5) diagram.

field, i.e. farther away from the field boundaries, and the 3 samples did more so in the within-plate field than the 5 samples of the collision field (qualitatively compare the mean values of 0.732 and 0.743 with 0.622; Table S12). Because most samples (22 out of 30) plotted in the arc field, the other diagrams of this set (Figures 4b–4e) can be used to discriminate the 2 types of arc setting (island and continental arcs).

A similarly high success rate of about 73% for the island arc field is obtained for the second diagram of this set (Figure 4b; Table S12), in which 22 samples out of 30 (with the mean p_{IA} value of about 0.547 for n = 22) plotted in the IA field. The remaining 8 samples were distributed between the continental arc (CA; 5 samples) and withinplate settings (3 samples; collision setting is absent from this diagram). This diagram (Figure 4b) indicates that the Indonesian samples likely represent an island arc setting rather than a continental arc.

The third diagram (Figure 4c), however, did not provide any decisive answer for the discrimination of these 2 very similar settings of IA and CA. Thirteen samples plotted in each of these 2 fields, with the remaining 4 in the collision field. The respective probabilities for the 2 fields (IA and CA) were also similar, although the mean value for IA was slightly greater ($p_{IA} = 0.584$ versus $p_{CA} = 0.557$) than that for the CA.

The fourth diagram (Figure 4d), from which the CA setting is missing, showed 21 samples in the IA field, whereas the fifth and final diagram (Figure 4e) showed 20 samples in the CA field. The respective mean probability values ($p_{IA} = 0.763$ for 21 samples of the IA field versus $p_{CA} = 0.711$ for 20 samples of the CA field) indicated that the Indonesian samples plotted somewhat more inside IA than CA (Figures 4d and 4e; Table S12).

From the consideration of all diagrams (Figures 4a– 4e), the fifth diagram (Figure 4e), from which the island arc setting is absent, can be considered as the inapplicable diagram for these samples. An alternative way to interpret these results is to evaluate the overall picture of all 5 diagrams (Figures 4a–4e), without actually discarding any of them, in terms of the probability estimates (Table S12).

The overall picture of the number of samples plotting in different fields and the respective probabilities are then summarized in Table S12. Out of the total number of data points (150) in the 5 diagrams (Figures 4a–4e), 22 belonged to the combined arc, 56 to the island arc, 38 to the continental arc, 12 to the within-plate, and 22 to the collision field (Table S12). Although one can consider the percentage of these samples to infer the tectonic setting, this percentage does not take into account the relative distance from the tectonic field boundaries the samples plot in a given field. Therefore, it is advisable for the overall picture that the total probability for each field should be calculated for each tectonic field occupied in all 5 diagrams. Nevertheless, the total probability of samples that plotted in the combined arc field (Figure 4a) must be subdivided and assigned proportionately to the 2 types of arc fields IA and CA, according to the weighing factors of total probabilities for these 2 arc fields in all the remaining diagrams (Figures 4b–4e). When this was done and the total percent probability (% prob) values for the 4 tectonic settings (IA, CA, CR+OI, and Col) were calculated, the results (Table S12) showed that the rock samples from the Ijen volcanic complex gave 46.3% total percent probability for the IA, 31.8% for the CA, 8.8% for the within-plate, and 13.1% for the collision setting. Therefore, from the first set of major element-based diagrams (Figures 1a–1e) an island arc setting can be inferred for these samples.

The second set of diagrams (Figures 2a–2e: Indonesian data are not shown here, because no additional diagram is presented in this paper) based on relatively immobile major and trace elements confirmed the result of an island arc setting for the samples from Indonesia under study (Table S12), because a large number of samples (13 to 24 out of 28) plotted in the IA field and the overall total probability percentage of 47.3% was obtained for this setting. This highest value was followed by 38.7% for the competing very similar tectonic setting of continental arc, but it was much greater than that for the collision setting (14.0%). No samples plotted in the continental rift setting, which means that the total probability of samples for this tectonic setting was zero (Table S12).

The third set of diagrams (Figures 3a–3e: Indonesian data are not shown here) also based on relatively immobile elements (trace elements in this case) fully confirmed a successful test of these multidimensional diagrams (Table S12). Sixteen to 24 samples (out of 28; success rates of about 57%–86%) plotted in the IA or combined IA+CA field. In this case, the fifth diagram (Figure 3e) can be clearly declared as the inapplicable diagram, because the inferred (and expected) island arc field is absent from it. Alternatively, the overall picture of total percent probability values (% prob of 48.6% for IA followed by 37.5% for CA and 13.9% for Col) can be used to infer an island arc setting for these Pleistocene samples from eastern Java, Indonesia.

Satisfactory functioning of all 3 sets of diagrams (Figures 1–3) for the island arc setting is confirmed from this example.

4.2.2. Samples from a continental arc setting

The functioning of our diagrams for continental arc setting was tested using 9 intermediate rock samples of Pleistocene age reported for the Huiqui volcano, southern Chile, by Watt *et al.* (2011). A continental arc setting is clearly known for this area of Chile.

In the first set of diagrams based on major elements (Figures 4a-4e; see data identified as Chile), all 9 samples

plotted in the combined arc field and showed relatively high probability ($p_{{\scriptscriptstyle IA+CA}})$ values of 0.8008 to 0.9949 (Table S13), testifying that the samples plotted well inside the IA+CA field (Figure 4a). In the next 2 diagrams, 8 out of 9 samples plotted in the CA field, with the remaining sample in the IA field (Figures 4b and 4c). In the other 2 diagrams, in which only 1 type of arc field is present (IA in Figure 4d and CA in Figure 4e), all the 9 samples plotted in the arc field. None of the samples plotted in withinplate or collision field in any of the 5 diagrams (Figures 4a-4e). Therefore, the continental arc setting expected for these samples is confirmed and Figure 4d is declared as the inapplicable diagram. Alternatively, the total probability estimates presented in Table S13 can be used to infer the tectonic setting of a continental arc, because the total percent probability (% prob) for this setting is the highest (70.8%) and that for the island arc setting is the complementary smaller value of 29.2%.

Geochemical data were also available for the second set of major and trace element-based diagrams (Table S13). A complete data set was not reported for our third set of diagrams (Th was the missing element; Watt et al. 2011), which meant that this third set based on immobile trace elements could not be tested for its functioning for the continental arc setting. Nevertheless, our second set of diagrams (Figure 2) provided exactly the same result as the first set, i.e. a continental arc setting for the Huiqui volcano, because the highest total percent probability of 70.1% was obtained for this field and the remaining much lower percent probability (29.9%) was shared by the IA (26.9%) and collision (3.0%) settings. Thus, satisfactory functioning of 2 sets of diagrams (Figures 1 and 2) for the discrimination of continental arc setting is safely inferred from this example.

4.2.3. Samples from a continental rift setting

Thirty-four samples of Pliocene-Holocene intermediate magmas from the Kilimanjaro volcano, Tanzania (Nonnotte *et al.* 2011) were successfully used to test all 3 sets of diagrams (Figures 1–3) for the continental rift setting (Table S14) from this largest volcano in Africa.

Complete major element data available for all 34 samples showed that all of them plotted in the within-plate (CR+OI) setting in the 4 diagrams in which this setting is present (Figures 4a, 4b, 4d, and 4e). In the inapplicable diagram (Figure 4c) from which this setting is absent, all samples plotted in the continental arc (CA) setting. Note that in all applicable diagrams, the samples plotted well inside the tectonic field. The corresponding probability values were very high (0.9703–0.9998; Table S14). The total percent probability estimates gave a high value of 83.5% for the within-plate setting.

For the second set of diagrams (Figure 2), only 23 samples (out of 34) had a complete data set (Ni

concentrations were missing for the remaining samples; Nonnotte *et al.* 2011). Nevertheless, these samples fully confirmed the expected continental rift setting for the Kilimanjaro volcano, because all 23 samples plotted in the within-plate field (Table S14). In the only diagram without the expected setting (Figure 2c), they belonged to the collision setting. The total percent probability of samples for the within-plate setting was high (79.9%).

All 34 samples from the Kilimanjaro volcano had complete data for the third set of trace element-based diagrams (Figure 3), which once again confirmed the within-plate setting (Table S14). All samples plotted in this field in all 4 applicable diagrams, whereas in the inapplicable diagram (Figure 3c), most of them plotted in the collision field, with a few samples belonging to the continental arc field. The total percent probability value for this setting was similarly high (80.3%).

Thus, we may conclude that all 3 sets of diagrams perform well for the continental rift setting discriminated as within-plate (CR+OI).

4.2.4. Samples from an ocean island setting

For evaluating our diagrams for the ocean island setting, samples of Pleistocene-Holocene rocks from the El Hierro and La Palma islands of the Canary Islands (Day *et al.* 2010) were compiled. Because most rocks from this setting are of ultrabasic and basic magmas, only 5 samples proved to be of intermediate magma type.

The first set of diagrams (Figure 4) successfully indicated a within-plate setting for these 5 samples (Table S15). The total percent probability (% prob) gave a very high value of 87.0%.

For the trace elements used in our second set of diagrams (Nb, Ni, V, Y, and Zr) based on the combination of immobile major and trace elements, Day et al. (2010) presented 2 sets of data by the analytical techniques used by them (X-ray fluorescence spectrometry [XRF] and inductively coupled plasma mass spectrometry [ICPMS]). Although the data for Nb, V, Y, and Zr generally showed only relatively small differences, those for Ni appeared to be drastically different (0–4 $\mu g~g^{\scriptscriptstyle -1}$ by XRF and 1.2–30.8 μ g g⁻¹ by ICPMS). These 2 sets of data (XRF and ICPMS) gave inconclusive and inconsistent results for the second set of diagrams (Figure 2). We report here only the results of our second diagram (Table S15) from the use of their ICPMS data. These results seem to be inconclusive because the samples are almost equally divided in within-plate and collision settings, with total percent probability (% prob) values of 48.2% and 51.8%, respectively.

Nevertheless, the third set of diagrams (Figure 3) provided conclusive results consistent with the first set of diagrams (Table S15). A within-plate setting was indicated for these ocean island samples with a high total percent probability of 79.6%, with the remaining probability of 20.4% for the collision setting.

4.2.5. Samples from a collision setting

For the evaluation of our diagrams (Figures 1-3) for the collision setting, Miocene ultrapotassic intermediate magmas from southern and southwestern Tibet, with 19 samples from Gao et al. (2007) and 35 from Zhao et al. (2009), clearly showed a collision setting in all 3 sets of diagrams. Most or all samples (52 to 54 out of 54 in the first set; Figures 4a and 4c-e; all 54 for the other 2 sets; Table S16) plotted in the collision field. When the collision field is absent in a diagram (Figure 4b; Table S16), the samples plotted in the within-plate field, except for the second set of diagrams (Figures 2a-2e; Table S16), in which some samples also plotted in the continental arc field. The total percent probability (% prob) values for the collision setting were therefore consistently high (78.8% to 84.1%; Table S16). Thus, all 3 sets of diagrams performed well for the collision tectonic setting.

4.2.6. Altered samples from the Central American Volcanic Arc

Seven samples of intermediate magma of corestone-shell complexes from Moyuta and Tecuamburro volcanoes of Guatemala (a part of the Central American Volcanic Arc; Patino et al. 2003) were used to evaluate the effects of spheroidal weathering in our multidimensional diagrams (Table S17). The samples from Tecuamburro are of Pliocene-Pleistocene age, whereas the age of the Moyuta samples may be Late Tertiary. A continental arc setting was still inferred for these highly altered rocks, because most of them (4 to 6 out of 7 samples; Figure 4; Table S17) plotted in the CA field. Although these authors did not report analyses of fresh rocks from these volcanoes, which might have helped to better understand the alteration effects in our multidimensional diagrams, we may hypothesize that these effects probably led some samples to plot in the collision field, with relatively high probabilities. Finally, from the total percent probability considerations, the samples showed 53.2% (% prob) total percent probability value for the continental arc setting, whereas the remaining probability (100 - 53.2 = 46.8%)was almost equally subdivided between the island arc and collision settings (23.7% and 23.1%, respectively; Table S17).

5. Application of discrimination diagrams to old terrains

We selected 7 case studies with ages varying from Archean to Phanerozoic to illustrate the application and excellent functioning of the multidimensional discrimination diagrams. The Archean to Proterozoic rocks were evaluated under the assumption of prevalence of plate tectonic processes and similar log_e-ratio geochemical variables for Archean to present-day tectonic regimes. For these applications, the plotting of samples in diagrams (Figures 1–3) was replaced by probability calculations (Table S18).

5.1. Wawa greenstone belt (Canada)

For the Late Archean Wawa greenstone belt in Canada, the 3 sets of diagrams for intermediate magma (32 samples; 14 from Polat et al. 1999 and 18 from Polat 2009) could be applied. The results are summarized in Table S18. The first set based on major elements (Figure 1) provided indecisive results because the samples were divided between arc and collision settings. The total percent probability values for island arc and collision settings (39.8% and 41.8%, respectively; Table S18) were very similar. The other 2 sets of diagrams based on relatively immobile elements, however, showed an island arc setting for the samples from the Wawa greenstone belt. The total percent probability values for this tectonic field were about 54.5% and 58.3%, respectively, for the second (Figure 2) and third (Figure 3) sets of diagrams. Therefore, an island arc setting can be inferred for this belt. This application to the Wawa greenstone belt also implies that similar plate tectonic processes as today might have been operative during the Archean (at about 2700 Ma; Table S18).

5.2. Southwestern Sweden

From the first set of diagrams applied to 13 intermediate samples of Paleoproterozoic intrusive rocks (1870–1780 Ma) of south-central Sweden (Rutanen & Andersson 2009), an arc setting could be certainly inferred (Table S18), although the discrimination of an island or continental arc was not decisive. The total percent probability estimates for these 2 settings were very similar (42.6% and 42.2%, respectively, for island and continental arcs; Table S18). No trace element data were published for these rocks. It is likely that the immobile element-based second and third sets of diagrams might provide a decision of island or continental arc setting for this area.

5.3. Adola (Ethiopia)

Twelve Neoproterozoic (885–765 Ma) intermediate rock samples from Adola, southern Ethiopia (Wolde *et al.* 1996), with complete major element data showed an island arc setting, because 8 to 10 samples had the highest probability for this field and the total percent probability (% prob) was 57.2% (Table S18). Eight of these samples had complete data for immobile element-based diagrams (Figures 2 and 3). An arc setting can be certainly inferred from these diagrams, as well. However, the major and trace element-based diagrams (Figure 2) indicated a continental arc setting with 60.8% total percent probability, whereas the trace element-based ones (Figure 3) showed an island arc setting with 59.1% total percent probability (Table S18).

5.4. Malani igneous complex (India)

Twenty-one samples of Neoproterozoic intermediate magma from the Malani igneous complex, Rajasthan, India (Maheshwari *et al.* 1996; Bhushan & Chandrasekaran 2002; Sharma 2004; Singh & Vallinayagam 2004), showed a within-plate setting, because 16 to 18 samples were discriminated as this tectonic environment and the

respective total percent probability was about 69.9% (Table S18). Only 2 samples had complete major and trace element data for our second set of diagrams, which also indicated a within-plate setting (results of too few samples, only 2, are not included in Table S18).

5.5. Tasmania (Australia)

Thirty-nine samples of Cambrian intermediate magma from western Tasmania, Australia (Brown & Jenner 1989), with complete data for only major elements, were discriminated as an island arc setting, because most (33 to 38 out of 39) samples showed high probabilities for this field. Their total percent probability (% prob) value for an island arc setting was about 68.5% (Table S18).

5.6. The Alps (Europe)

Six samples of intermediate rocks of about 295 Ma from the Alps (France-Italy-Switzerland; Debon & Lemmet 1999) clearly showed a collision setting during the Late Carboniferous, because in the major element-based diagrams (Figure 1) all 6 samples plotted in this field with high probabilities (total percent probability of 83.1%; Table S18). This result was fully consistent with the other 2 sets of diagrams (Figures 2 and 3), in which all samples (5 out of 5 in Figure 2 and 6 out of 6 in Figure 3) plotted in the collision field (Table S18). The corresponding total percent probability values were very high (83.3% and 80.9%, respectively, for these 2 sets of diagrams based on immobile elements) for the Col setting.

5.7. Chichijima Island (Japan)

Finally, our last case study concerns the Bonin Archipelago, which represents an uplifted fore-arc area exposing the products of Eocene suprasubduction zone magmatism, with Chichijima Island being the type locality for boninite rocks (Taylor *et al.* 1994). An island arc setting was fully confirmed for the Chichijima Island during the Eocene, because all 35 intermediate rock samples plotted in the arc field with very high probabilities (0.6453–0.9998; Table S18). The total percent probability for the island arc field was also very high (77.3%; Table S18).

6. Evaluation of discrimination diagrams for element mobility and petrogenetic processes

We now briefly present the evaluation of our diagrams for compositional changes related to element mobility and petrogenetic processes of fractional crystallization (FC) and combined assimilation and fractional crystallization (AFC). Instead of plotting the data in diagrams (Figures 1–3), the probabilities for the 3 tectonic settings in a given diagram were calculated. The interpretation was based on these probability estimates.

6.1. Analytical errors, mobility of elements, and alteration effects

Extreme models of compositional changes were considered that may arise from analytical errors, mobility of elements

caused by postemplacement processes such as weathering, Fe-oxidation, and low or even high temperature rock alteration. For simplicity and better understanding of the results, only changes (both gain and loss) of one element at a time were considered. From our 5-part database (see Tables S1 and S2), the mean compositions (centroid values) of compiled rocks for each tectonic setting were calculated and the models were evaluated for changes in these centroid compositions. For the first set of diagrams (Figure 1), these extreme models included $\pm 10\%$ changes for SiO₂; ±20% for TiO₂, Al₂O₃, Fe₂O₃, FeO, MgO, CaO, and P2O5; and ±40% for MnO, Na2O, and K2O. Similarly, for immobile element-based diagrams of the second and third sets (Figures 2 and 3), large gains or losses of $\pm 20\%$ were modeled for all corresponding major and trace elements. Greater than ±10% changes in SiO₂ were not considered realistic because the magma type may change to acid (from the gain of SiO₂) or basic (from the loss of SiO₂), which will render the present diagrams inapplicable to the modified or altered rocks. The results are summarized in Tables S19-S21 for the 3 sets of diagrams.

6.1.1. First set of diagrams

The first example of element mobility (SiO₂; Table S19) is described in detail. The probabilities for the expected tectonic field of the centroids (see the boldface probability values in the first row for the diagram type 1+2-3+4-5 in Table S19) for the IA discriminated as the combined arc (IA+CA) setting, the CA discriminated as IA+CA, the CR discriminated as within-plate, the OI discriminated as within-plate, and the Col discriminated as Col, were, respectively, 0.92046, 0.88378, 0.92458, 0.98888, and 0.94785. Although all centroids should plot well within the respective tectonic field (all probability values >> 0.5), the CA centroid (probability of 0.88378) would be somewhat closer to one of the tectonic field boundaries, whereas the OI centroid (probability of 0.98888) would be the much more inside the within-plate tectonic field, even more so than the CR centroid (probability of 0.92458) or the Col centroid (probability of 0.94785). For +10% change (gain) in SiO₂ (see the first value in all columns of the second row of Table S19), these probability values changed to about 0.8898, 0.8402, 0.8624, 0.9803, and 0.9710, respectively. Thus, the 10% increase in SiO, caused a probability change in the IA centroid of about (0.8898 - 0.92046) = -0.0306(about -3.3%). For the other centroids, the probability changes were -0.0436 (-4.9%) for CA, -0.0622 (-6.7%) for CR, -0.0085 (-0.9%) for OI, and +0.0231 (+2.4%) for Col. All centroids remained within the original tectonic field, because the new probability values (range: 0.8402-0.9803; see the first value in each column of the second row of Table S19) for their respective fields were still very high (>>0.5). For 4 tectonic settings (IA, CA, CR, and OI) the centroid probability slightly decreased (by about

-0.0085 to -0.0622, amounting to about -0.9% to -6.7%). In other words, this SiO₂ mobility caused these centroids to move towards one of the boundaries (Figure 1a). For the Col setting, however, the centroid probability slightly increased from about 0.94785 to 0.9710 (about +0.0231; +2.4%), causing this centroid to plot still more inside this tectonic field.

Similarly, the -10% change (loss) in SiO₂ rendered the IA, CA, CR, OI, and Col centroid probabilities to become 0.9363, 0.9075, 0.9599, 0.9936, and 0.9005 (see the second value in each column of the second row of Table S19), i.e. the 10% decrease in SiO₂ caused probability changes of about +0.0158 (+1.7%), +0.0237 (+2.7%), +0.0353 (+3.8%), 0.0047 (+0.5%), and -0.0473 (-5.0%), respectively. These probability changes and the centroid movements are just in the opposite direction as compared to those for the SiO₂ gain, but the percent probability changes are not exactly the same. More importantly, for both SiO₂ gain as well as its loss, the centroids remained well within the respective tectonic fields and the percent probability changes (-6.7% to +3.8%) were much less than the changes of SiO₂ concentration (±10%).

For even larger changes in other major elements ($\pm 20\%$ to $\pm 40\%$; Table S19), none of the compositional changes caused any of the centroids in this first major elementbased diagram (Figure 1a) to move outside the respective tectonic field. Therefore, we can safely conclude that the performance of this diagram (Figure 1a) is not seriously affected by element mobility from $\pm 10\%$ to $\pm 40\%$. In other words, this diagram is particularly robust against such extreme concentration changes.

In the behavior of the second diagram of the first set (Figure 1b; see diagram type 1-2-3+4 in Table S19), in which both IA and CA fields are discriminated in the presence of the within-plate (CR+OI) field, the effects of compositional changes were less robust for these 2 very similar tectonic settings (IA and CA). The IA and CA centroids showed relatively low probabilities (0.61392 and 0.59320, respectively; see the second part of Table S19) and, consequently, would plot in Figure 1b closer to the tectonic field boundaries than the other 2 centroids (CR and OI, with probabilities of 0.95535 and 0.98472, respectively). The latter 2 centroid values obviously plotted well inside the within-plate field, away from the field boundaries (Figure 1b). The collision field is absent from this second diagram. The changes in SiO₂, TiO₂, Fe₂O₃, MgO, K₂O, and P_2O_5 were large, but did not cause any of the arc centroids to move outside their tectonic fields, whereas the changes modeled for the other elements (+20% for Al₂O₃, +40% for Na₂O, -40% for MnO, and -20% for CaO) led the IA centroid to move into the CA field (Table S19). Similarly, the CA centroid moved into the IA setting for +20% FeO, +40% MnO, +20% CaO, -20% Al₂O₃, and -40% Na₂O.

For a given sample, however, there can be either a gain or a loss of an element. Therefore, misdiscrimination will occur only for a lower number of cases than those listed above. For example, if there were a gain of Al₂O₂ of about +20%, a sample from only the island arc setting is likely to be misdiscriminated in the continental arc setting, but not a sample from the continental arc setting; in fact, as a result of Al₂O₃ gain, this latter sample is likely to plot still more inside the continental arc field (the new probability value of 0.7344 is greater than the initial value of 0.59320 for the CA centroid; see Table S19). Nevertheless, because these 2 environments (IA and CA) are subduction-related settings, the misdiscrimination is not of too serious consequences. Note also that none of the compositional changes significantly affect the CR and OI centroids. All probability values remain consistently very high, 0.8115-0.9958; see the second part of Table S19.

In the third diagram of this set (Figure 1c; 1-2-5 type), the behavior of IA and CA was similar to the earlier diagram (Figure 1b), but for the Col setting, the discrimination results could be considered more robust against such compositional changes (Table S19). The misdiscrimination of the IA centroid as the CA setting was for Al_2O_3 gain (+20%), Na_2O gain (+40%), and MnO loss (-40%). Similarly, the CA centroid moved into the IA field for MnO gain (+40%), Al_2O_3 loss (-20%), and Na_2O loss (-40%). On the other hand, the Col centroid (Figure 1c) was little affected by any of the changes listed in Table S19; in all cases, it remained in the same tectonic field with high probability values of 0.7803–0.9949.

The fourth and fifth diagrams (Figures 1d and 1e; 1-3+4-5 and 2-3+4-5), in which both arc settings are not simultaneously present (Figure 1d has only IA whereas Figure 1e has only CA, along with the other 2 within-plate and Col settings), were observed to be totally immune to all the above-mentioned compositional changes. All centroids remained well within their respective fields and generally showed very high probability values (Table S19).

The major element-based diagrams perform well in spite of the large gains or losses modeled for any of these major elements. A possible explanation of such a good performance of our first set of diagrams may be related to the processing of the chemical data in SINCLAS and also the log_e-ratio transformation that is involved in all of them; see Eqs. (1) through (10) above.

Simultaneous gains or losses of 2 or more elements will not really change our conclusions. In fact, because some log_e-ratio terms in Eqs. (1) through (10) have positive signs, whereas the others have negative signs, simultaneous gains or losses of 2 elements may affect the final probability values even less; see Eqs. (31) through (39). For other cases, simultaneous gains and losses of 2 elements that appear in Eqs. (1) through (10) with the same sign may also keep the final probability changes to small values. The simple oxidation process of FeO to Fe_2O_3 , without any significant gain or loss of total Fe, will not affect our diagrams because all major element data are always readjusted from the SINCLAS computer program (Verma *et al.* 2002) to 100% on an anhydrous basis along with a prior adjustment of Fe_2O_3 /FeO according to Middlemost's proposal (1989) for the least oxidized rock samples. The adjusted data should always be used for plotting the samples in Figures 1a–1e and calculating the respective probabilities in Eqs. (31) through (39).

6.1.2. Second and third sets of diagrams

Our results of element mobility in the remaining 2 sets of diagrams (Figures 2 and 3; Tables S20 and S21) are now briefly presented. Because both sets of diagrams are based on relatively immobile elements, the calculations for $\pm 20\%$ changes in the concentration of these elements probably represent extreme variations not likely to occur in most actual situations. The second set of diagrams based on 3 major and 5 trace elements was shown to be generally robust for all tectonic settings. The centroids remained in the expected field in practically all cases. The few exceptions were as follows (Table S20): MgO loss (-20%) caused the CR centroid to move to the Col setting in the first, fourth, and fifth diagrams (Figures 2a, 2d, and 2e); and P₂O₅ gain (+20%) and Y loss (-20%) caused the IA centroid to move to the within-plate (CR+OI) setting in the second and third diagrams (Figures 2b and 2c). However, the centroids remained rather close to the boundaries of the tectonic field to which they moved.

The third set of diagrams (Figures 3a-3e) based on immobile trace elements proved to be totally immune to these compositional changes (Table S21). The extremely large changes (gains or losses of ±20%) did not cause even a single centroid to move to a different tectonic field; all centroids remained well inside the original tectonic setting in all diagrams. Because concentration changes of only 1 element at a time were modeled, the probability values represent the highest changes compared to the simultaneous changes of 2 or more elements; see Eqs. (21) through (30) for DF1-DF2 functions and (31) through (39) for probability calculations. For example, because Yb was used as the common denominator, its gain or loss will affect most mathematical terms in Eqs. (21) through (30), and will probably cause more changes in the resulting probability values than the other elements. However, the probability changes caused by Yb gain or loss could be lower if other elements also changed simultaneously, which could be a more likely process to occur in nature. For the changes in other trace elements, the probability values of the IA, CA, CR, OI, and Col centroids (Figure 3a) changed respectively from 0.97541, 0.91223, 0.97804, 0.99661, and 0.98297 to about 0.9088-0.9899, 0.7884-0.9733, 0.9421-0.9933, 0.9908-0.9990, and 0.9523-0.9917. Similarly,

small changes in probabilities were also observed in all other diagrams (Figures 3b–3e; Table S21).

The best performance of this set of diagrams as compared to the other 2 sets is an extremely important result of our modeling. This also implies that in case of inconsistency in the inferences of these 3 sets of diagrams for practical applications, this third set should be given more weight in decision making, i.e. in the case of inconsistent results, our decision can be based on this set of diagrams unless other independent geological, geochemical, or geophysical evidence were available to favor the results of other diagrams.

6.2. Petrogenetic process of bulk assimilation

Bulk assimilation of crust may be a petrogenetic process worth evaluating for its effects in our diagrams. For illustration purposes, we used the average upper continental crust (Taylor & McLennan 1995) and mixed 10% and 20% of this crust (UCC) with the centroids of our database. Still greater percentages of bulk assimilation were not modeled for 2 reasons: the magma type might change from intermediate to acid, in which case these diagrams should not be used; and the intermediate magma may not have a sufficient heat budget to assimilate greater proportions of crust. Other crustal compositions summarized by Taylor and McLennan 1995) could not be used because of the lack of P data for all of them.

In the first diagram (figure type 1+2-3+4-5; Table S22), UCC would plot well within the collision field (probability of 0.98306 for Col). From mixing of UCC, all centroids moved towards the boundary with the Col setting, but even with 20% UCC all of them remained in their respective fields (Table S22). As expected, the Col centroid showed only the smallest change in its probability. In the second diagram (figure type 1-2-3+4), UCC plotted in the withinplate field, whereas in all the remaining diagrams of this set, UCC plotted well within the Col setting. None of the centroids moved outside their fields in any of the major element-based diagrams (Table S22).

In the second set of diagrams, the results of bulk assimilation of UCC were practically similar, although for a few cases of 20% bulk assimilation the centroids moved to a different field. These include the following instances: the IA and CA moved to the Col setting in the first (figure type 1-2-3+4-5) and third (figure type 1-2-5) diagrams; the IA moved to Col in the fourth (figure type 1-3+4-5) diagram; and the CA moved to Col in the fifth (figure type 2-3+4-5) diagram.

In the third set of diagrams, the UCC plotted in the within-plate field except in diagram 1-2-5, where UCC plotted in the Col field. However, the centroids remained in their original fields (Table S22). Once again, this trace element-based diagram showed an excellent performance and robustness against the bulk assimilation process.

6.3. Petrogenetic process of fractional crystallization

Basic magma may undergo FC to produce intermediate magma. To model the effects of this process in our trace element-based diagrams (third set), the mean compositions of basic magma (see footnote of Table S23) from 3 tectonic settings (arc, continental rift, and ocean island) from the extensive database of Verma and Agrawal (2011) were estimated. For modeling the FC of common minerals (olivine, clinopyroxene [cpx], orthopyroxene [opx], and plagioclase [plg]), the partition coefficient data compiled by Torres-Alvarado *et al.* (2003) were used for extreme mineral fractionation of 50% (Table S23).

Verma and Agrawal (2011) had not made any distinction between island and continental arcs. The average composition (centroid) of arc basic rocks from their compilation plotted in the IA+CA field in diagram 1+2-3+4-5 (probability of 0.86271; Table S23); in the CA field in 1-2-3+4 (0.55888), 1-2-5 (0.48481) and 2-3+4-5 (0.88619) diagrams; and in the IA field in diagram 1-3+4-5 (0.80111). Similarly, the average composition of basic magma from the CR or OI setting plotted in the withinplate setting in all applicable diagrams (probability values of 0.97864-0.99620 for CR and 0.98237-0.99730 for OI). The initial probability for basic magma from the arc setting was distributed between the IA and CA settings in diagrams in which both IA and CA fields were present (0.42952 and 0.55888 in diagram 1-2-3+4, and 0.46586 and 0.48481 in diagram 1-2-5; Table S23).

The FC process generally did not drastically change the probability values for the basic magmas. For example, in the first diagram (1+2-3+4-5), the initial probability for the arc magma changed from 0.86271 to 0.8240, 0.5298, 0.9485, and 0.8598 for FC of olivine, cpx, opx, and plg, respectively. For the within-plate setting, the CR and OI basic magmas showed even much smaller changes. As an example, in the first diagram (1+2-3+4-5), the probability values for CR changed from 0.98273 to 0.9795–0.9847 and for OI from 0.98691 to 0.9845–0.9884.

In diagrams 1-2-3+4 and 1-2-5, in which both IA and CA settings are present as separate fields, the probabilities of arc basic magma after the FC process still showed that the evolved magma should plot in either of these 2 fields. For all basic magmas, thus, the evolved (probably intermediate) magmas obtained from the FC process remained within the expected field (Table S23). The only exception to this was in the fourth diagram (1-3+4-5) for the IA field, for which the evolved magma after 50% FC of cpx moved from the IA to Col setting (Table S23).

6.4. Petrogenetic process of assimilation coupled with fractional crystallization

The AFC process (DePaolo 1981) was also modeled for the basic magma compositions of the above section. More complex petrogenetic processes, such as those put forth by Spera and Bohrson (2004), were not considered because our aim was to understand the behavior of our complex diagrams for simple petrogenetic processes. Evaluation of more complex petrogenetic processes should constitute a separate study.

Two probably extreme models were considered and the results are presented in Table S24. The first model (r = 0.2 and $F_{remain} = 0.7$; Table S24) showed only a few cases in which the arc basic magma centroid moved to a different field. This took place for the arc centroid in diagram 1-3+4-5, where for the AFC process (A of UCC and FC of cpx) this centroid moved from the IA field to the collision setting, but only very close to the field boundary (the probabilities for IA and Col were about 0.4304 and 0.4355, respectively). For the second extreme model (r = 0.4 and $F_{remain} = 0.5$; Table S24), more cases of the arc centroid were misdiscriminated (Table S24). However, none of the 2 models affected the CR and OI centroids in any of the 5 diagrams. Nevertheless, the second AFC model should be considered as an extreme situation and less likely to occur in nature, because under such circumstances the evolved magma may even change to the acid type, rendering the present diagrams inapplicable to them.

7. Reasons for the good functioning of multidimensional diagrams

Why do the multidimensional diagrams based on LDA of log_-transformed ratios work so well? The high success rates documented above for all diagrams (Figures 1-3; Tables S5, S8, and S11); the excellent performance obtained for the 3 sets of diagrams from the testing examples (Figure 4; Tables S12-S17); the generally consistent inferences from the 7 application studies for Archean to Phanerozoic rocks (Table S18); and the overall best performance and minimal effects from compositional changes caused by analytical errors, element mobility, Fe-oxidation, and rock alteration (Tables S19-S21), as well as from bulk assimilation of crust (Table S22), fractional crystallization of common minerals (Table S23), and assimilation of upper crust coupled with fractional crystallization of common minerals (Table S24), are all worthy of mention. More important, however, would be the possible reasons for these favorable results.

There may be several reasons for such an excellent functioning of these diagrams. First, the basic condition of representativeness of the database is fulfilled when the samples from all over the world (Table S1) are compiled. All 5 tectonic groups are well chosen and represented (Table S2). Other reasons may be related to coherent statistical handling of compositional data (Verma 2012b; see also Aitchison 1986). Besides these reasons, the multivariate technique of LDA is centered around minimizing the effects of petrogenetic processes and maximizing the separation among the different tectonic groups being discriminated (Verma 2012a). The complex multiplication factors with both positive and negative signs in Eqs. (1) through (30) may also be considered an asset rather than a disadvantage of these multidimensional diagrams. The probabilitybased boundaries further provide a better objective statistical method in comparison to the commonly used subjective method of determining the boundaries by eye judgment (Agrawal 1999; Agrawal & Verma 2007). Probability-based decisions in Eqs. (31) through (39) also constitute an important aspect of the new diagrams. The total percent probability calculations seem to provide an innovative way to interpret geochemical discrimination diagrams (Verma 2012a). Our interpretation in terms of these total percent probability estimates instead of simply counting the number of samples also seems helpful in this respect.

A computer program for efficiently processing the geochemical data for new applications is currently under preparation, which should be available in the future to potential users of our diagrams. In the meantime, we have developed a Statistica spreadsheet to facilitate such applications.

8. Conclusions

The 15 multidimensional diagrams with high success rates for intermediate magma, put forth in this work from correct statistical treatment of \log_{e} -ratio transformation, discordant outlier-free database, multivariate technique of

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LDA, probability-based boundaries, and associated sample probability and total percent probability calculations as a replacement for plotting samples, are shown to work well for relatively fresh to highly altered rocks of almost all ages from several areas around the world, and are therefore recommended to be used to decipher the tectonic settings of any area of interest. The robustness of all diagrams, especially those based on immobile trace elements, against the compositional changes from analytical errors and element mobility, as well as petrogenetic processes, is also well documented. This implies that these multidimensional diagrams can be safely used for deciphering the tectonic setting of old terrains as well as tectonically complex areas.

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Region	References, arranged chronologically
	Island arcs
Aegean	Huijsmans et al. 1988; Mitropoulos et al. 1987; Zellmer et al. 2000; Vespa et al. 2006
Alaskan peninsula	Hildreth <i>et al.</i> 2004
Aleutians	Kay <i>et al.</i> 1982; Myers <i>et al.</i> 1985, 2002; Brophy 1986; Nye & Reid 1986; Romick <i>et al.</i> 1990; Singer <i>et al.</i> 1992; Kay & Kay 1994
Barren Islands	Alam <i>et al.</i> 2004; Luhr & Haldar 2006
Burma	Stephenson & Marshall 1984
Indonesian islands (Java, Sangihe, Sua, Sulawesi, Sunda- Banda)	Foden & Varne 1980; Wheller <i>et al.</i> 1987; Stolz <i>et al.</i> 1990; Tatsumi <i>et al.</i> 1991; van Bergen <i>et al.</i> 1992; Edwards <i>et al.</i> 1994; Hoogewerff <i>et al.</i> 1997; Elburg & Foden 1998; Turner & Foden 2001; Elburg <i>et al.</i> 2003; Toya <i>et al.</i> 2005; Chadwick <i>et al.</i> 2007; Sendjaja <i>et al.</i> 2009; Takanashi <i>et al.</i> 2011
Izu-Bonin	Tatsumi et al. 1992; Taylor & Nesbitt 1998; Ishizuka et al. 2003, 2006; Shukuno et al. 2006; Tamura et al. 2007
Japan	 Hickey & Frey 1982; Sakuyama & Nesbitt 1986; Togashi <i>et al.</i> 1992; Tamura 1994; Taylor <i>et al.</i> 1994; Ujike & Stix 2000; Kita <i>et al.</i> 2001; Sano <i>et al.</i> 2001; Kimura <i>et al.</i> 2002; Tamura <i>et al.</i> 2003; Moriguti <i>et al.</i> 2004; Toya <i>et al.</i> 2005; Shuto <i>et al.</i> 2004, 2006; Kuritani <i>et al.</i> 2005, 2008; Hirotani & Ban 2006; Kimura & Yoshida 2006; Ban <i>et al.</i> 2007; Ohba <i>et al.</i> 2007, 2009; Sato <i>et al.</i> 2007; Suzuki & Nakada 2007; Hoang <i>et al.</i> 2011; Takanashi <i>et al.</i> 2011
Kamchatka	Kepezhinskas et al. 1997; Dorendorf et al. 2000; Churikova et al. 2001; Ishikawa et al. 2001; Izbekov et al. 2004
Kuril	Zhuravlev et al. 1987; Nakagawa et al. 2002
Lau	Tian <i>et al.</i> 2008
Lesser Antilles	Brown <i>et al.</i> 1977; Thirlwall & Graham 1984; Smith <i>et al.</i> 1996; Thirlwall <i>et al.</i> 1996; Turner <i>et al.</i> 1996; Defant <i>et al.</i> 2001; Zellmer <i>et al.</i> 2003; Lindsay <i>et al.</i> 2005; Halama et al. 2006
Marianas	Hickey & Frey 1982; Hole <i>et al.</i> 1984; Reagan & Meijer 1984; Woodhead 1988; Bloomer 1987; Bloomer & Hawkins 1987; Bloomer <i>et al.</i> 1989; Elliott <i>et al.</i> 1997; Wade <i>et al.</i> 2005; Reagan <i>et al.</i> 2008
New Britain	Woodhead et al. 1998; Woodhead & Johnson 1993
New Caledonia	Cameron 1989
New Hebrides	Dupuy et al. 1982; Monzier et al. 1993, 1997
New Zealand (Northland, Taupo)	Cole 1981; Gamble et al. 1993; Huang et al. 2000; Schmitz & Smith 2004; Booden et al. 2011
Papua New Guinea	Hickey & Frey 1982
Philippines (Arayat, Bataan, Bicol, Luzon)	Defant <i>et al.</i> 1989, 1991b; Bau & Knittel 1993; Knittel <i>et al.</i> 1997; Castillo & Newhall 2004; McDermott <i>et al.</i> 2005; DuFrane <i>et al.</i> 2006
Ryukyu	Shinjo 1998, 1999; Shinjo et al. 2000
Solomon	Chadwick et al. 2009
South Shetland	Smellie 1983
Taiwan	Lai <i>et al.</i> 2008
Tonga-Kermadec	Bryan <i>et al.</i> 1972; Ewart & Bryan 1972; Ewart <i>et al.</i> 1977; Gamble <i>et al.</i> 1993, 1995; Haase <i>et al.</i> 2002; Smith <i>et al.</i> 2003; Wright <i>et al.</i> 2006; Hergt & Woodhead 2007
Vanuatu	Barsdell 1988; Barsdell & Berry 1990; Peate et al. 1997
Yap arc system	Ohara <i>et al.</i> 2002
	Continental arcs
Argentina	Déruelle 1982; Sruoga et al. 2005; Bruni et al. 2008
Antarctica	Kelly et al. 2008
Bolivia	Vezzoli <i>et al.</i> 2008
Chile	Saunders <i>et al.</i> 1979; López-Escobar <i>et al.</i> 1981, 1991, 1993; Déruelle 1982; Frey <i>et al.</i> 1984; Hickey <i>et al.</i> 1986; Kay <i>et al.</i> 1987, 1988; Davidson <i>et al.</i> 1988; Gerlach <i>et al.</i> 1988; Hickey-Vargas <i>et al.</i> 1989; de Silva 1991; Tormey <i>et al.</i> 1991; Vergara <i>et al.</i> 1991, 2004; Walker <i>et al.</i> 1991; Rodríguez <i>et al.</i> 2007; Vezzoli <i>et al.</i> 2008
Costa Rica	Reagan & Gill 1989; Chan et al. 1999; Alvarado et al. 2006; Bolge et al. 2006; Ryder et al. 2006
Ecuador	Bryant et al. 2006; Hidalgo et al. 2007; Robin et al. 2009; Samaniego et al. 2012

Table S1. Locations and literature sources for the 5-part database.

Table S1. (continued).

El Salvador	Carr 1984; González Partida et al. 1997; Rotolo & Castorina 1998; Chan et al. 1999; Agostini et al. 2006
Guatemala	Bardintzeff & Deniel 1992; Duffield et al. 1992; Chan et al. 1999; Walker et al. 2000; Cameron et al. 2002
Honduras	Walker et al. 2000
Mexico (Sierra Madre	Albrecht & Coldstein 2000
Occidental)	Abrent & Goldstein 2000
Nicaragua	Sussman 1985; Hazlett 1987; Carr et al. 1990; Chan et al. 1999; Walker et al. 2001; Pardo et al. 2008
Panama	Defant <i>et al.</i> 1991a, 1991c
USA (Alaska,	Reagan et al. 2003
California, Oregon)	
	Continental rifts and break-up regions
Afar	Barberi <i>et al.</i> 1975; Deniel <i>et al.</i> 1994
Australia	Johnson et al. 1989; Price et al. 1997
China	Peng et al. 1986; Zhi et al. 1990; Basu et al. 1991; Fan & Hooper 1991; Liu et al. 1992; Chung et al. 1995; Zhang et al. 1995; Han et al. 1999; Ho et al. 2000; Hsu et al. 2000; Zou et al. 2000; Y.G. Xu et al. 2005
Ethiopia	Hart <i>et al.</i> 1989; Trua <i>et al.</i> 1999; Peccerillo <i>et al.</i> 2003, 2007; Ayalew <i>et al.</i> 2006; Rooney <i>et al.</i> 2007; Ronga <i>et al.</i> 2010
France	Chauvel & Jahn 1984
Germany	Haase <i>et al.</i> 2004
Kenya	Bell & Peterson 1991; Kampunzu & Mohr 1991; Macdonald <i>et al.</i> 1995, 2008; Kabeto <i>et al.</i> 2001; Le Roex <i>et al.</i> 2001; Rogers <i>et al.</i> 2004
Japan (Beppu- Shimbara graben)	Kita et al. 2001; Sakuyama et al. 2009
Mali and Morocco Mexico (Fastern	Bertrand 1991
Alkaline Province, Tepic-Zacoalco rift)	Nick 1988; Frey et al. 2007
New Zealand	Timm <i>et al.</i> 2009
Philippines	Arpa <i>et al.</i> 2008
Republic of Congo	de Mulder <i>et al.</i> 1986
Saudi Arabia	Camp et al. 1991
Sudan	Davidson & Wilson 1989
Tanzania	Paslick et al. 1995; Mollel et al. 2008; Fontijn et al. 2010
Turkey	Besang et al. 1977; Karsli et al. 2008
Uganda	Llvod <i>et al.</i> 1991
USA (Basin and Range, Colorado, Fish Canyon, Nevada, Rio Grande Rift)	Singer & Kudo 1986; Johnson & Lipman 1988; Moyer & Esperança 1989; Perry <i>et al.</i> 1990; Duncker <i>et al.</i> 1991; Fitton <i>et al.</i> 1991; Kempton <i>et al.</i> 1991; Gibson <i>et al.</i> 1992; Feuerbach <i>et al.</i> 1993; Potter 1996; Bachmann <i>et al.</i> 2002; McMillan <i>et al.</i> 2000; Parat <i>et al.</i> 2005; Maldonado <i>et al.</i> 2006; Brueseke & Hart 2009
Zaire	Auchapt et al. 1987
	Ocean islands
Atlantic (Tropic seamount)	Blum <i>et al.</i> 1996
Azores (Sao Miguel)	Turner et al. 1997; Beier et al. 2006
Bouvet	Verwoerd <i>et al.</i> 1976
Canary Islands (Granadilla, Gran Canaria, La Palma, Tenerife)	Palacz & Wolff 1989; Bryan 2006; Praegel & Holm 2006; Jutzeler <i>et al.</i> 2010
Cape Verde	Holm <i>et al.</i> 2006
French Polynesia (Cook-Austral)	Palacz & Saunders 1986

Table S1. (continued).

Hawaiian Islands	Feigenson <i>et al.</i> 1983; Spengler & Garcia 1988; Lipman <i>et al.</i> 1990; West <i>et al.</i> 1992; Frey <i>et al.</i> 1994; Cousens <i>et al.</i> 2003; G. Xu <i>et al.</i> 2005, 2007					
Heard	Barling et al. 1994					
Kerguelen	Weis <i>et al.</i> 1993					
Madeira	Geldmacher & Hoernle 2000					
Pitcairn	Hekinian <i>et al.</i> 2003					
Réunion	Albarède et al. 1997					
Socorro	Bohrson & Reid 1995, 1997					
Collision						
Azerbaijan	Dilek <i>et al.</i> 2010					
Greece	Seymore & Vlassopoulos 1992; Pe-Piper & Moulton 2008					
India (Himalayas)	Reichardt et al. 2010					
Indonesia (Sulawesi)	Elburg & Foden 1999; Elburg et al. 2003					
Iran	Omrani et al. 2008					
Italy	Bellieni et al. 1981; Dini et al. 2002; Cadoux & Pinti 2009					
Pakistan (Karakorum)	Mahéo <i>et al.</i> 2009					
Tibet	Arnaud et al. 1992; Chen et al. 2010					
Turkey	Borsi <i>et al.</i> 1972; Innocenti & Mazzuoli 1972; Besang <i>et al.</i> 1977; Ercan <i>et al.</i> 1979, 1985, 1997; Ertürk 1990; Esder 1992; Güleç 1991; Seyitoglu <i>et al.</i> 1997; Aydar <i>et al.</i> 1998; Keskin <i>et al.</i> 1998; Temel <i>et al.</i> 1998; Aldanmaz <i>et al.</i> 2000; Delaloye & Bingol 2000; Ilbeyli <i>et al.</i> 2004; Innocenti <i>et al.</i> 2005; Aydin <i>et al.</i> 2008; Ekici <i>et al.</i> 2009; Agostini <i>et al.</i> 2010					

		Tot	al number of sam	ples
Tectonic setting §	Group number §	Major elements	Major and trace elements	Trace elements
IA	1	1552	873	671
CA	2	726	340	301
CR	3	517	221	241
OI	4	277	77	136
Col	5	592	357	163
Sum	1-5	3664	1868	1512

Table S2. Number of samples in the training set of normally distributed discordant outlier-free database.

IA = island arc (group number 1); CA = continental arc (group number 2); CR = continental rift (group number 3); OI = ocean island (group number 4); Col = collision (group number 5).

Original (wt.% or μg g ⁻¹) or log _e -transformed ratio variable	IA (n = 1	(1) 1552)	CA (n =	(2) 726)	CR (n =	(3) 517)	OI (n =	(4) 277)	Col (n =	(5) 592)
	\overline{X}	S	\overline{X}	S	\overline{X}	S	\overline{X}	S	\overline{X}	S
(SiO ₂) _{adj}	56.23	3.17	56.39	3.17	56.55	3.55	56.69	3.66	58.45	3.00
(TiO ₂) _{adj}	0.838	0.217	0.862	0.276	1.48	0.66	1.46	0.77	0.938	0.317
$(Al_2O_3)_{adi}$	17.52	1.38	18.16	1.41	16.19	1.91	17.57	2.63	16.76	1.55
$(\mathrm{Fe}_{2}\mathrm{O}_{3})_{\mathrm{adj}}$	1.960	0.301	1.860	0.281	2.18	0.50	1.94	0.64	1.637	0.281
(FeO ₂) _{adi}	6.15	1.15	5.81	1.10	6.03	1.78	5.19	2.48	4.47	0.92
(MnO) _{adi}	0.1664	0.0291	0.1489	0.0325	0.174	0.066	0.206	0.071	0.1135	0.0312
(MgO) _{adi}	4.41	1.76	4.02	1.30	3.69	2.41	2.74	2.61	3.84	1.74
(CaO) _{adi}	8.33	1.59	7.89	1.51	6.09	2.64	4.76	3.23	6.73	1.44
(Na ₂ O) _{adi}	3.15	0.65	3.50	0.57	4.27	1.50	5.50	2.08	3.43	0.74
$(K_2O)_{adi}$	1.06	0.65	1.14	0.66	2.89	1.89	3.57	2.25	3.25	1.63
$(P_2O_5)_{adj}$	0.189	0.102	0.220	0.077	0.438	0.321	0.379	0.350	0.383	0.256
ln(TiO ₂ /SiO ₂) _{adj}	-4.237	0.276	-4.227	0.328	-3.75	0.55	-3.85	0.72	-4.180	0.338
$\ln(Al_2O_3/SiO_2)_{adi}$	-1.168	0.108	-1.135	0.111	-1.256	0.120	-1.181	0.128	-1.252	0.107
ln(Fe ₂ O ₃ /SiO ₂) _{adj}	-3.367	0.180	-3.421	0.184	-3.285	0.283	-3.436	0.417	-3.588	0.197
$\ln(\text{FeO}_2/\text{SiO}_2)_{adj}$	-2.229	0.231	-2.289	0.239	-2.289	0.390	-2.52	0.60	-2.589	0.238
$\ln(MnO/SiO_2)_{adj}$	-5.836	0.190	-5.961	0.263	-5.843	0.350	-5.668	0.293	-6.278	0.291
ln(MgO/SiO ₂) _{adi}	-2.620	0.429	-2.696	0.388	-3.06	1.00	-3.55	1.14	-2.81	0.46
ln(CaO/SiO ₂) _{adi}	-1.928	0.252	-1.986	0.254	-2.38	0.69	-2.81	0.98	-2.183	0.257
$\ln(\text{Na}_2\text{O}/\text{SiO}_2)_{adi}$	-2.901	0.188	-2.790	0.139	-2.635	0.294	-2.415	0.394	-2.860	0.227
ln(K ₂ O/SiO ₂) _{adi}	-4.15	0.59	-4.04	0.50	-3.21	0.71	-3.14	1.02	-3.01	0.50
$\ln(P_2O_5/SiO_2)_{adi}$	-5.82	0.50	-5.598	0.326	-5.12	0.80	-5.49	1.12	-5.19	0.58

Table S3. Mean and standard deviation of adjusted major elements and log-transformed ratios for the 5 tectonic settings (IA, CA, CR, OI, and Col) for discordant outlier-free samples.

 \overline{X} = mean; *s* = standard deviation. The data are presented as rounded values obtained from the flexible rules summarized by Verma (2005).

Table S4. Test of equality of group means for 10 \log_{e} -transformed major element ratio variables in the discordant outlier-free samples summarized in Table S3.

Variable	Wilks' lambda	F-ratio	Significance
ln(TiO ₂ /SiO ₂) _{adj}	0.2522	247.53	0.000000
$\ln(Al_2O_3/SiO_2)_{adj}$	0.2053	31.97	0.000000
$\ln(Fe_2O_3/SiO_2)_{adj}$	0.2016	14.75	0.000000
ln(FeO/SiO ₂) _{adj}	0.2061	35.77	0.000000
ln(MnO/SiO ₂) _{adj}	0.2240	118.15	0.000000
ln(MgO/SiO ₂) _{adj}	0.2002	8.43	0.000001
ln(CaO/SiO ₂) _{adj}	0.2121	63.20	0.000000
ln(Na ₂ O/SiO ₂) _{adj}	0.2096	51.75	0.000000
$\ln(K_2O/SiO_2)_{adj}$	0.2159	80.81	0.000000
$\ln(P_2O_5/SiO_2)_{adj}$	0.2053	31.83	0.000000

Wilks' lambda (U-statistic) and F-ratio with degree of freedom df1 = v1 = g - 1 = 5 - 1 = 4 and df2 = v2 = n - g = 3664 - 5 = 3659, where g is the number of groups and n is total number of samples.

Actual	Discrimination	Total no. of	Predicted tectonic affinity and number of discriminated samples (%)						
affinity	(Figures 1a–1e) §	samples	IA+CA (1+2)	IA (1)	CA (2)	CR+OI (3+4)	Col (5)		
IA (1)	1+2-3+4-5	1552	1398 (90.1)			61 (3.9)	93 (6.0)		
IA (1)	1-2-3+4	1552		1106 (71.3)	380 (24.5)	66 (4.2)			
IA (1)	1-2-5	1552		1072 (69.1)	407 (26.2)		73 (4.7)		
IA (1)	1-3+4-5	1552		1383 (89.1)		71 (4.6)	98 (6.3)		
IA (1)	2-3+4-5*	1552			1311 (84.5)	117 (7.5)	124 (8.0)		
CA (2)	1+2-3+4-5	726	576 (79.3)			50 (6.9)	100 (13.8)		
CA (2)	1-2-3+4	726		148 (20.4)	526 (72.5)	52 (7.1)			
CA (2)	1-2-5	726		158 (21.8)	502 (69.1)		66 (9.1)		
CA (2)	1-3+4-5*	726		530 (73.0)		61 (8.4)	135 (18.6)		
CA (2)	2-3+4-5	726			581 (80.0)	57 (7.9)	88 (12.1)		
CR (3)	1+2-3+4-5	517	62 (12.0)			371 (72.1)	82 (15.9)		
CR (3)	1-2-3+4	517		51 (9.9)	70 (13.5)	396 (76.6)			
CR (3)	1-2-5*	517		206 (39.8)	128 (24.8)		183 (35.4)		
CR (3)	1-3+4-5	517		53 (10.3)		388 (75.0)	76 (14.7)		
CR (3)	2-3+4-5	517			64 (12.4)	368 (71.2)	85 (16.4)		
OI (4)	1+2-3+4-5	277	7 (2.5)			267 (96.4)	3 (1.1)		
OI (4)	1-2-3+4	277		6 (2.1)	11 (4.0)	260 (93.9)			
OI (4)	1-2-5*	277		149 (53.8)	82 (29.6)		46 (16.6)		
OI (4)	1-3+4-5	277		9 (3.2)		263 (95.0)	5 (1.8)		
OI (4)	2-3+4-5	277			7 (2.5)	266 (96.0)	4 (1.5)		
Col (5)	1+2-3+4-5	592	54 (9.1)			24 (4.1)	514 (86.8)		
Col (5)	1-2-3+4*	592		147 (24.8)	273 (46.1)	172 (29.1)			
Col (5)	1-2-5	592		30 (5.1)	57 (9.6)		505 (85.3)		
Col (5)	1-3+4-5	592		51 (8.6)		28 (4.7)	513 (86.7)		
Col (5)	2-3+4-5	592			59 (10.0)	26 (4.4)	507 (85.6)		

Table S5. Assessment of correct discrimination (success rate %) of 4 tectonic settings from the set of 5 diagrams based on major elements.

§ The groups discriminated in discriminant-function-based multidimensional diagrams are as follows: island arc (group 1–IA), continental arc (group 2–CA), continental rift (group 3–CR), ocean island (group 4–OI), and collision (group 5–Col); the numbers in the parentheses are the percentages of samples plotting in a given field and the correct discrimination can be seen in the column with italic boldface numbers; *: inapplicable diagram.

Original (wt.% or μg g ⁻¹) or log _e -transformed ratio variable	IA (n =	(1) 873)	CA (n =	(2) 340)	CR (n =	(3) 221)	OI (n =	(4) - 77)	Col (n =	(5) 357)
	\overline{X}	\$	\overline{X}	s	\overline{X}	\$	\overline{x}	\$	\overline{X}	s
$(TiO_2)_{adj}$	0.846	0.249	0.808	0.278	1.64	0.50	2.134	0.256	0.971	0.329
(MgO) _{adj}	4.58	1.81	4.386	1.203	5.14	2.10	6.26	2.00	3.95	1.76
$(P_2O_5)_{adj}$	0.188	0.108	0.210	0.072	0.455	0.276	0.376	0.227	0.380	0.249
Nb	4.19	3.54	4.04	2.85	23.9	17.8	27.1	35.5	17.1	9.0
Ni	36	58	33.0	23.9	81	64	111	64	56	72
V	211	73	176	51	165	62	216	63	142.2	37.5
Y	23.6	7.6	18.2	5.1	30.1	11.5	27.1	10.8	24.5	7.5
Zr	96	47	89.7	38.1	220	111	231	173	254	198
ln(MgO/TiO ₂) _{adi}	1.65	0.48	1.703	0.316	1.08	0.54	1.00	0.47	1.368	0.396
$\ln(P_2O_5/TiO_2)_{adi}$	-1.598	0.435	-1.341	0.254	-1.39	0.48	-1.86	0.47	-1.045	0.383
ln(Nb/(TiO ₂) _{adi})	-7.89	0.82	-7.66	0.49	-6.71	0.53	-7.25	0.94	-6.410	0.367
$\ln(\text{Ni}/(\text{TiO}_2)_{adi})$	-6.12	1.27	-5.81	0.93	-5.84	1.30	-5.67	1.27	-5.67	0.99
$\ln(V/(TiO_2)_{adi})$	-3.713	0.356	-3.822	0.251	-4.62	0.46	-4.651	0.408	-4.208	0.290
$\ln(Y/(TiO_2)_{adi})$	-5.894	0.291	-6.078	0.272	-6.319	0.403	-6.715	0.293	-5.967	0.356
$\ln(Zr/(TiO_2)_{adj})$	-4.541	0.432	-4.538	0.342	-4.38	0.48	-4.71	0.55	-3.770	0.403

Table S6. Mean and standard deviation of major and trace elements as well as log-transformed ratios for the 5 tectonic settings (IA, CA, CR, OI, and Col) for discordant outlier-free samples.

 \overline{X} = mean; *s* = standard deviation. The data are presented as rounded values obtained from the flexible rules summarized by Verma (2005).

Table S7. Test of equality of group means for $7 \log_e$ -transformed major and trace element ratio variables in the discordant outlier-free samples summarized in Table S6.

Element	Wilks' lambda	F-ratio	Significance
ln(MgO/TiO ₂) _{adj}	0.2119	25.1	0.000000
$\ln(P_2O_5/TiO_2)_{adj}$	0.2268	59.5	0.000000
$\ln(Nb/(TiO_2)_{adj})$	0.2354	79.4	0.000000
ln(Ni/(TiO ₂) _{adj})	0.2156	33.7	0.000000
$\ln(V/(TiO_2)_{adj})$	0.2391	88.0	0.000000
$\ln(Y/(TiO_2)_{adj})$	0.2139	29.8	0.000000
$\ln(Zr/(TiO_2)_{adi})$	0.2298	66.4	0.000000

Wilks' lambda (U-statistic) and F-ratio with degree of freedom df1 = v1 = g - 1 = 5 - 1 = 4 and df2 = v2 = n - g = 1868 - 5 = 1863, where g is the number of groups and n is total number of samples.

Actual	Discrimination	Total no. of	Predicted tectonic affinity and number of discriminated samples (%)					
affinity	diagram (Figures 2a–2e) §	samples	IA+CA (1+2)	IA (1)	CA (2)	CR+OI (3+4)	Col (5)	
IA (1)	1+2-3+4-5	873	753 (86.3)			17 (1.9)	103 (11.8)	
IA (1)	1-2-3+4	873		615 (70.4)	156 (17.9)	102 (11.7)		
IA (1)	1-2-5	873		548 (62.8)	220 (25.2)		105 (12.0)	
IA (1)	1-3+4-5	873		746 (85.5)		15 (1.7)	112 (12.8)	
IA (1)	2-3+4-5*	873			727 (83.3)	22 (2.5)	124 (14.2)	
CA (2)	1+2-3+4-5	340	301 (88.5)			7 (2.1)	32 (9.4)	
CA (2)	1-2-3+4	340		54 (15.9)	278 (81.8)	8 (2.3)		
CA (2)	1-2-5	340		60 (17.6)	259 (76.2)		21 (6.2)	
CA (2)	1-3+4-5*	340		284 (83.5)		13 (3.9)	43 (12.6)	
CA (2)	2-3+4-5	340			322 (94.7)	4 (1.2)	14 (4.1)	
CR (3)	1+2-3+4-5	221	20 (9.0)			161 (72.9)	40 (18.1)	
CR (3)	1-2-3+4	221		14 (6.3)	32 (14.5)	175 (79.2)		
CR (3)	1-2-5*	221		11 (4.9)	47 (21.3)		163 (73.8)	
CR (3)	1-3+4-5	221		19 (8.6)		164 (74.2)	38 (17.2)	
CR (3)	2-3+4-5	221			21 (9.5)	161 (72.9)	39 (17.6)	
OI (4)	1+2-3+4-5	77	0 (0.0)			77 (100.0)	0 (0.0)	
OI (4)	1-2-3+4	77		0 (0.0)	0 (0.0)	77 (100.0)		
OI (4)	1-2-5*	77		4 (5.2)	54 (70.3)		19 (24.5)	
OI (4)	1-3+4-5	77		0 (0.0)		76 (98.7)	1 (0.3)	
OI (4)	2-3+4-5	77		0 (0.0)		76 (98.7)	1 (0.3)	
Col (5)	1+2-3+4-5	357	16 (4.5)			19 (5.3)	322 (90.2)	
Col (5)	1-2-3+4*	357		100 (28.0)	154 (43.1)	103 (28.9)		
Col (5)	1-2-5	357		11 (3.1)	15 (4.2)		331 (92.7)	
Col (5)	1-3+4-5	357		16 (4.5)		19 (5.3)	322 (90.2)	
Col (5)	2-3+4-5	357			14 (3.9)	19 (5.3)	324 (90.8)	

Table S8. Assessment of correct discrimination (success rate %) of 4 tectonic settings from the set of 5 diagrams based on immobile major and trace elements.

Original (µg g ⁻¹) or log -	IA	(1)	CA	. (2)	CR	. (3)	OI	(4)	Co	l (5)
transformed ratio variable	(n =	671)	(n =	301)	(n =	241)	(n =	136)	(n =	163)
	(•••=)	()	(/	((
	$\overline{\mathcal{X}}$	S	\overline{X}	S	\overline{X}	S	\overline{X}	S	\overline{X}	S
Yb	2.40	0.81	1.90	0.66	3.93	3.01	3.71	2.11	2.14	0.75
La	9.9	6.5	11.5	4.8	59	57	82	63	48.2	29.6
Ce	21.8	12.7	25.0	9.9	111	105	150	105	92	53
Sm	3.40	1.27	3.47	1.07	9.2	5.7	10.5	5.9	6.90	3.23
Nb	3.36	2.68	3.92	2.74	71	97	135	124	16.4	10.7
Th	2.28	2.42	1.67	1.20	10.7	11.0	13.0	14.1	18.0	18.0
Y	23.8	8.0	19.5	6.5	45.8	37.6	43.2	22.2	24.9	8.2
Zr	89.9	43.4	86.0	41.3	363	355	680	499	208	113
ln(La/Yb)	1.27	0.60	1.787	0.381	2.51	0.56	2.76	0.80	2.97	0.63
ln(Ce/Yb)	2.10	0.52	2.571	0.328	3.18	0.56	3.48	0.63	3.63	0.61
ln(Sm/Yb)	0.332	0.253	0.613	0.180	0.897	0.324	1.030	0.333	1.113	0.437
ln(Nb/Yb)	0.09	0.80	0.66	0.49	2.30	0.98	3.02	1.05	1.89	0.63
ln(Th/Yb)	-0.45	0.93	-0.25	0.48	0.77	0.64	0.42	1.40	1.76	0.90
ln(Y/Yb)	2.291	0.115	2.333	0.093	2.476	0.195	2.480	0.169	2.451	0.156
ln(Zr/Yb)	3.568	0.387	3.767	0.309	4.38	0.57	5.02	0.58	4.50	0.49

Table S9. Mean and standard deviation of trace elements and log-transformed ratios for discordant outlier-free samples.

 \overline{X} = mean; *s* = standard deviation. The data are presented as rounded values obtained from the flexible rules summarized by Verma (2005).

Element	Wilks' lambda	F-ratio	Significance
ln(La/Yb)	0.1466	5.0	0.000490
ln(Ce/Yb)	0.1475	7.3	0.000008
ln(Sm/Yb)	0.1496	12.7	0.000000
ln(Nb/Yb)	0.1986	140.0	0.000000
ln(Th/Yb)	0.1892	115.6	0.000000
ln(Y/Yb)	0.1515	17.8	0.000000
ln(Y/Yb)	0.1691	63.5	0.000000

Table S10. Test of equality of group means for $10 \log_{e}$ -transformed trace element ratio variables in the discordant outlier-free samples summarized in Table S9.

Wilks' lambda (U-statistic) and univariate-ratio with degree of freedom df1 = v1 = g - 1 = 5 - 1 = 4 and df2 = v2 = n - g = 1512 - 5 = 1507, where g is the number of groups and n is total number of samples.

Actual Discrimination		Total no. of	Predicted tectonic affinity and number of discriminated samples (%)						
affinity	(Figures 3a–3e) §	samples	IA+CA (1+2)	IA (1)	CA (2)	CR+OI (3+4)	Col (5)		
IA (1)	1+2-3+4-5	671	613 (91.4)			33 (4.9)	25 (3.7)		
IA (1)	1-2-3+4	671		508 (75.7)	144 (21.5)	19 (2.8)			
IA (1)	1-2-5	671		488 (72.7)	163 (24.3)		20 (3.0)		
IA (1)	1-3+4-5	671		606 (90.3)		37 (5.5)	28 (4.2)		
IA (1)	2-3+4-5*	671			623 (92.8)	26 (3.9)	22 (3.3)		
CA (2)	1+2-3+4-5	301	272 (90.4)			10 (3.3)	19 (6.3)		
CA (2)	1-2-3+4	301		95 (31.6)	198 (65.8)	8 (2.6)			
CA (2)	1-2-5	301		95 (31.6)	194 (64.5)		12 (3.9)		
CA (2)	1-3+4-5*	301		262 (87.0)		15 (5.0)	24 (8.0)		
CA (2)	2-3+4-5	301			288 (95.7)	9 (3.0)	4 (1.3)		
CR (3)	1+2-3+4-5	241	16 (6.6)			179 (74.3)	46 (19.1)		
CR (3)	1-2-3+4	241		7 (2.9)	40 (16.6)	194 (80.5)			
CR (3)	1-2-5*	241		19 (7.9)	61 (25.3)		161 (66.8)		
CR (3)	1-3+4-5	241		17 (7.0)		180 (74.7)	44 (18.3)		
CR (3)	2-3+4-5	241			24 (9.9)	179 (74.3)	38 (15.8)		
OI (4)	1+2-3+4-5	136	0 (0.0)			136 (100.0)	0 (0.0)		
OI (4)	1-2-3+4	136		0 (0.0)	0 (0.0)	136 (100.0)			
OI (4)	1-2-5*	136		1 (0.7)	54 (39.7)		81 (59.6)		
OI (4)	1-3+4-5	136		0 (0.0)	0 (0.0)	136 (100.0)			
OI (4)	2-3+4-5	136		7 (5.1)		128 (94.1)	1 (0.8)		
Col (5)	1+2-3+4-5	163	17 (10.4)			14 (8.6)	132 (81.0)		
Col (5)	1-2-3+4*	163		13 (8.0)	76 (46.6)	74 (45.4)			
Col (5)	1-2-5	163		11 (6.8)	15 (9.2)		137 (84.0)		
Col (5)	1-3+4-5	163		12 (7.3)		13 (8.0)	138 (84.7)		
Col (5)	2-3+4-5	163			17 (10.4)	14 (8.6)	132 (81.0)		

Table S11. Assessment of correct discrimination (success rate %) of 4 tectonic settings from the set of 5 diagrams based on immobile trace elements.

		Total		Numb	er of discriminated s	amples		
				Arc		Within-plate	Collision	
Figure name §	of s		$\begin{array}{ccc} \text{IA+CA} \left[\ \overline{X} \pm S \ \right] & \text{IA} \left[\ \overline{X} \pm S \ \right] & \text{CA} \left[\ \overline{X} \pm S \ \right] \\ (p_{\text{IA+CA}}) \Theta & [p_{\text{IA}}] \Theta & [p_{\text{CA}}] \Theta \end{array}$		CA [$\overline{X} \pm S$] [p_{CA}] Θ	$CR+OI [\overline{X} \pm S]$ $[p_{CR+OI}] \Theta$	Col [$\overline{X} \pm S$] [p_{Col}] Θ	
	1+2-3+4-5	30	22 [0.732 ± 0.181] (0.5010-0.9925)			3 [0.743 ± 0.122] (0.6157-0.8597)	$5 [0.622 \pm 0.131] (0.4832 - 0.8280)$	
	1-2-3+4	30		22 [0.547 ± 0.108] (0.3754-0.7278)	5 [0.603 ± 0.086] (0.5403-0.7452)	3 [0.694 ± 0.125] (0.5914-0.8333)		
Major elements	1-2-5	30		13 [0.584 ± 0.134] (0.3636–0.8590)	13 [0.557 ± 0.083] (0.4594–0.7058)		$\begin{array}{l} 4 \; [0.457 \pm 0.076] \\ (0.3956 0.5657) \end{array}$	
	1-3+4-5	30		21 [0.763 ± 0.174] (0.5218–0.9884)		$\begin{array}{c} 3 \; [0.690 \pm 0.106] \\ (0.6089 {-} 0.8096) \end{array}$	$\begin{array}{l} 6 \; [0.588 \pm 0.152] \\ (0.4853 {-} 0.8943) \end{array}$	
	2-3+4-5 *	30			20 [0.711 ± 0.153] (0.4570-0.9278)	3 [0.738 ± 0.214] (0.4917-0.8649)	$7 \ [0.611 \pm 0.129] \\ (0.4887 - 0.8799)$	
All major element- based diagrams	$\begin{array}{l} \{\Sigma n\} \ \{\Sigma prob\} \\ [\% prob] \end{array}$	{150}	{22} {16.1099} []	{56} {35.6611} [46.3%]	{38} {24.5093} [31.8%]	{12} {8.5942} [8.8%]	{22} {12.7441} [13.1%]	
	1+2-3+4-5	28	23 [0.780 ± 0.156] (0.5001–0.9935)			0	$5 \ [0.687 \pm 0.134] \\ (0.5519 - 0.9047)$	
	1-2-3+4	28		19 [0.628 ± 0.125] (0.5013–0.9463)	9 [0.581 ± 0.045] (0.4916-0.6405)	0		
Major and trace elements	1-2-5	28		13 [0.462 ± 0.055] (0.4062-0.5810)	9 [0.550 ± 0.059] (0.4579–0.6339)		6 [0.569 ±0.135] (0.4345-0.7984)	
	1-3+4-5	28		24 [0.755 ± 0.146] (0.5251-0.9496)		0	$\begin{array}{l} 4 \; [0.648 \pm 0.124] \\ (0.5270 {-} 0.7958) \end{array}$	
	2-3+4-5 *	28			$22 \ [0.879 \pm 0.134] \\ (0.5296 - 0.9972)$	0	$\begin{array}{l} 6 \ [0.697 \pm 0.179] \\ (0.5256 - 0.9818) \end{array}$	
All major and trace element-based diagrams	{Σn} {Σprob} [%prob]	{140}	{23} {17.9474} []	{56} {36.0589} [47.3%]	{40} {29.5188} [38.7%]	{0} {0.0} [0%]	{21} {13.6219} [14.0%]	
	1+2-3+4-5	28	21 [0.601 ± 0.121] (0.4595–0.8424)			0	7 [0.4975 ± 0.0281] (0.5519-0.9047)	
	1-2-3+4	28		17 [0.534 ± 0.047] (0.4616-0.6314)	10 [0.588 ± 0.091] (0.4500-0.6973)	0		
Trace elements	1-2-5	28		<i>16</i> [0.441 ± 0.046] (0.3730–0.5461)	10 [0.501 ± 0.068] (0.4011-0.6168)		$\begin{array}{l} 2 \; [0.406 \pm 0.067] \\ (0.3581 {-} 0.4535) \end{array}$	
	1-3+4-5	28		24 [0.575 ± 0.080] (0.4795-0.7795)		0	$\begin{array}{c} 4 \; [0.4888 \pm 0.0111] \\ (0.4752 {-} 0.5021) \end{array}$	
	2-3+4-5 *	28			$\begin{array}{c} 19 \; [0.612 \pm 0.137] \\ (0.4348 0.9021) \end{array}$	0	9 $[0.483 \pm 0.050]$ (0.4424-0.6001)	
All trace element- based diagrams	{Σn} {Σprob} [%prob]	{140}	{21} {12.6207} []	{57} {29.9301} [48.6%]	{40} {23.1159} [37.5%]	{0} {0.0} [0%]	{22} {10.5924} [13.9%]	

Table S12. Evaluation of the new multidimensional diagrams from Pleistocene (Quaternary) intermediate magmas from the Ijen volcanic complex, eastern Java, Indonesia (island arc setting).

§ "Figure name" corresponds to 1 of the 3 sets of diagrams based on major elements, immobile major and trace elements, and immobile trace elements, respectively, whereas "Figure type" gives the tectonic fields being discriminated where the tectonic group numbers are as follows: 1–IA (island arc), 2–CA (continental arc), 3–CR (continental rift) and 4–OI (ocean island) together as within-plate, and 5–Col (collision); $\overline{X} \pm S = \text{mean} \pm 1$ standard deviation of the probability estimates for all samples discriminated in a given tectonic setting reported in square brackets; $\Theta = \text{probability estimates for different tectonic groups are summarized after the number of discriminated samples as follows: [<math>p_{\text{IA+CA}}$]–range of probability values estimated for IA+CA combined setting, [p_{IA}]–for IA, [p_{CA}]–for CA, [$p_{\text{CR+OI}}$]–for CR+OI, and [p_{Col}]–for CO. Boldface italic font shows the expected or more probable tectonic setting; *: inapplicable diagram identified whenever it is clearly established, although this diagram is used in the overall total number of samples and probability estimates (see the next explanation); the final row gives a synthesis of results as { Σn } { $\Sigma prob$ } [% prob] where { Σn } = number of samples plotting in all 5 diagrams reported in the column of total number of samples, whereas the sum of samples plotting in a given tectonic field are reported in the respective tectonic field column; { $\Sigma prob$ } = sum of probability values for all samples plotting in a given tectonic field reported in the respective tectonic field column; { $\Sigma prob$ } = sum of probability values for all samples plotting in a given tectonic field reported in the respective tectonic field column; [% prob] = total probability of a given tectonic setting expressed in percent after assigning the probability of IA+CA to IA and CA (using weighing factors explained in the text).

		Total	Number of discriminated samples						
				Arc		Within-plate	Collision		
Figure name §	Figure type §	number of samples	IA+CA [$\overline{X} \pm S$] (p_{IA+CA}) Θ	IA [$\overline{X} \pm S$] [p_{IA}] Θ	CA [$\overline{X} \pm S$] [p_{CA}] Θ	CR+OI [$\overline{x} \pm S$] [p_{CR+OI}] Θ	Col [$\overline{X} \pm S$] [p_{Col}] Θ		
	1+2-3+4-5	9	9 [0.915 ± 0.075] (0.8008-0.9949)			0	0		
	1-2-3+4	9		1 [] (0.4989)	8 [0.785 ± 0.165] (0.5573-0.9111)	0			
Major elements	1-2-5	9		1 [] (0.5286)	$8 [0.756 \pm 0.157]$ (0.5491–0.8787)		0		
	1-3+4-5 *	9		9 [0.839 ± 0.156] (0.5850-0.9970)		0	0		
	2-3+4-5	9			$9[0.942 \pm 0.050]$ (0.8244-0.9877)	0	0		
All major element- based diagrams	{Σn} {Σprob} [%prob]	{45}	{9} {8.2361} []	{11} {8.5774} [29.2%]	{25} {20.8001} [70.8%]	{0} {0} [0%]	{0} {0} [0%]		
	1+2-3+4-5	9	8 [0.805 ± 0.115] (0.6486–0.9461)			0	1 [] (0.4585)		
	1-2-3+4	9		0	9 [0.587 ± 0.054] (0.5035-0.7050)	0			
Major and trace elements	1-2-5	9		0	$8 [0.534 \pm 0.095]$ (0.4081-0.7075)		1 [] (0.4952)		
	1-3+4-5 *	9		9 [0.737 ± 0.150] (0.4444-0.9169)		0	0		
	2-3+4-5	9			9 [0.859 ± 0.150] (0.5246-0.9832)	0	0		
All major and trace element-based diagrams	{Σn} {Σprob} [%prob]	{45 }	{8} {6.4391} []	{9} {6.6362} [26.9%]	{26} {17.2886} [70.1%]	{0} {0} [0%]	{2} {0.9537} [3.0%]		

Table S13. Evaluation of the new multidimensional diagrams from Pleistocene (Quaternary) intermediate magmas from the Huequi volcano, Chile (continental arc setting).

		Total number of samples	Number of discriminated samples							
				Arc		Within-plate	Collision			
Figure name §	rigure type y		IA+CA [$\overline{X} \pm S$] (p_{IA+CA}) Θ	IA [$\overline{X} \pm S$] [p_{IA}] Θ	CA [$\overline{x} \pm S$] [p_{CA}] Θ	$CR+OI [\overline{X} \pm S] \\ [p_{CR+OI}] \Theta$	$\begin{array}{c} \text{Col} \left[\overline{X} \pm S \right] \\ \left[p_{\text{Col}} \right] \Theta \end{array}$			
	1+2-3+4-5	34	0			34 [0.9974 ± 0.0018] (0.9943-0.9998)	0			
	1-2-3+4	34		0	0	34 [0.9948 ± 0.0049] (0.9838-0.9998)				
Major elements	1-2-5 *	34		0	34 [0.787 ± 0.092] (0.5999-0.9409)		0			
	1-3+4-5	34		0		34 [0.9965 ± 0.0024] (0.9910-0.9996)	0			
	2-3+4-5	34			0	34 [0.9874 ± 0.0076] (0.9703-0.9989)	0			
All major element- based diagrams	$\begin{array}{l} \{\Sigma n\} \left\{\Sigma prob\right\} \\ [\% prob] \end{array}$	{170}	{0} {0} [0%]	{0} {0} [0%]	{34} {26.7449} [16.5%]	{136} {135.1858} [83.5%]	{0} {0} [0%]			
	1+2-3+4-5	23	0			23 [0.9968 ± 0.0060] (0.9756-1.0000)	0			
	1-2-3+4	23		0	0	23 [1.0000 ± 0.0000] (1.0000-1.0000)				
Major and trace elements	1-2-5 *	23		0	0		23 [0.9998 ± 0.0002] (0.9992-1.0000)			
	1-3+4-5	23		0		23 [0.9949 ± 0.0092] (0.9635-1.0000)	0			
	2-3+4-5	23			0	23 [0.9874 ± 0.0234] (0.9093-1.0000)	0			
All major and trace element-based diagrams	{Σn} {Σprob} [%prob]	{115}	{0} {0} [0%]	{0} {0} [0%]	{0} {0} [0%]	{92} {91.5175} [79.9%]	{23} {22.9961} [20.1%]			
	1+2-3+4-5	34	0			34 [0.9908 ± 0.0139] (0.9358-0.9999)	0			
	1-2-3+4	34		0	0	34 [0.9988 ± 0.0025] (0.9870-1.0000)				
Trace elements	1-2-5 *	34		0	4 [0.863 ± 0.142] (0.6653-0.9756)		$\begin{array}{c} 30 \; [0.965 \pm 0.048] \\ (0.8178 0.9978) \end{array}$			
	1-3+4-5	34		0		34 [0.9868 ± 0.0174] (0.9189–1.0000)	0			
	2-3+4-5	34			0	34 [0.9842 ± 0.0185] (0.9097-0.9985)	0			
All trace element- based diagrams	{Σn} {Σprob} [%prob]	{170}	{0} {0} [0%]	{0} {0} [0%]	{4} {3.4522} [2.1%]	{133} {131.7091} [80.3%]	{30} {28.9438} [17.6%]			

Table S14. Evaluation of the new multidimensional diagrams from Pliocene-Holocene (Quaternary) intermediate magmas from the Kilimanjaro volcano, Tanzania (continental rift setting).

Table S15. Evaluation of the new multidimensional diagrams from Pleistocene-Holocene (Quaternary) intermediate magmas from the Cana	ary Islands
(ocean island setting).	

				Nu	mber of discriminat	ed samples	
		Total		Arc		TAT: 1 . 1 .	
Figure name §	Figure type §	number of samples	IA+CA [$\overline{X} \pm S$] (p_{IA+CA}) Θ	IA [$\overline{X} \pm S$] [p_{IA}] Θ	CA [$\overline{X} \pm S$] [p_{CA}] Θ	Within-plate CR+OI [$\mathbf{X} \pm \mathbf{S}$] [\mathbf{p}_{CR+OI}] Θ	Collision Col [$\overline{X} \pm S$] [p_{Col}] Θ
	1+2-3+4-5	5	0			$5 \begin{bmatrix} 0.9959 \pm 0.0041 \end{bmatrix} \\ (0.9886 - 0.9982)$	0
	1-2-3+4	5		0	0	5 [0.9883 ± 0.0168] (0.9586-0.9977)	
Major elements	1-2-5 *	5		1 [] (0.7600)	$\begin{array}{l} 4 \; [0.554 \pm 0.143] \\ (0.4737 {-} 0.7683) \end{array}$		0
	1-3+4-5	5		0		5 [0.9937 ± 0.0070] (0.9813-0.9976)	0
	2-3+4-5	5			0	5 [0.9878 ±0.0051] (0.9788-0.9911)	0
All major element- based diagrams	$\begin{array}{l} \{\Sigma n\} \{\Sigma prob\} \\ [\% prob] \end{array}$	{25}	{0} {0} [0%]	{1} {0.7600} [3.3%]	{4} {2.2165} [9.7%]	{20} {19.8285} [87.0%]	{0} {0} [0%]
	1+2-3+4-5	5	0			$\begin{array}{l} 4 \; [0.679 \pm 0.196] \\ (0.5381 {-} 0.9633) \end{array}$	1 [] (0.9859)
	1-2-3+4	5		0	0	5 [1.0000 ± 0.0000] (1.0000-1.0000)	
Major and trace elements	1-2-5	5		0	0		5 [1.0000 ± 0.0000] (1.0000-1.0000)
	1-3+4-5	5		0		$\begin{array}{l} 2 \; [0.726 \pm 0.293] \\ (0.5183 {-} 0.9331) \end{array}$	3 [0.711 ± 0.243] (0.5545-0.9901)
	2-3+4-5	5			0	1 [] (0.9344)	4 [0.689 ± 0.209] (0.5178-0.9938)
All major and trace element-based	{Σn} {Σprob} [%prob]	{25}	{0} {0} [0%]	{0} {0} [0%]	{0} {0} [0%]	{12} {10.1008} [48.2%]	{13} {10.8758} [51.8%]
ulagranis	1+2-3+4-5	5	0			5 [0.9745 ± 0.0106] (0.9639-0.9908)	0
	1-2-3+4	5		0	0	5 [0.9986 ± 0.0011] (0.9976-0.9998)	
Trace elements	1-2-5 *	5		0	0		5 [0.9871 ± 0.0066] (0.9817-0.9983)
	1-3+4-5	5		0		5 [0.9639 ± 0.0137] (0.9509-0.9851)	0
	2-3+4-5	5			0	5 [0.9167 ± 0.0394] (0.8875-0.9852)	0
All trace element- based diagrams	$\begin{array}{l} \{\Sigma n\} \{\Sigma prob\} \\ [\% prob] \end{array}$	{25}	{0} {0} [0%]	{0} {0} [0%]	{0} {0} [0%]	{20} {19.2690} [79.6%]	{5} {4.9356} [20.4%]

Table S16. Evaluation of the new multidimensional diagrams from Miocene (Neogene) ultrapotassic intermediate magmas from southern and southwestern Tibet (collision setting).

			Number of discriminated samples							
		Total		Arc		- Within plate	Collision			
Figure name §	Figure type §	samples	IA+CA [$\overline{X} \pm S$] (p_{IA+CA}) Θ	IA [$\overline{\mathbf{X}} \pm S$] [\mathbf{p}_{IA}] Θ	CA [$\overline{X} \pm S$] [p_{CA}] Θ	$CR+OI [\mathbf{X} \pm S]$ $[p_{CR+OI}] \Theta$	Col [$\overline{x} \pm S$] [p_{Col}] Θ			
	1+2-3+4-5	54	0			$\begin{array}{c} 2 \; [0.571 \pm 0.061] \\ (0.5281 {-} 0.6145) \end{array}$	52 [0.9858 ± 0.0200] (0.9180-0.9995)			
	1-2-3+4 *	54		0	0	54 [0.9809 ± 0.0229] (0.8785-0.9998)				
Major elements	1-2-5	54		0	0		$54 \begin{bmatrix} 0.9965 \pm 0.0083 \end{bmatrix} \\ (0.9547 1.0000)$			
	1-3+4-5	54		0		$\begin{array}{c} 2 \; [0.595 \pm 0.098] \\ (0.5256 {-} 0.6642) \end{array}$	$52 \begin{bmatrix} 0.9780 \pm 0.0286 \end{bmatrix} \\ (0.8842 0.9993)$			
	2-3+4-5	54			0	1 [] (0.5017)	$53 [0.971 \pm 0.060] (0.5749 - 0.9976) (0.5749 - $			
All major element- based diagrams	$\begin{array}{l} \{\Sigma n\} \{\Sigma prob\} \\ [\% prob] \end{array}$	{270}	{0} {0} [0%]	{0} {0} [0%]	{0} {0} [0%]	{59} {55.8040} [21.2%]	{211} {207.3658} [78.8%]			
	1+2-3+4-5	54	0			0	54 [0.9819 ± 0.0240] (0.8759–0.9996)			
	1-2-3+4 *	54		0	$11 [0.635 \pm 0.071] \\ (0.5163 - 0.7466)$	43 [0.769 ± 0.155] (0.4964–0.9902)				
Major and trace elements	1-2-5	54		0	0		$54 \begin{bmatrix} 0.9901 \pm 0.0125 \end{bmatrix} \\ (0.9536 1.0000)$			
	1-3+4-5	54		0		0	$54 \begin{bmatrix} 0.9753 \pm 0.0330 \end{bmatrix} \\ (0.8366 - 0.9995)$			
	2-3+4-5	54			0	0	54 [0.9819 ± 0.0263] (0.8598-0.9996)			
All major and trace element-based diagrams	{Σn} {Σprob} [%prob]	{270}	{0} {0} [0%]	{0} {0} [0%]	{11} {6.9832} [2.8%]	{43} {33.0767} [13.1%]	{216} {212.1850} [84.1%]			
	1+2-3+4-5	54	0			0	54 [0.9973 ± 0.0046] (0.9818-1.0000)			
	1-2-3+4 *	54		0	0	54 [0.9997 ± 0.0006] (0.9963-1.0000)				
Trace elements	1-2-5	54		0	0		$54 \begin{bmatrix} 1.0000 \pm 0.0000 \end{bmatrix} \\ (1.0000 - 1.0000)$			
	1-3+4-5	54		0		0	$54 \begin{bmatrix} 0.9942 \pm 0.0095 \end{bmatrix} \\ (0.9679 1.0000)$			
	2-3+4-5	54			0	0	$54 [0.9939 \pm 0.0099] \\ (0.9634 - 1.0000) \\ ($			
All trace element- based diagrams	$\begin{array}{l} \{\Sigma n\} \ \{\Sigma prob\} \\ [\% prob] \end{array}$	{270}	{0} {0} [0%]	{0} {0} [0%]	{0} {0} [0%]	{54} {53.9838} [20.1%]	{216} {215.2133} [79.9%]			

	Figure type §	Total	Number of discriminated samples						
				Arc		Within-plate	Callisian		
Figure name		number of samples	IA+CA [$\overline{\mathbf{X}} \pm \mathbf{S}$] ($\mathbf{p}_{\text{IA+CA}}$) Θ	IA [$\overline{\mathbf{x}} \pm \mathbf{s}$] [\mathbf{p}_{IA}] Θ	CA [$\overline{X} \pm S$] [p_{CA}] Θ	CR+OI [$\overline{x} \pm S$] [p_{CR+OI}] Θ	Col [$\overline{X} \pm S$] [p_{col}] Θ		
	1+2-3+4-5	7	$\begin{array}{l} \textbf{4} \left[0.773 \pm 0.165 \right] \\ (0.5746 {-} 0.9468) \end{array}$			0	3 [0.6091 ± 0.0320] (0.5733-0.6349)		
	1-2-3+4	7		1 [] (0.4997)	$6 [0.645 \pm 0.129]$ (0.4947-0.5423)	0			
Major elements	1-2-5	7		2 [0.507 ± 0.050] (0.4711-0.5423)	$5 \begin{bmatrix} 0.5226 \pm 0.0433 \end{bmatrix} \\ (0.4768 - 0.5900)$		0		
	1-3+4-5*	7		$\begin{array}{l} 4 \; [0.736 \pm 0.219] \\ (0.5185 {-} 0.9339) \end{array}$		0	3 [0.807 ± 0.071] (0.7244-0.8512)		
	2-3+4-5	7			5 [0.707 ± 0.161] (0.5429–0.8961)	0	2 [0.5155 ± 0.0026] (0.5136-0.5173)		
All major element- based diagrams	$\begin{array}{l} \{\Sigma n\} \ \{\Sigma prob\} \\ [\% prob] \end{array}$	{35}	{4} {3.0921} []	{7} { 4.4555 } [23.7%]	{16} {10.0154} [53.2%]	{0} {0} [0%]	{8} {5.2782} [23.1%]		

 Table S17. Evaluation and testing of one set of new multidimensional diagrams from Late Tertiary to Quaternary altered intermediate magmas from the Central American Volcanic Arc (continental arc setting).

Number of discriminated samples							
Area country (reference):		Total		Arc		TAT: 1 . 1 .	
age; figure name	Figure type	number of samples	IA+CA [$\overline{X} \pm S$] (p_{IA+CA}) Θ	IA [$\overline{X} \pm S$] [p_{IA}] Θ	CA [$\overline{X} \pm S$] [p_{CA}] Θ	CR+OI [$\overline{X} \pm S$] [p_{CR+OI}] Θ	Collision Col [$\overline{X} \pm S$] [p_{Col}] Θ
	1+2-3+4-5	32	10 [0.920 ± 0.090] (0.7113-0.9952)			$\begin{array}{c} 4 \; [0.870 \pm 0.231] \\ (0.5249 - 0.9986) \end{array}$	$18 \ [0.962 \pm 0.072] \\ (0.6977 - 0.9995)$
Wawa greenstone belt,	1-2-3+4	32		25 [0.898 ± 0.116] (0.5729-0.9988)	0	7 [0.837 ± 0.202] (0.4539-0.9979)	
Canada (Polat <i>et al.</i> , 1999; Polat, 2009); Late Archean, 2700 Ma: major elements	1-2-5	32		18 [0.856 ± 0.150] (0.5272-0.9981)	1 [] (0.7845)		13 [0.903 ±0.124] (0.6264-0.9997)
2,00 11,20, 11,201 010110110	1-3+4-5	32		12 [0.910 ±0.117] (0.6257-0.9982)		$\begin{array}{l} 4 \; [0.887 \pm 0.203] \\ (0.5829 0.9994) \end{array}$	$\begin{array}{c} 16 \; [0.812 \pm 0.143] \\ (0.5118 {-} 0.9933) \end{array}$
	2-3+4-5	32			9 $[0.849 \pm 0.147]$ (0.5696-0.9824)	$\begin{array}{l} 4 \; [0.869 \pm 0.237] \\ (0.5133 {-} 0.9971) \end{array}$	$19 \ [0.925 \pm 0.124] \\ (0.5378 - 0.9994)$
All major element-based diagrams	{Σn} {Σprob} [%prob]	{160}	{10} {9.1982} []	{55} {48.7725} [39.8%]	{10} {8.4248} [6.9%]	{19} {16.3630} [11.5%]	{66} {59.6018} [41.8%]
	1+2-3+4-5	32	22 [0.808 ± 0.163] (0.4463-0.9905)			10 [0.943 ± 0.068] (0.7796-0.9983)	0
Wawa greenstone belt, Canada (Polat <i>et al.</i> , 1999:	1-2-3+4	32		22 [0.810 ± 0.103] (0.6564–0.9386)	0	10 [0.920 ± 0.127] (0.6000-0.9998)	
Polat, 2009); Late Archean, 2700 Ma; major and trace	1-2-5	32		27 [0.775 ± 0.120] (0.4438–0.9142)	0		$5 [0.756 \pm 0.174] (0.5252 - 0.9589)$
elements	1-3+4-5	32		22 [0.854 ± 0.126] (0.5555-0.9877)		10 [0.914 ± 0.095] (0.7053-0.9973)	0
	2-3+4-5*	32			$18 \ [0.739 \pm 0.207] \\ (0.4326 - 0.9981)$	$\begin{array}{c} 14 \; [0.842 \pm 0.184] \\ (0.5217 {-} 0.9988) \end{array}$	0
All major and trace element-based diagrams	{Σn} {Σprob} [%prob]	{160}	{22} {17.7694} []	{71} {57.5270} [54.5%]	{18} {13.3033} [12.6%]	{44} {39.5541} [30.0%]	{5} {3.7792} [2.9%]
	1+2-3+4-5	32	27 [0.9412 ± 0.0431] (0.8536-0.9978)			$5 [0.680 \pm 0.053] (0.6324 - 0.7564)$	0
Wawa greenstone belt,	1-2-3+4	32		24 [0.793 ± 0.068] (0.6401-0.9285)	6 [0.563 ± 0.063] (0.4770-0.6429)	$\begin{array}{l} 2 \; [0.509 \pm 0.033] \\ (0.4854 0.5324) \end{array}$	
Canada (Polat <i>et al.</i> , 1999; Polat, 2009); Late Archean, 2700 Ma; trace elements	1-2-5	32		24 [0.722 ± 0.076] (0.5552-0.8928)	8 [0.811 ± 0.116] (0.6587-0.9384)		0
	1-3+4-5	32		27 [0.9499 ± 0.0409] (0.8233-0.9977)		$5 [0.779 \pm 0.067] (0.6755 - 0.8423)$	0
	2-3+4-5 *	32			30 [0.903 ± 0.071] (0.5612-0.9983)	2 [0.548 ± 0.071] (0.4979-0.5978)	0
All trace element-based diagrams	{Σn} {Σprob} [%prob]	{160}	{27} {25.4114} []	{75} { 62.0089 } [58.3%]	{44} {36.9603} [34.7%]	{14} {39.5541} [7.2%]	{0} {0} [0%]
	1+2-3+4-5	13	11 [0.796 ± 0.114] (0.5903–0.9700)			0	$\begin{array}{l} 2 \; [0.809 \pm 0.178] \\ (0.6831 0.9350) \end{array}$
South-central Sweden (Butanen & Andersson	1-2-3+4	13		5 [0.741 ± 0.120] (0.6376-0.9412)	8 [0.579 ± 0.115] (0.3494-0.7459)	0	
2009); Paleoproterozoic, 1870–1780 Ma; major	1-2-5	13		5 [0.642 ± 0.156] (0.5008-0.9007)	7 $[0.602 \pm 0.078]$ (0.4885-0.7290)		1 [] (0.8784)
elements	1-3+4-5	13		11 [0.789 ± 0.127] (0.6035-0.9670)		0	$\begin{array}{c} 2 \; [0.839 \pm 0.142] \\ (0.7390 {-} 0.9399) \end{array}$
	2-3+4-5	13			9 [0.736 ± 0.155] (0.5250-0.9367)	0	$4 [0.735 \pm 0.138]$ (0.5546-0.8908)

Table S18. Application of the new multidimensional diagrams to Archean to Phanerozoic igneous rocks.

Table S18. (continued).

All major element-based diagrams	{Σn} {Σprob} [%prob]	{65}	{11} {8.7553} []	{21} {15.5963} [42.6%]	{24} {15.4717} [42.2%]	{0} {0} [0%]	{9} {7.1160} [15.2%]
	1+2-3+4-5	12	$7 \begin{bmatrix} 0.9967 \pm 0.0065 \end{bmatrix}$ (0.9824-1.0000)			0	5 [0.644 ± 0.234] (0.3928-0.9997)
Adola, southern Ethiopia	1-2-3+4	12		9 [0.899 ± 0.131] (0.6498–1.0000)	2 [0.785 ± 0.121] (0.6992-0.8706)	1 [] (0.5881)	
(Wolde <i>et al.</i> , 1996); Neoproterozoic, 885–765	1-2-5	12		10 [0.882 ± 0.136] (0.6590–1.0000)	$\begin{array}{c} 2 \; [0.664 \pm 0.142] \\ (0.5641 {-} 0.7645) \end{array}$		0
Ma; major elements	1-3+4-5	12		8 [0.9968 ± 0.0077] (0.9780-1.0000)		1 [] (0.3879)	3 [0.765 ± 0.208] (0.5813-0.9900)
	2-3+4-5 *	12			$7 [0.9701 \pm 0.0425] \\ (0.8842 - 1.0000)$	0	5 [0.842 ± 0.250] (0.4036-1.0000)
All major element-based diagrams	{Σn} {Σprob} [%prob]	{60}	{7} { 6.9770 } []	{27} {24.8922} [57.2%]	{11} {9.6890} [22.3%]	{2} {0.9760} [1.9%]	{13} {9.7239} [18.6%]
	1+2-3+4-5	8	7 [0.884 ± 0.172] (0.5379–0.9945)			1 [] (0.9992)	0
Adola, southern Ethiopia	1-2-3+4	8		0	$7 \begin{bmatrix} 0.738 \pm 0.098 \end{bmatrix}$ (0.5406-0.8256)	1 [] (0.9981)	
(Wolde <i>et al.</i> , 1996); Neoproterozoic, 885–765 Ma; major and trace	1-2-5	8		0	8 [0.742 ± 0.096] (0.5452–0.8277)		0
elements	1-3+4-5 *	8		6 [0.888 ± 0.135] (0.6276–0.9856)		1 [] (0.9991)	1 [] (0.5164)
	2-3+4-5	8			$\begin{array}{c} 5 \; [0.879 \pm 0.174] \\ (0.5879 {-} 0.9909) \end{array}$	0	$\begin{array}{c} 2 \; [0.78 \pm 0.31] \\ (0.5563 {-} 0.9962) \end{array}$
All major and trace element-based diagrams	{Σn} {Σprob} [%prob]	{40}	{7} { 6.1921 } []	{6} {5.3295} [20.9%]	{20} {15.5044} [60.8%]	{4} {3.9930} [12.1%]	{3} {2.0689} [6.2%]
	1+2-3+4-5	8	7 [0.9916 ± 0.0144] (0.9601-0.9998)			1 [] (0.9521)	0
Adola, southern Ethiopia	1-2-3+4	8		6 [0.810 ± 0.115] (0.6251–0.9664)	1 [] (0.5023)	1 [] (0.8820)	
(Wolde <i>et al.</i> , 1996); Neoproterozoic, 885–765	1-2-5	8		6 [0.759 ± 0.129] (0.5568-0.9283)	$\begin{array}{c} 2 \; [0.674 \pm 0.199] \\ (0.5329 {-} 0.8142) \end{array}$		0
Ma; trace elements	1-3+4-5	8		7 [0.9904 ± 0.0170] (0.9527-0.9997)		1 [] (0.9647)	0
	2-3+4-5 *	8			7 [0.933 ±0.097] (0.7566-0.9989)	1 [] (0.9503)	0
All trace element-based diagrams	{Σn} {Σprob} [%prob]	{40}	{7} { 6.9411 } []	{19} {16.3458} [59.1%]	{10} {8.3815} [30.3%]	{4} {3.7491} [10.6%]	{0} {0} [0%]
	1+2-3+4-5	21	3 [0.618 ± 0.231] (0.4442-0.8799)			<i>18</i> [0.883 ± 0.171] (0.4683–1.0000)	0
Malani igneous complex, Rajasthan, India (Maheshwari <i>et</i>	1-2-3+4	21		0	3 [0.745 ± 0.247] (0.5057-0.9985)	<i>18</i> [0.831 ± 0.185] (0.4611–0.9999)	
India (Maheshwari <i>et al.</i> , 1996; Bhushan & Chandrasekharam, 2002; Singh & Vallinanyagam, 2004); Neoproterozoic, 750 Ma: maior elements	1-2-5 *	21		3 [0.831 ± 0.213] (0.5871-0.9825)	17 [0.783 ± 0.213] (0.3816-0.9977)		1 [] (0.5083)
	1-3+4-5	21		$\begin{array}{l} 4 \; [0.660 \pm 0.135] \\ (0.5195 {-} 0.8428) \end{array}$		17 [0.910 ± 0.129] (0.5878-1.0000)	0
,	2-3+4-5	21			$5 [0.612 \pm 0.214] (0.4755 - 0.9796)$	16 [0.890 ± 0.122] (0.6670–0.9998)	0
All major element-based diagrams	{Σn} {Σprob} [%prob]	{105}	{3} {1.8531} []	{7} {5.1345} [6.4%]	{25} {18.5987} [23.1%]	{69} {60.5147} [69.9%]	{1} {0.5083} [0.6%]

Table S18. (continued).

	1+2-3+4-5	39	33 [0.9811 ± 0.0319] (0.8849-1.0000)			0	6 [0.871 ± 0.148] (0.6857-0.9994)
Wastern Tasmania	1-2-3+4	39		33 [0.903 ± 0.146] (0.5562–1.0000)	$\begin{array}{c} 6 \; [0.758 \pm 0.201] \\ (0.5344 {-} 0.9948) \end{array}$	0	
Australia (Brown & Jenner, 1989); Cambrian; major	1-2-5	39		35 [0.889 ± 0.145] (0.5197–1.0000)	$\begin{array}{l} 3 \; [0.840 \pm 0.235] \\ (0.5685 {-} 0.9762) \end{array}$		1 [] (0.5234)
elements	1-3+4-5	39		38 [0.9805 ± 0.0254] (0.8657–1.0000)		0	1 [] (0.9038)
	2-3+4-5 *	39			28 [0.931 ± 0.129] (0.5537-1.0000)	0	$\begin{array}{c} 11 \; [0.844 \pm 0.160] \\ (0.5664 {-} 0.9981) \end{array}$
All major element-based diagrams	{Σn} {Σprob} [%prob]	{195}	{33} {32.3754} []	{106} {98.5682} [68.5%]	{36} {32.5718} [22.6%]	{0} {0} [0%]	{19} {15.9407} [8.9%]
	1+2-3+4-5	6	0			0	6 [0.981 ± 0.034] (0.9116–0.9995)
Alps, France-Italy-	1-2-3+4 *	6		0	0	6 [0.796 ± 0.264] (0.3700-0.9969)	
Switzerland (Debon & Lemmet, 1999); Late Carboniferous, 295 Ma:	1-2-5	6		0	0		6 [0.977 ± 0.051] (0.8728–1.0000)
major elements	1-3+4-5	6		0		0	6 [0.983 ± 0.028] (0.9256-0.9993)
	2-3+4-5	6			0	0	6 [0.973 ± 0.042] (0.8903-0.9991)
All major element-based diagrams	{Σn} {Σprob} [%prob]	{30}	{0} {0} [0%]	{0} {0} [0%]	{0} {0} [0%]	{6} {4.7760} [16.9%]	{24} {23.4834} [83.1%]
	1+2-3+4-5	5	0			0	5 [0.925 ± 0.083] (0.7936-0.9859)
Alps, France-Italy-	1-2-3+4	5		1 [] (0.5085)	$\begin{array}{c} 2 \; [0.979 \pm 0.008] \\ (0.9736 {-} 0.9850) \end{array}$	2 [0.8100 ± 0.053] (0.7723-0.8476)	
Switzerland (Debon & Lemmet, 1999); Late Carboniferous, 295 Ma:	1-2-5	5		0	0		5 [0.846 ± 0.163] (0.6011–0.9959)
major and trace elements	1-3+4-5	5		0		0	5 [0.913 ± 0.111] (0.7312-0.9924)
	2-3+4-5	5			0	0	5 [0.927 ± 0.077] (0.8299-0.9943)
All major and trace element-based diagrams	{Σn} {Σprob} [%prob]	{25}	{0} {0} [0%]	{1} {0.5857} [2.6%]	{2} {1.9586} [8.8%]	{2} {1.6200} [7.3%]	{20} {23.4834} [83.3%]
	1+2-3+4-5	6	0			0	6 [0.957 ± 0.102] (0.7485–0.9993)
Alps, France-Italy-	1-2-3+4	6		0	1 [] (0.5602)	$5 [0.970 \pm 0.045] (0.8940 - 1.0000)$	
Switzerland (Debon & Lemmet, 1999); Late Carboniferous, 295 Ma;	1-2-5	6		0	0		6 [0.953 ± 0.113] (0.7228–1.0000)
trace elements	1-3+4-5	6		0		0	6 [0.95613 ± 0.099] (0.7549-0.9983)
	2-3+4-5	6			0	0	6 [0.950 ± 0.114] (0.7184–0.9988)
All trace element-based diagrams	{Σn} {Σprob} [%prob]	{30}	{0} {0} [0%]	{0} {0} [0%]	{1} {0.5602} [2.0%]	{5} { 4.8494 } [17.1%]	{24} {22.9374} [80.9%]

Table S18. (continued).

Chichijima Island, Bonin Islands, Japan (Taylor <i>et</i> <i>al.</i> , 1994); Eocene, 48–40 Ma; major elements	1+2-3+4-5	35	35 [0.989 ± 0.040] (0.7583-0.9993)			0	0
	1-2-3+4	35		35 [0.944 ± 0.081] (0.6617-0.9994)	0	0	
	1-2-5	35		35 [0.941 ± 0.087] (0.6453-0.9995)	0		0
	1-3+4-5	35		35 [0.988 ± 0.058] (0.6535-0.9998)		0	0
	2-3+4-5	35			33 [0.873 ± 0.123] (0.5252-0.9810)	0	$\begin{array}{l} 2 \; [0.525 \pm 0.019] \\ (0.5156 {-} 0.5389) \end{array}$
All major element-based diagrams	{Σn} {Σprob} [%prob]	{175}	{35} {34.6104} []	{105} {100.5573} [77.3%]	{33} {28.7943} [22.1%]	{0} {0} [0%]	{2} {1.0504} [0.6%]

Table S19. Evaluation of the first new major element-based multidimensional diagram for changes related to analytical errors, mobility, or alteration.

		Probability chang	e of the centroid [p _{gain} , p _{loss}] caused l	by element concen	tration changes Θ	
Element [+gain%, _loss%]	IA+	-CA	А	rc	Within-pla	te (CR+OI)	Collision
]	IA	CA	IA	CA	CR	OI	Col
No change (1+2-3+4-5)	0.92046	0.88378			0.92458	0.98888	0.94785
SiO ₂ [+10%, -10%]	[0.8898, 0.9363]	[0.8402, 0.9075]			[0.8624, 0.9599]	[0.9803, 0.9936]	[0.9710, 0.9005]
TiO_{2} [+20%, -20%]	[0.8515, 0.9562]	[0.7928, 0.9341]			[0.9720, 0.7679]	[0.9963, 0.9568]	[0.9348, 0.9400]
Al ₂ O ₃ [+20%, -20%]	[0.9420, 0.8818]	[0.9140, 0.8314]			[0.8914, 0.9515]	[0.9827, 0.9934]	[0.9415, 0.9505]
Fe ₂ O ₃ [+20%, -20%]	[0.9343, 0.9460]	[0.9046, 0.9213]			[0.9333, 0.9454]	[0.9904, 0.9917]	[0.9644, 0.9534]
FeO [+20%, -20%]	[0.9124, 0.9562]	[0.7612, 0.9364]			[0.9162, 0.9541]	[0.9885, 0.9925]	[0.9748, 0.9401]
MnO [+40%, -40%]	[0.9466, 0.7373]	[0.9229, 0.6445]			[0.9706, 0.6257]	[0.9949, 0.9389]	[0.8366, 0.9915]
MgO [+20%, -20%]	[0.9128, 0.9288]	[0.8729, 0.8957]			[0.9192, 0.9304]	[0.9883, 0.9895]	[0.9538, 0.9395
CaO [+20%, -20%]	[0.9301, 0.8942]	[0.8966, 0.8494]			[0.8570, 0.9671]	[0.9776, 0.9953]	[0.9561, 0.9264]
Na ₂ O [+40%, -40%]	[0.9444, 0.7324]	[0.9199, 0.6386]			[0.9729, 0.5918]	[0.9953, 0.9334]	[0.8295, 0.9919]
K ₂ O [+40%, -40%]	[0.8559, 0.9663]	[0.7949, 0.9502]			[0.9000, 0.9374]	[0.9868, 0.9888]	[0.9733, 0.8599]
P ₂ O ₅ [+20%, -20%]	[0.9144, 0.9268]	[0.8751, 0.8930]			[0.9159, 0.9338]	[0.9878, 0.9901]	[0.9540, 0.9392]
No change (1-2-3+4)			0.61392	0.59320	0.95535	0.98472	
SiO ₂ [+10%, -10%]			[0.6580, 0.5626]	[0.5513, 0.6365]	[0.9409, 0.9671]	[0.9798, 0.9887]	
TiO ₂ [+20%, -20%]			[0.6261, 0.5745]	[0.5312, 0.6466]	[0.9875, 0.8115]	[0.9958, 0.9275]	
Al ₂ O ₃ [+20%, -20%]			[0.4618, 0.7668]	[0.7344, 0.3998]	[0.9329, 0.9695]	[0.9756, 0.9902]	
Fe ₂ O ₃ [+20%, -20%]			[0.5831, 0.5533]	[0.6391, 0.6664]	[0.9854, 0.9851]	[0.9930, 0.9927]	
FeO [+20%, -20%]			[0.6207, 0.5157]	[0.4423, 0.6957]	[0.9858, 0.9847]	[0.9932, 0.9924]	
MnO [+40%, -40%]			[0.8294, 0.2098]	[0.3053, 0.9001]	[0.9689, 0.8657]	[0.9902, 0.9459]	
MgO [+20%, -20%]			[0.5962, 0.6352]	[0.6095, 0.5728]	[0.9585, 0.9511]	[0.9858, 0.9833]	
CaO [+20%, -20%]			[0.7110, 0.4800]	[0.4942, 0.6953]	[0.9158, 0.9788]	[0.9712, 0.9926]	
Na ₂ O [+40%, -40%]			[0.3659, 0.8747]	[0.8027, 0.2344]	[0.9343, 0.9614]	[0.9756, 0.9880]	
K ₂ O [+40%, -40%]			[0.6699, 0.5209]	[0.5275, 0.6860]	[0.9646, 0.9350]	[0.9882, 0.9768]	
P ₂ O ₅ [+20%, -20%]			[0.5665, 0.6689]	[0.6395, 0.5342]	[0.9553, 0.9548]	[0.9845, 0.9848]	
No change (1-2-5)			0.59424	0.59364			0.95095
SiO ₂ [+10%, -10%]			[0.6574, 0.5167]	[0.5130, 0.6763]			[0.9666, 0.9240]
TiO ₂ [+20%, -20%]			[0.6426, 0.5252]	[0.5206, 0.6738]			[0.9712, 0.9061]
Al ₂ O ₃ [+20%, -20%]			[0.3942, 0.7970]	[0.7586, 0.3571]			[0.9458, 0.9474]
Fe ₂ O ₃ [+20%, -20%]			[0.5870, 0.5549]	[0.6139, 0.6532]			[0.9819, 0.9702]
FeO [+20%, -20%]			[0.6226, 0.5127]	[0.4204, 0.6929]			[0.9901, 0.9527]
MnO [+40%, -40%]			[0.8355, 0.1693]	[0.3209, 0.7570]			[0.8268, 0.9895]
MgO [+20%, -20%]			[0.5705, 0.6224]	[0.6105, 0.5715]			[0.9571, 0.9421]
CaO [+20%, -20%]			[0.6638, 0.4966]	[0.5000, 0.6971]			[0.9704, 0.9079]
Na ₂ O [+40%, -40%]			[0.4067, 0.7213]	[0.7771, 0.2366]			[0.7803, 0.9949]
K ₂ O [+40%, -40%]			[0.6145, 0.5455]	[0.5327, 0.6640]			[0.9776, 0.8484]
P ₂ O ₅ [+20%, -20%]			[0.5281, 0.6705]	[0.6501, 0.5191]			[0.9547, 0.9448]
No change (1-3+4-5)			0.92792		0.93414	0.98914	0.95117
SiO ₂ [+10%, -10%]			[0.8947, 0.9450]		[0.8745, 0.9662]	[0.9798, 0.9940]	[0.9751, 0.8985]
TiO ₂ [+20%, -20%]			[0.8580, 0.9628]		[0.9751, 0.7970]	[0.9963, 0.9590]	[0.9299, 0.9486]
Al ₂ O ₂ [+20%, -20%]			[0.9567, 0.8655]		[0.8973, 0.9605]	[0.9812, 0.9941]	[0.9419, 0.9522]

Table S19. (continued).

Fe ₂ O ₃ [+20%, -20%]	 	[0.9361, 0.9433]		[0.9387, 0.9505]	[0.9897, 0.9915]	[0.9598, 0.9501]
FeO [+20%, -20%]	 	[0.9232, 0.9492]		[0.9221, 0.9593]	[0.9873, 0.9928]	[0.9700, 0.9390]
MnO [+40%, -40%]	 	[0.9725, 0.5531]		[0.9665, 0.6457]	[0.9930, 0.9354]	[0.7864, 0.9958]
MgO [+20%, -20%]	 	[0.9224, 0.9340]		[0.9297, 0.9390]	[0.9885, 0.9898]	[0.9558, 0.9449]
CaO [+20%, -20%]	 	[0.9419, 0.8972]		[0.8824, 0.9686]	[0.9794, 0.9951]	[0.9580, 0.9319]
Na ₂ O [+40%, -40%]	 	[0.9153, 0.8890]		[0.9812, 0.6406]	[0.9968, 0.9269]	[0.8731, 0.9845]
$K_{2}O$ [+40%, -40%]	 	[0.8669, 0.9712]		[0.9164, 0.9425]	[0.9874, 0.9886]	[0.9730, 0.8782]
P ₂ O ₅ [+20%, -20%]	 	[0.9254, 0.9304]		[0.9251, 0.9437]	[0.9877, 0.9907]	[0.9562, 0.9441]
No change (2-3+4-5)	 		0.84611	0.86404	0.96601	0.91793
SiO ₂ [+10%, -10%]	 		[0.7704, 0.8992]	[0.8144, 0.8975]	[0.9543, 0.9729]	[0.9523, 0.8544]
TiO ₂ [+20%, -20%]	 		[0.7647, 0.8938]	[0.9424, 0.6647]	[0.9868, 0.8964]	[0.8912, 0.9223]
$Al_{2}O_{3}$ [+20%, -20%]	 		[0.9443, 0.5761]	[0.7633, 0.9161]	[0.9266, 0.9820]	[0.8356, 0.9468]
Fe ₂ O ₃ [+20%, -20%]	 		[0.8347, 0.8660]	[0.8687, 0.8822]	[0.9668, 0.9695]	[0.9283, 0.9071]
FeO [+20%, -20%]	 		[0.7641, 0.8942]	[0.8499, 0.8919]	[0.9630, 0.9708]	[0.9496, 0.8821]
MnO [+40%, -40%]	 		[0.8292, 0.8141]	[0.9443, 0.5795]	[0.9865, 0.8665]	[0.8553, 0.9593]
MgO [+20%, -20%]	 		[0.8423, 0.8477]	[0.8311, 0.8966]	[0.9570, 0.9745]	[0.9291, 0.9012]
CaO [+20%, -20%]	 		[0.8385, 0.8451]	[0.7975, 0.9187]	[0.9473, 0.9801]	[0.9369, 0.8843]
Na ₂ O [+40%, -40%]	 		[0.8736, 0.7187]	[0.9367, 0.5981]	[0.9838, 0.8798]	[0.8297, 0.9737]
$K_{2}O$ [+40%, -40%]	 		[0.7119, 0.9396]	[0.7991, 0.9005]	[0.9511, 0.9713]	[0.9630, 0.7492]
P ₂ O ₅ [+20%, -20%]	 		[0.8410, 0.8520]	[0.8581, 0.8709]	[0.9646, 0.9677]	[0.9223, 0.9122]

 Θ p_{gain} and p_{loss} here refer to the probability of the modified concentrations from the gain or loss of an element; the probability values in *italics* underlined are for the centroids that are misdiscriminated in a given diagram, generally as the other arc setting (i.e. IA was misdiscriminated as CA and vice versa).

Table S20. Evaluation of the second set of major and trace element-based multidimensional diagrams for compositional changes related to analytical errors, mobility, or alteration.

Probability change of the centroid $[p_{gain}, p_{loss}]$ caused by element concentration changes							
Element [+gain%, -loss%]	IA+	-CA	А	rc	Within-pla	te (CR+OI)	Collision
	IA	CA	IA	CA	CR	OI	Col
No change (1+2-3+4-5)	0.86377	0.84043			0.92193	0.99002	0.96549
TiO ₂ [+20%, -20%]	[0.9031, 0.7965]	[0.8867, 0.7623]			[0.8970, 0.9431]	[0.9862, 0.9930]	[0.9577, 0.9702]
MgO [+20%, -20%]	[0.8419, 0.8361]	[0.7720, 0.8148]			[0.9934, 0.3425]	[0.9992, 0.8156]	[0.8453, 0.9813]
P ₂ O ₅ [+20%, -20%]	[0.8732, 0.8505]	[0.8526, 0.8224]			[0.8894, 0.9497]	[0.9854, 0.9937]	[0.9674, 0.9609]
Nb [+20%, -20%]	[0.8075, 0.9131]	[0.7763, 0.8976]			[0.9304, 0.9093]	[0.9912, 0.9883]	[0.9718, 0.9525]
Ni [+20%, -20%]	[0.8414, 0.8874]	[0.8148, 0.8678]			[0.9264, 0.9160]	[0.9906, 0.9892]	[0.9685, 0.9609]
V [+20%, -20%]	[0.8739, 0.8395]	[0.8554, 0.7970]			[0.7843, 0.9804]	[0.9683, 0.9976]	[0.9717, 0.9330]
Y [+20%, -20%]	[0.8870, 0.8300]	[0.8672, 0.8020]			[0.9189, 0.9253]	[0.9896, 0.9905]	[0.9606, 0.9702]
Zr [+20%, -20%]	[0.8154, 0.9029]	[0.7899, 0.8771]			[0.8140, 0.9753]	[0.9735, 0.9970]	[0.9798, 0.9268]
No change (1-2-3+4)			0.58700	0.64616	0.98474	0.99858	
TiO ₂ [+20%, -20%]			[0.5623, 0.6167]	[0.6728, 0.6078]	[0.9698, 0.9933]	[0.9969, 0.9993]	
MgO [+20%, -20%]			[0.5509, 0.6096]	[0.6106, 0.6320]	[0.9985, 0.7923]	[0.9998, 0.9749]	
P_2O_5 [+20%, -20%]			[0.4775, 0.7082]	[0.7413, 0.5122]	[0.9729, 0.9921]	[0.9973, 0.9992]	
Nb [+20%, -20%]			[0.5794, 0.5958]	[0.6492, 0.6410]	[0.9898, 0.9752]	[0.9990, 0.9975]	
Ni [+20%, -20%]			[0.5839, 0.5906]	[0.6470, 0.6447]	[0.9878, 0.9800]	[0.9988, 0.9980]	
V [+20%, -20%]			[0.6200, 0.5413]	[0.6197, 0.6640]	[0.9554, 0.9960]	[0.9954, 0.9996]	
Y [+20%, -20%]			[0.6848, 0.4581]	[0.5475, 0.7492]	[0.9805, 0.9883]	[0.9980, 0.9988]	
Zr [+20%, -20%]			[0.6220, 0.5425]	[0.6153, 0.6800]	[0.9768, 0.9908]	[0.9977, 0.9991]	
No change (1-2-5)			0 54861	0 59639			0 94769
TiO $[\pm 20\% - 20\%]$			[0 5292 0 5626]	[0.6412_0.5318]			[0.921/ 0.9687]
M_{2} [+20%, -20%]			[0.5292, 0.5020]	[0.6266_0.5576]			[0.9214, 0.9087]
$\frac{1}{1000} \left[\frac{1}{200}, \frac{200}{200} \right]$			[0.3231, 0.3703]	[0.6248, 0.4700]			[0.9378, 0.9377]
$P_{2}O_{5}[+20\%, -20\%]$			[0.5100, 0.5785]	[0.5873 0.5000]			[0.9570, 0.9500]
ND [+20%, -20%]			[0.5190, 0.5785]	[0.5073, 0.3990]			[0.9638, 0.9187]
NI [+20%, -20%]			[0.5422, 0.5555]	[0.5902, 0.6029]			[0.9343, 0.9381]
V [+20%, -20%]			[0.3940, 0.4912]	[0.5584, 0.6596]			[0.9446, 0.9508]
1 [+20%, -20%]			[0.0575, 0.4305]	[0.5175, 0.0815]			[0.9432, 0.9309]
Zr[+20%, -20%]			[0.5714, 0.5098]	[0.5552, 0.6650]	0.01525	0.09629	[0.9636, 0.9129]
T:O [1200/ 200/]			0.83940		0.91525	0.98028	0.96261
M_{2} [+20%, -20%]			[0.8795, 0.7755]		[0.0014_0.2714]	[0.9817, 0.9900]	[0.9372, 0.9635]
MgO [+20%, -20%]			[0.8094, 0.8161]			[0.9987, 0.7981]	[0.8551, 0.9806]
$P_2O_5[+20\%, -20\%]$			[0.8347, 0.8444]		[0.8896, 0.9391]	[0.9817, 0.9903]	[0.9673, 0.9532]
ND $[+20\%, -20\%]$			[0.0150.00050]		[0.9237, 0.9031]	[0.9877, 0.9842]	
N1 [+20%, -20%]			[0.8158, 0.8650]		[0.9198, 0.9093]	[0.98/1, 0.9852]	[0.9651, 0.9588]
V [+20%, -20%]			[0.8481, 0.8155]		[0.7788, 0.9770]	[0.9591, 0.9965]	[0.9716, 0.9230]
Y [+20%, -20%]			[0.8840, 0.7673]		[0.9114, 0.9192]	[0.9856, 0.9869]	[0.9533, 0.9701]
Zr [+20%, -20%]			[0.7929, 0.8775]		[0.8024, 0.9726]	[0.9643, 0.9958]	[0.9782, 0.9195]
No change (2-3+4-5)				0.94673	0.89487	0.97756	0.97595

Table S20. (continued).

TiO ₂ [+20%, -20%]	 	 [0.9653, 0.9084] [0.8506, 0.9314] [0.9661, 0.9861] [0.9771, 0.9703]
MgO [+20%, -20%]	 	 [0.9293, 0.9098] [0.9891, 0.3172] [0.9978, 0.7060] [0.8353, 0.9952]
P ₂ O ₅ [+20%, -20%]	 	 [0.9645, 0.9125] $[0.8653, 0.9227]$ $[0.9705, 0.9839]$ $[0.9762, 0.9726]$
Nb [+20%, -20%]	 	 [0.8856, 0.9800] [0.8916, 0.8970] [0.9768, 0.9781] [0.9809, 0.9618]
Ni [+20%, -20%]	 	 [0.9311, 0.9613] [0.8996, 0.8886] [0.9787, 0.9761] [0.9769, 0.9740]
V [+20%, -20%]	 	 [0.9546, 0.9223] [0.7475, 0.9688] [0.9381, 0.9937] [0.9859, 0.9362]
Y [+20%, -20%]	 	 [0.9403, 0.9537] [0.9044, 0.8820] [0.9798, 0.9745] [0.9750, 0.9768]
Zr [+20%, -20%]	 	 [0.9338, 0.9532] [0.7751, 0.9625] [0.9463, 0.9924] [0.9877, 0.9410]

For more explanation, see Table S19.

Table S21. Evaluation of the third set of major and trace element-based multidimensional diagrams for compositional changes related to analytical errors, mobility, or alteration.

Probability change of the centroid $[p_{gain}, p_{loss}]$ caused by element concentration changes							
Element [+gain%, -loss%]	IA+	-CA	А	rc	Within-pla	te (CR+OI)	Collision
	IA	CA	IA	CA	CR	OI	Col
No change (1+2-3+4-5)	0.96541	0.91223			0.97804	0.99661	0.98297
Yb [+20%, -20%]	[0.9951, 0.7020]	[0.9868, 0.4732]			[0.9636, 0.9729]	[0.9962, 0.9953]	[0.9484, 0.9911]
La [+20%, -20%]	[0.9693, 0.9599]	[0.9213, 0.8997]			[0.9792, 0.9765]	[0.9968, 0.9963]	[0.9812, 0.9849]
Ce [+20%, -20%]	[0.9681, 0.9485]	[0.9226, 0.8636]			[0.9433, 0.9933]	[0.9908, 0.9990]	[0.9917, 0.9523]
Sm [+20%, -20%]	[0.9343, 0.9845]	[0.8413, 0.9595]			[0.9798, 0.9733]	[0.9967, 0.9963]	[0.9851, 0.9775]
Nb [+20%, -20%]	[0.9494, 0.9738]	[0.8688, 0.9359]			[0.9902, 0.9421]	[0.9985, 0.9908]	[0.9675, 0.9908]
Th [+20%, -20%]	[0.9521, 0.9757]	[0.8835, 0.9355]			[0.9697, 0.9846]	[0.9951, 0.9978]	[0.9887, 0.9720]
Y [+20%, -20%]	[0.9088, 0.9899]	[0.7884, 0.9733]			[0.9793, 0.9703]	[0.9966, 0.9963]	[0.9865, 0.9710]
Zr [+20%, -20%]	[0.9659, 0.9641]	[0.9122, 0.9105]			[0.9826, 0.9708]	[0.9974, 0.9954]	[0.9788, 0.9869]
No change (1-2-3+4)			0.71546	0.64256	0.98757	0.99908	
Yb [+20%, -20%]			[0.7870, 0.5795]	[0.5673, 0.6142]	[0.9233, 0.9987]	[0.9941, 0.9999]	
La [+20%, -20%]			[0.6275, 0.8036]	[0.7289, 0.5233]	[0.9835, 0.9909]	[0.9987, 0.9994]	
Ce [+20%, -20%]			[0.6716, 0.7590]	[0.6974, 0.5597]	[0.9697, 0.9958]	[0.9977, 0.9997]	
Sm [+20%, -20%]			[0.6413, 0.7899]	[0.6900, 0.5595]	[0.9944, 0.9668]	[0.9996, 0.9976]	
Nb [+20%, -20%]			[0.7135, 0.7144]	[0.6238, 0.6548]	[0.9944, 0.9677]	[0.9996, 0.9976]	
Th [+20%, -20%]			[0.7600, 0.6545]	[0.5870, 0.7055]	[0.9896, 0.9844]	[0.9992, 0.9988]	
Y [+20%, -20%]			[0.7366, 0.6816]	[0.5890, 0.6903]	[0.9956, 0.9569]	[0.9997, 0.9967]	
Zr [+20%, -20%]			[0.7500, 0.6692]	[0.5986, 0.6931]	[0.9901, 0.9835]	[0.9993, 0.9988]	
No change (1-2-5)			0.71670	0.63668			0.98681
Yb [+20%, -20%]			[0.7825, 0.5642]	[0.5778, 0.5512]			[0.9154, 0.9987]
La [+20%, -20%]			[0.6392, 0.7955]	[0.7165, 0.5282]			[0.9821, 0.9908]
Ce [+20%, -20%]			[0.6866, 0.7502]	[0.6566, 0.6070]			[0.9905, 0.9804]
Sm [+20%, -20%]			[0.6322, 0.8023]	[0.7087, 0.5331]			[0.9890, 0.9832]
Nb [+20%, -20%]			[0.7097, 0.7251]	[0.6429, 0.6289]			[0.9874, 0.9861]
Th [+20%, -20%]			[0.7624, 0.6514]	[0.5691, 0.7112]			[0.9917, 0.9767]
Y [+20%, -20%]			[0.7503, 0.6575]	[0.5491, 0.7152]			[0.9957, 0.9485]
Zr [+20%, -20%]			[0.7326, 0.6965]	[0.6177, 0.6594]			[0.9876, 0.9958]
No change (1-3+4-5)			0.96450		0.97209	0.99371	0.97546
Yb [+20%, -20%]			[0.9946, 0.7164]		[0.9657, 0.9622]	[0.9944, 0.9908]	[0.9434, 0.9859]
La [+20%, -20%]			[0.9526, 0.9749]		[0.9778, 0.9630]	[0.9949, 0.9918]	[0.9714, 0.9789]
Ce [+20%, -20%]			[0.9685, 0.9418]		[0.9218, 0.9924]	[0.9815, 0.9983]	[0.9897, 0.9205]
Sm [+20%, -20%]			[0.9305, 0.9847]		[0.9759, 0.9646]	[0.9944, 0.9926]	[0.9753, 0.9729]
Nb [+20%, -20%]			[0.9498, 0.9725]		[0.9869, 0.9315]	[0.9971, 0.9841]	[0.9527, 0.9879]
Th [+20%, -20%]			[0.9593, 0.9689]		[0.9621, 0.9807]	[0.9912, 0.9958]	[0.9822, 0.9637]
Y [+20%, -20%]			[0.9170, 0.9879]		[0.9708, 0.9701]	[0.9931, 0.9941]	[0.9800, 0.9645]
Zr [+20%, -20%]			[0.9693, 0.9574]		[0.9751, 0.9677]	[0.9945, 0.9926]	[0.9715, 0.9795]
No change (2-3+4-5)				0.94219	0.97245	0.99233	0.97787

Table S21. (continued).

Yb [+20%, -20%]	 	 [0.9878, 0.6863]	[0.9637, 0.9635]	[0.9917, 0.9890]	[0.9428, 0.9890]
La [+20%, -20%]	 	 [0.9604, 0.9082]	[0.9648, 0.9792]	[0.9904, 0.9941]	[0.9786, 0.9755]
Ce [+20%, -20%]	 	 [0.9533, 0.9091]	[0.9414, 0.9893]	[0.9832, 0.9971]	[0.9874, 0.9509]
Sm [+20%, -20%]	 	 [0.8980, 0.9717]	[0.9782, 0.9613]	[0.9938, 0.9897]	[0.9774, 0.9756]
Nb [+20%, -20%]	 	 [0.8958, 0.9663]	[0.9879, 0.9265]	[0.9966, 0.9791]	[0.9589, 0.9870]
Th [+20%, -20%]	 	 [0.9105, 0.9654]	[0.9649, 0.9778]	[0.9898, 0.9943]	[0.9852, 0.9632]
Y [+20%, -20%]	 	 [0.8688, 0.9799]	[0.9725, 0.9665]	[0.9920, 0.9917]	[0.9832, 0.9630]
 Zr [+20%, -20%]	 	 [0.9522, 0.9270]	[0.9736, 0.9705]	[0.9928, 0.9916]	[0.9746, 0.9812]

For more explanation, see Table S19.

	Probability change of the centroid $[\mathrm{p}_{gain},\mathrm{p}_{loss}]$ caused by element concentration changes Θ							
Diagram type [Assimilation %, %]	IA+	CA	А	rc	Within-pla	te (CR+OI)	Collision	
	IA	CA	IA	CA	CR	OI	Col	
Major element-based diagrams								
(1+2-3+4-5) UCC							0.98306	
(1+2-3+4-5) No change	0.92046	0.88378			0.92458	0.98888	0.94785	
(1+2-3+4-5) [10%, 20%]	[0.8618, 0.7701]	[0.8084, 0.6991]			[0.8681, 0.7698]	[0.9778, 0.9531]	[0.9546, 0.9604]	
(1-2-3+4) UCC					0.74	1767		
(1-2-3+4) No change			0.61392	0.59320	0.95535	0.98472		
(1-2-3+4) [10%, 20%]			[0.6044, 0.5867]	[0.5861, 0.5859]	[0.9336, 0.8995]	[0.9752, 0.9587]		
(1-2-5) UCC							0.91900	
(1-2-5) No change			0.59424	0.59364			0.95095	
(1-2-5) [10%, 20%]			[0.5700, 0.5320]	[0.5699, 0.5398]			[0.9503, 0.9495]	
(1-3+4-5) UCC							0.99496	
(1-3+4-5) No change			0.92792		0.93414	0.98914	0.95117	
(1-3+4-5) [10%, 20%]			[0.8596, 0.7436]		[0.8825, 0.7892]	[0.9782, 0.9531]	[0.9610, 0.9689]	
(2-3+4-5) UCC							0.97334	
(2-3+4-5) No change				0.84611	0.86404	0.96601	0.91793	
(2-3+4-5) [10%, 20%]				[0.7492, 0.6220]	[0.7936, 0.6900]	[0.9415, 0.8958]	[0.9278, 0.9365]	
Major and trace elements- based diagrams								
(1+2-3+4-5) UCC							0.98581	
(1+2-3+4-5) No change	0.86377	0.84043			0.92193	0.99002	0.96549	
(1+2-3+4-5) [10%, 20%]	[0.6037, 0.4021]	[0.5970, 0.3562]			[0.8937, 0.8520]	[0.9854, 0.9776]	[0.9697, 0.9731]	
(1-2-3+4) UCC					0.47	7778		
(1-2-3+4) No change			0.58701	0.64616	0.98474	0.99848		
(1-2-3+4) [10%, 20%]			[0.5944, 0.6032]	[0.6089, 0.5675]	[0.9827, 0.9798]	[0.9981, 0.9976]		
(1-2-5) UCC							0.99520	
(1-2-5) No change			0.54861	0.59639			0.94769	
(1-2-5) [10%, 20%]			[0.4666, 0.3467]	[0.4828, 0.3289]			[0.9581, 0.9665]	
(1-3+4-5) UCC							0.98058	
(1-3+4-5) No change			0.83946		0.91525	0.98628	0.96261	
(1-3+4-5) [10%, 20%]			[0.6287, 0.4129]		[0.8854, 0.8421]	[0.9802, 0.9701]	[0.9657, 0.9684]	
(2-3+4-5) UCC							0.99072	
(2-3+4-5) No change				0.94673	0.89487	0.99756	0.97595	
(2-3+4-5) [10%, 20%]				[0.6347, 0.2257]	[0.8579, 0.8047]	[0.9680, 0.9526]	[0.9798, 0.9826]	
Trace element-based diagrams								
(1+2-3+4-5) UCC					0.57	7012		
(1+2-3+4-5) No change	0.96541	0.91223			0.97804	0.99661	0.98297	
(1+2-3+4-5) [10%, 20%]	[0.8800, 0.7376]	[0.7379, 0.5410]			[0.9733, 0.9669]	[0.9958, 0.9947]	[0.9739, 0.9601]	
(1-2-3+4) UCC					0.79	0084		
(1-2-3+4) No change			0.71546	0.64256	0.98757	0.99908		

Table S22. Evaluation of the 3 sets of multidimensional diagrams for bulk assimilation of upper continental crust (UCC).

Table S22. (continued).

(1-2-3+4) [10%, 20%]	 	[0.6666, 0.5930]	[0.5585, 0.4788]	[0.9858, 0.9834]	[0.9989, 0.9986]	
(1-2-5) UCC						0.82762
(1-2-5) No change	 	0.71670	0.63668			0.98681
(1-2-5) [10%, 20%]	 	[0.6646, 0.5970]	[0.5619, 0.4943]			[0.9835, 0.9791]
(1-3+4-5) UCC				0.54	1487	
(1-3+4-5) No change	 	0.96450		0.97209	0.99371	0.97546
(1-3+4-5) [10%, 20%]	 	[0.8882, 0.7628]		[0.9663, 0.9588]	[0.9925, 0.9907]	[0.9635, 0.9461]
(2-3+4-5) UCC				0.61	370	
(2-3+4-5) No change	 		0.94219	0.97245	0.99233	0.97787
(2-3+4-5) [10%, 20%]	 		[0.7382, 0.4818]	[0.9675, 0.9611]	[0.9910, 0.9892]	[0.9671, 0.9511]

For more explanation, see Table S19.

Diagram type [petrogenetic	Probability ch	Probability change of the centroid $[p_{gain}, p_{loss}]$ caused by fractional crystallization applied to basic magmas *								
process of fractional		Arc		CR	OI	Collision				
crystallization	IA+CA	IA	CA	Within-pla	te (CR+OI)	Col				
(1+2-3+4-5) Centroid of basic magmas	0.86271			0.98273 (CR)	0.98691 (OI)	No data				
[FC of olivine: $F = 0.50$]	[0.8240]			[0.9827]	[0.9869]					
[FC of cpx: F = 0.50]	[0.5298]			[0.9795]	[0.9845]					
[FC of opx: F = 0.50]	[0.9484]			[0.9803]	[0.9850]					
[FC of plg: F = 0.50]	[0.8598]			[0.9847]	[0.9884]					
(1-2-3+4) Centroid of basic magmas		0.42952-	- 0.55888	0.99620	0.99730					
[FC of olivine: $F = 0.50$]		[0.4290]	[0.5585]	[0.9966]	[0.9976]					
[FC of cpx: F = 0.50]		[0.3384]	[0.6214]	[0.9988]	[0.9992]					
[FC of opx: F = 0.50]		[0.3612]	[0.6356]	[0.9853]	[0.9895]					
[FC of plg: F = 0.50]		[0.4785]	[0.5107]	[0.9964]	[0.9974]					
(1-2-5) Centroid of basic magmas		0.46586-0.48481				No data				
[FC of olivine: $F = 0.50$]		[0.4686]	[0.4653]							
[FC of cpx: F = 0.50]		[0.3045]	[0.4228]							
[FC of opx: F = 0.50]		[0.3826]	[0.6001]							
[FC of plg: F = 0.50]		[0.5185]	[0.4318]							
(1-3+4-5) Centroid of basic magmas		0.80111		0.97864	0.98237	No data				
[FC of olivine: $F = 0.50$]		[0.7545]		[0.9785]	[0.9822]					
[FC of cpx: F = 0.50]		[<u>0.4338]</u>		[0.9730]	[0.9776]					
[FC of opx: F = 0.50]		[0.9093]		[0.9794]	[0.9831]					
[FC of plg: F = 0.50]		[0.8137]		[0.9808]	[0.9842]					
(2-3+4-5) Centroid of basic magmas			0.88619	0.98231	0.98649	No data				
[FC of olivine: $F = 0.50$]			[0.8500]	[0.9823]	[0.9865]					
[FC of cpx: F = 0.50]			[0.5926]	[0.9747]	[0.9818]					
[FC of opx: F = 0.50]			[0.9517]	[0.9800]	[0.9827]					
[FC of plg: F = 0.50]			[0.8696]	[0.9849]	[0.9884]					

Table S23. Evaluation of the third trace element-based multidimensional diagrams for petrogenetic process of fractional crystallization applied to basic magmas.

Diagram type	Probabilit	y change of the ce	ntroid $[p_{gain}, p_{loss}]$	caused by AFC a	pplied to basic mag	gmas*
mineral [petrogenetic process		Arc		CR	OI	Collision
of AFC; $r-F_{remain}$]	IA+CA	IA	CA	Within-pla	te (CR+OI)	Col
(1+2-3+4-5) Centroid of basic magmas	0.86271			0.98273 (CR)	0.98691 (OI)	No data
olivine [0.2-0.7, 0.4-0.5]	[0.7007, 0.3509]			[0.9774, 0.9567]	[0.9814, 0.9589]	
cpx [0.2–0.7, 0.4–0.5]	[0.4986, 0.0773]			[0.9752, 0.9455]	[0.9795, 0.9472]	
opx [0.2-0.7, 0.4-0.5]	[0.8450, 0.7934]			[0.9760, 0.9437]	[0.9803, 0.9492]	
plg [0.2–0.7, 0.4–0.5]	[0.7315, 0.4229]			[0.9791, 0.9633]	[0.9828, 0.9654]	
(1-2-3+4) Centroid of basic magmas		0.42952-	-0.55888	0.99620	0.99730	
olivine [0.2–0.7, 0.4–0.5]		[0.4273, 0.3047]	[0.5218, 0.3975]	[0.9958, 0.9934]	[0.9971, 0.9959]	
cpx [0.2–0.7, 0.4–0.5]		[0.3568, 0.1002]	[0.5428, 0.2208]	[0.9978, 0.9984]	[0. 9985, 0.9990]	
opx [0.2-0.7, 0.4-0.5]		[0.3955, 0.3133]	[0.5819, 0.6311]	[0.9894, 0.9438]	[0.9928, 0.9627]	
plg [0.2–0.7, 0.4–0.5]		[0.4574, 0.3725]	[0.4957, 0.3719]	[0.9956, 0.9925]	[0.9970, 0.9954]	
(1-2-5) Centroid of basic magmas		0.46586-	-0.48481			No data
olivine [0.2–0.7, 0.4–0.5]		[0.4382, 0.2952]	[0.4399, 0.3487]			
cpx [0.2-0.7, 0.4-0.5]		[0.3205, 0.0513]	[0.3995, 0.1019]			
opx [0.2-0.7, 0.4-0.5]		[0.4049, 0.2841]	[0.5395, 0.6494]			
plg [0.2–0.7, 0.4–0.5]		[0.4708, 0.3787]	[0.4254, 0.3532]			
(1-3+4-5) Centroid of basic magmas		0.80111		0.97864	0.98237	No data
olivine [0.2–0.7, 0.4–0.5]		[0.6347, 0.3267]		[0.9725, 0.9492]	[0.9757, 0.9497]	
cpx [0.2-0.7, 0.4-0.5]		[0.4304, 0.0731]		[0.9685, 0.9315]	[0.9720, 0.9310]	
opx [0.2-0.7, 0.4-0.5]		[0.7818, 0.7169]		[0.9733, 0.9496]	[0.9765, 0.9516]	
plg [0.2–0.7, 0.4–0.5]		[0.6798, 0.4250]		[0.9743, 0.9561]	[0.9773, 0.9567]	
(2-3+4-5) Centroid of basic magmas			0.88619	0.98231	0.98649	No data
olivine [0.2–0.7, 0.4–0.5]			[0.6675, 0.2492]	[0.9775, 0.9588]	[0.9821, 0.9636]	
cpx [0.2-0.7, 0.4-0.5]			[0.4794, 0.0609]	[0.9721, 0.9301]	[0.9783, 0.9375]	
opx [0.2-0.7, 0.4-0.5]			[0.8113, 0.6542]	[0.9765, 0.9512]	[0.9804, 0.9548]	
plg [0.2–0.7, 0.4–0.5]			[0.6843, 0.2727]	[0.9797, 0.9575]	[0.9837, 0.9712]	

Table S24. Evaluation of the third trace element-based multidimensional diagrams for petrogenetic process of assimilation and fractional crystallization (AFC) applied to basic magmas.