J Soils Sediments
DOI 10.1007/s11368-013-0798-8

SEDIMENTS, SEC 1 • SEDIMENT QUALITY AND IMPACT ASSESSMENT • RESEARCH ARTICLE

Geochemistry of sediments in three sectors of Trincomalee Bay, Sri Lanka: provenance, modifying factors and present environmental status

Sansfica M. Young · Hiroaki Ishiga · Barry P. Roser · Amarasooriya Pitawala

Received: 11 December 2012 / Accepted: 18 October 2013

Abstract
Purpose The geochemical compositions of sediments from three sectors in Trincomalee Bay (Koddiyar Bay, Thambalagam Bay and the Inner Harbour) in Sri Lanka were examined to determine fluvial and marine contributions and the effects of sorting and heavy mineral concentration. The present environmental status of the bay was also assessed.
Materials and methods Forty-nine sediment samples were collected from Trincomalee Bay and analysed by X-ray fluorescence, yielding data for the major elements and 17 trace elements. Mean grain size and sorting were also measured. Data were compared with the compositions of sediments from the lower Mahaweli River, which supplies most of the clastic detritus to Trincomalee Bay.
Results and discussion Sediments in the three sectors differ significantly in chemical composition, according to position relative to the Mahaweli River delta source, depositional environment, heavy mineral concentration and marine influences. According to accepted sediment quality guidelines, some As contamination may have occurred in the Inner Harbour and Thambalagam Bay and Cr contamination in all three sectors.
Conclusions Proximal Koddiyar Bay sediments compare closely with Mahaweli River bedload. Although the clastic component in the more distal Thambalagam Bay and the Inner Harbour is also derived from the Mahaweli River, compositions are modified significantly by marine contributions. High concentrations of elements including Ti, Zr, Ce, Nb and Y in NW Koddiyar Bay are consistent with heavy mineral concentration by winnowing in high-energy zones. Some decoupling of Fe–Ti- and Zr-bearing heavy mineral assemblages may occur within the bay. Al-normalized metal enrichment factors and contour maps show that apparent contamination by As and Cr is spurious and is caused by locally high background levels from Mahaweli River detritus. This illustrates the importance of establishing local background levels of elements during environmental studies.

Keywords Geochemistry · Pollution · Provenance · Sediments · Sri Lanka · Trincomalee Bay

Responsible editor: Marc Babut

Electronic supplementary material The online version of this article (doi:10.1007/s11368-013-0798-8) contains supplementary material, which is available to authorized users.

S. M. Young (✉) · H. Ishiga · B. P. Roser
Department of Geoscience, Shimane University,
690-8504 Matsue, Japan
e-mail: sansfica@sansfica.com

A. Pitawala
Department of Geology, University of Peradeniya, Peradeniya,
Kandy, Sri Lanka

1 Introduction

Estuaries are sites where the energy available to transport sediments decreases abruptly, and tidal influences can produce ebb and flow of sediments. The environment of such estuarine and coastal zones is thus both dynamic and complex (Morris et al. 1995). Interactions between freshwater and saltwater bodies in this land–sea interface, and resultant changes in physical, chemical and biogenic inputs, can strongly affect the transport and deposition of trace elements (Ladipo et al. 2011). Transport of trace elements from rivers, through estuaries, and into the open ocean is influenced by partitioning between dissolved and particulate phases (Ip et al. 2007). Modern or historic anthropogenic inputs of trace metals can

Published online: 06 November 2013

be identified in river and bay sediments (Lin et al. 2007, 2012), and contamination of these sensitive aquatic ecosystems is unfortunately not uncommon. Major and trace element compositions of sediments are often used to study the geochemical impacts of provenance, environmental issues, transport of weathering products and climatic events (e.g. Hirst 1962; Pattan et al. 1995; Dellwig et al. 2000; Borrego et al. 2002; Ip et al. 2007).

Trincomalee Bay is located in northeast Sri Lanka (Fig. 1). The sheltered deep-water port of Trincomalee Bay has been used for centuries and has a European history dating back to the days of Marco Polo. Trincomalee Bay comprises an estuarine system open to the Indian Ocean. Physiographically, the bay can be divided into three distinct sectors: Koddiyar Bay in the south; Thambalagam Bay in the west; and the Inner Harbour in the north (Fig. 1). Four major channels of the Mahaweli River—the longest in Sri Lanka—enter Koddiyar Bay in a delta system in its south section. Koddiyar Bay thus receives voluminous clastic detritus from these river systems. In contrast, Thambalagam Bay is almost fully enclosed and is not fed by any major rivers. The Inner Harbour also lacks major river inflow and is more open to the sea. Sediment supply and estuarine dynamics should thus differ in these three parts of Trincomalee Bay.

Utilization of the three parts of the bay also differs. The Inner Harbour is the main site of port and shipbuilding facilities, and the area surrounding it is urbanized and industrialized. The shallow waters of Thambalagam Bay restrict activity mainly to small-scale fishing, and Koddiyar Bay is the main estuary zone of the Mahaweli River delta. These contrasting uses may also have caused varying anthropogenic impacts.

With the exception of studies of stratigraphy and groundwater availability in the delta sediments of the Mahaweli River (e.g. Jayawardena 2005) and the basement geology around Trincomalee Bay (Fig. 2, e.g. Wijayananda 1985), no other major studies have been carried out in the area. Hydrogeological investigations by Jayawardena (2005) found that the sediments in the Mahaweli delta were mainly deposits of the river itself and not a mixture of sea sediments. Our present study sets out to test that hypothesis, utilizing the first sediment composition data from this major fluvial–estuarine system, which is the most important in Sri Lanka.

We determined the geochemical characteristics of surface sediments in the three sectors of Trincomalee Bay to (a) determine their provenance, by comparison with data for main river channel sediments in the lower Mahaweli River; (b) evaluate the possible roles of circulation and oceanic influence within the bay in modifying sediment compositions; (c) assess

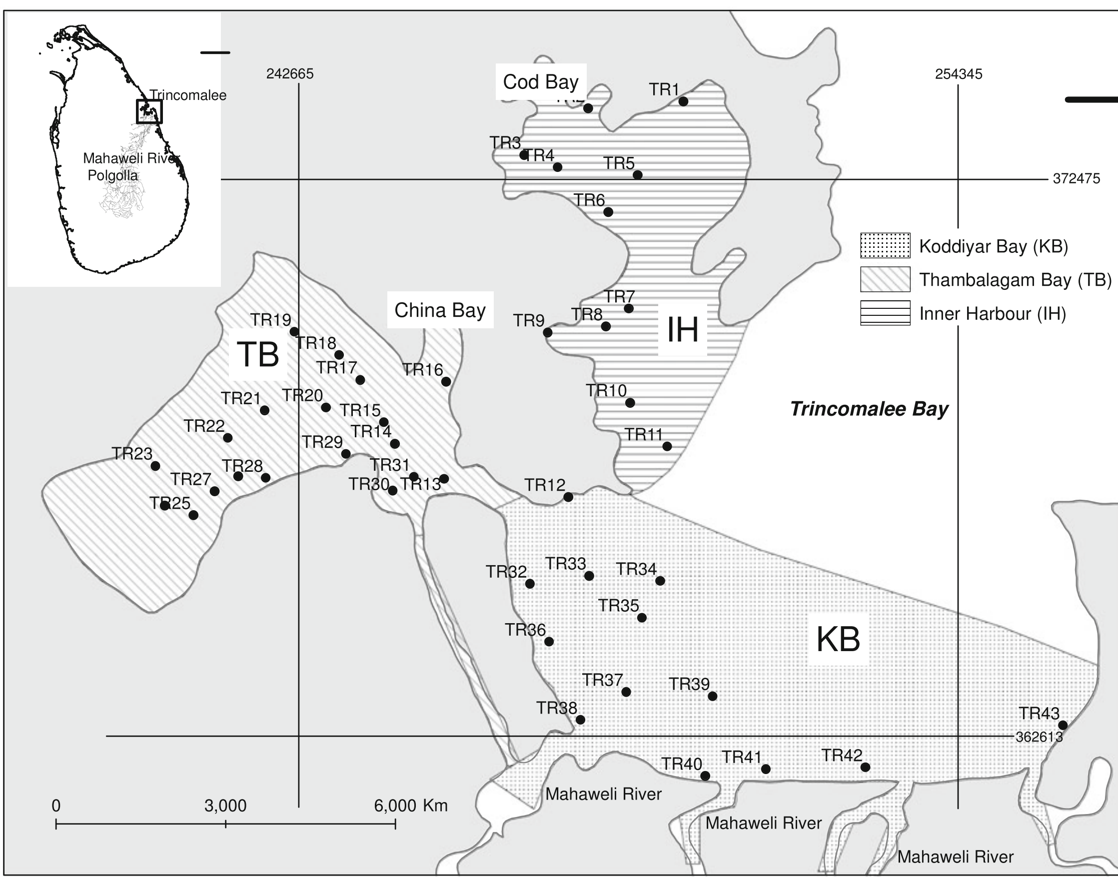


Fig. 1 Location of Trincomalee Bay, Sri Lanka and sample sites within the Inner Harbour (*IH*), Thambalagam Bay (*TB*) and Koddiyar Bay (*KB*)

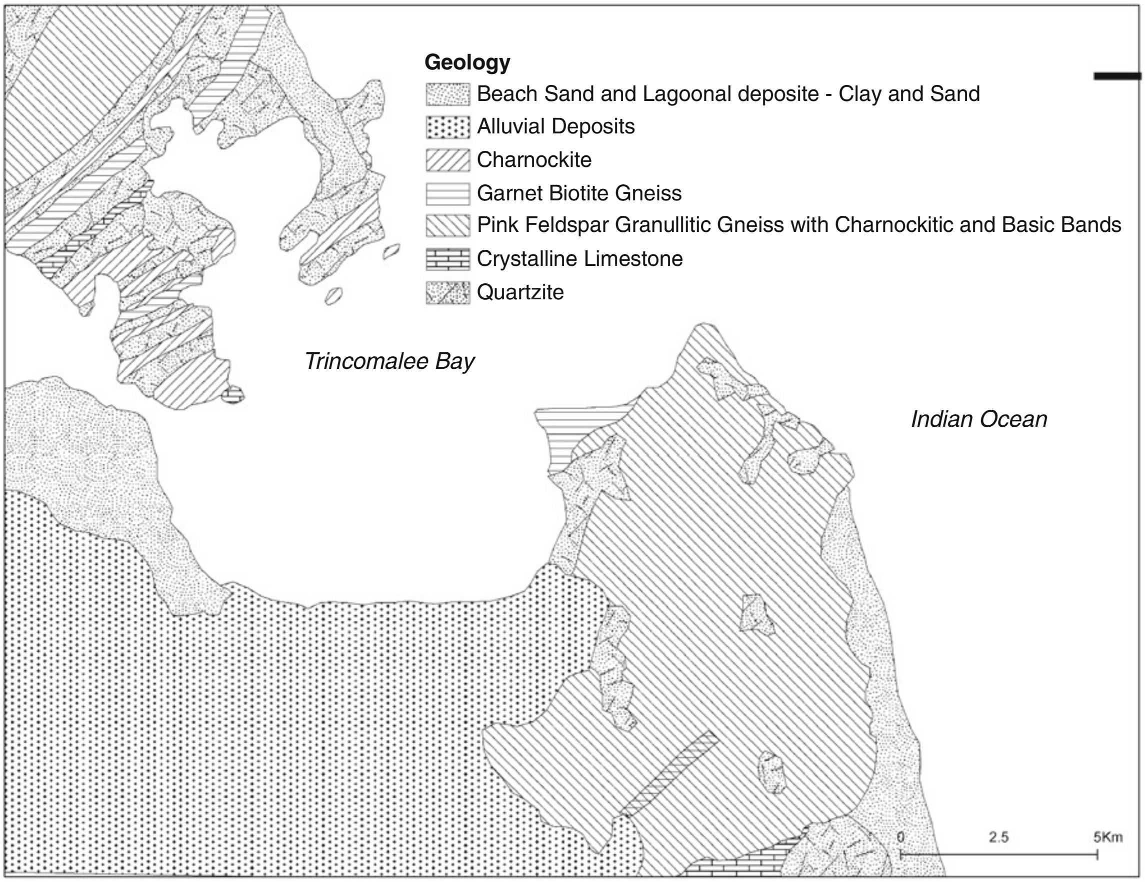


Fig. 2 Simplified geological map of the area surrounding Trincomalee Bay (after Wijayananda 1985)

present environmental conditions by comparison with established sediment quality guidelines; and (d) evaluate the results from those guidelines compared to those using local background values derived from sediment data from the Mahaweli River.

2 Study area

Trincomalee Harbour is a natural bay trending NE–SW, with a gentle average slope of about 3° (Wijayananda 1985). The three sectors of the bay developed due to the configuration of the local basement rocks and operation of coastal and fluvial processes. The dimensions of the Inner Harbour are mainly controlled by the basement geology, whereas those of Thambalagam Bay are influenced by beach deposits, and the more open Koddiyar Bay is dominated by deposits of the Mahaweli River delta.

The inland area is slightly undulating, with small hills forming 'turtle back' topography. The topographic highs are mantled by soils, whereas the lows are characterized by alluvial deposits, peaty clays developed due to marshy conditions and thick soils derived from gneissic basement rocks. Mean annual rainfall is more than 900 mm, and most precipitation falls during the NE monsoons from October to January. Lowest rainfall occurs from March to June. Mean monthly temperatures vary from 25.6 to 30.0 °C.

Basement in the study area consists of Precambrian Highland Complex rocks (Fig. 2). The Highland Complex consists of upper amphibolite to granulite facies metamorphic rocks and minor igneous rocks (Cooray 1994). Garnet-cordierite gneisses, meta-quartzites, marbles, orthogneisses and charnockitic gneisses are common lithotypes. The general trend of the basement rocks is NW–SE, and the area is characterized by megascale deformational features such as synforms and an antiform (Wijayananda 1985). Quartzites are the most common rocks in the Trincomalee Bay area (Fig. 2). These are highly resistant to weathering and form ridges along the coast. Interbedded charnockite, the next most prominent lithology, is less resistant and underlies areas of lower elevation. Marbles occur as limited bands or patches in the southeastern part of the bay. Pink feldspar granulitic gneiss occurs north of the Inner Harbour and east of Koddiyar Bay.

3 Methodology

Surface sediments in Trincomalee Bay were collected taking the proximity of the Mahaweli River mouth into account and location in Koddiyar Bay, Thambalagam Bay and the Inner Harbour (Fig. 1). Samples from the Inner Harbour ($n=12$) and Thambalagam Bay ($n=19$) were collected using an Ekman-Birge bottom sampler. Water depths at sampling points ranged up to 11.5 m. Sample positions were recorded using global positioning system. The grab samples (1–2 kg) were subsampled (about 500 g) at a depth of 3–6 cm below surface. Some samples from Koddiyar Bay ($n=17$) were taken by free diving, as strong current activity at the time of sampling precluded use of the Ekman-Birge sampler.

The samples were air dried and then halved by coning and quartering. One split was archived, and the other was used for textural and geochemical analysis. This split was oven dried at 120 °C for 1 week at the University of Peradeniya, Sri Lanka. All analyses were carried out at Shimane University. Grain size analysis was determined using a laser diffraction particle size analyser (SALD-3000). Oven-dried sediments were treated with 30% H_2O_2 for at least 24 h prior to measurement. Calculations of grain size and sorting were made following Folk and Ward (1957) and are presented in phi (ϕ) units.

Approximately 50 g of each sample was oven dried at 160 °C for 48 h before crushing in a tungsten carbide ring mill. Portions (7–10 g) of the crushed materials were transferred to glass vials and dried at 110 °C for 24 h prior to determination of loss on ignition (LOI). The LOI values were calculated from the net weight loss after ignition in a muffle furnace at 1,020 °C for more than 2 h. Abundances of major elements and 14 trace elements were determined from glass fusion beads using a Rigaku RIX-2000 X-ray fluorescence (XRF) spectrometer, using the methods described by Kimura and Yamada (1996). Abundances of three additional trace elements (As, Cu, Zn) were determined from pressed powder briquettes, following Ogasawara (1987). Additional description of the XRF analysis including standard analyses and estimates of precision is given in the Electronic Supplementary Material 1.

Statistical analyses (p values, t values) were calculated using Minitab 14 software to determine if differences were present between the three sectors. Principal component analysis (PCA) was carried out using the Pearson method in XLSTAT 12. Geographic information system (GIS) contour maps of element distributions were generated using ARC-GIS 9.2. The maps were generated using the nearest neighbor method with inverse distance-weighted interpolation, with contours in five classes.

4 Results

Averages and ranges of grain size and geochemical compositions in the Inner Harbour, Thambalagam Bay and Koddiyar Bay are listed in Table 1 and compared to average upper continental crust (UCC; Taylor and McLennan 1985) and stream sediments from the lower Mahaweli River (Young et al. 2012). Individual Trincomalee analyses are contained in the Electronic Supplementary Material (Table OR1). Values of LOI are variable, but are higher on average in the Inner Harbour (12.9 wt%) than in Thambalagam and Koddiyar Bays (3.18 and 2.69 wt%, respectively; Table OR1). Total organic carbon (TOC) contents of selected samples analysed for a separate Ostracode study are low (<0.49 wt%; Young, unpublished data), indicating that TOC contents are not responsible for the higher LOI values.

4.1 Texture

Mean grain size of the Trincomalee Bay sediments ranged from −0.13 to 4.60 ϕ (Table 1), equivalent to very coarse sand to coarse silt. Average mean grain size of the three sectors show limited contrast, with values of 1.29 ϕ (Inner Harbour), 1.71 ϕ (Thambalagam Bay) and 1.77 ϕ (Koddiyar Bay). The sediments in Thambalagam Bay show the least variability (0.16–3.47 ϕ) (Fig. 3). Clay contents (<9 Φ, 2 μm) are generally low (<2% for most samples), but combined silt and clay contents can be significant, with the <4 Φ fraction (clay and silt) averaging 9.05, 8.08 and 6.85 wt% in the Inner Harbour, Thambalagam Bay and Koddiyar Bay (Electronic Supplementary Material 1). The sediments are also generally well sorted, with sorting greatest in the Inner Harbour (average 2.08, range 0.41–2.63), compared to 1.64 (0.30–2.48) and 1.51 (0.81–2.59) in Thambalagam and Koddiyar Bays, respectively (Table 1 and Fig. 3).

4.2 Major elements

Major element concentrations show some contrast between the three sectors. Average SiO_2 contents in the Inner Harbour, Thambalagam Bay and Koddiyar Bay are 62.69, 74.38 and 69.76 wt%, respectively, intermediate between the composition of UCC (66.0 wt%) and sediments from the lower reaches of the Mahaweli River (78.95 wt%; Table 1). Average concentrations of Al_2O_3 are 8.18, 11.43 and 11.68 wt%, respectively, less than in UCC (15.20 wt%), but similar to lower Mahaweli River sediments (9.90 wt%; Table 1, data from Young et al. 2012).

Among the other major elements, CaO contents show the greatest contrast (Table 1), with much higher levels and greater range in the Inner Harbour (average 17.52 wt%, range 3.02–40.60 wt%) than in Thambalagam (average 3.61; range 1.31–13.90 wt%) or Koddiyar Bay (average 4.58; range 1.38–22.33 wt%). The higher CaO contents are due to the presence of shell fragments. Average Fe_2O_3 and TiO_2 contents in Koddiyar Bay (6.71 and 1.43 wt%, respectively) are significantly greater than in the two other sectors, UCC and the lower Mahaweli sediments (Table 1). In contrast, average MgO, Na_2O and K_2O contents in all three sectors are

Table 1 Average, minimum and maximum elemental concentrations in the three sectors of Trincomalee Bay, compared to sediments from the lower Mahaweli River (data from Young et al. 2012) and upper continental crust (Taylor and McLennan 1985)

	Inner Harbour (n=12)				Thambalagam Bay (n=19)				Koddiyar Bay (n=17)				LMR	UCC	p value			T value		
	Mean	STDEV	Min	Max	Mean	STDEV	Min	Max	Mean	STDEV	Min	Max	(n=18)		IH-TB	TB-KB	KB-IH	IH-TB	TB-KB	KB-IH
SiO_2	**62.69**	16.42	39.04	85.65	**74.38**	8.28	59.25	86.30	**69.76**	11.93	37.06	83.37	**78.95**	66.00	**0.037**	0.209	0.209	**2.30**	1.31	1.30
TiO_2	**1.09**	0.48	0.32	2.15	**0.73**	0.52	0.14	2.14	**1.43**	1.17	0.13	5.18	**0.87**	0.50	0.944	**0.038**	0.425	1.64	1.86	0.81
Al_2O_3	**8.18**	2.62	2.67	11.70	**11.43**	2.58	7.68	19.00	**11.68**	2.88	5.32	15.89	**9.90**	15.20	**0.002**	0.547	**0.002**	**3.24**	0.12	**3.09**
Fe_2O_3[a]	**4.79**	2.27	1.52	8.49	**4.19**	3.62	0.82	12.97	**6.71**	7.34	0.80	32.91	**4.97**	4.50	0.708	0.115	0.167	0.55	1.24	0.99
MnO	**0.06**	0.03	0.02	0.13	**0.06**	0.04	0.01	0.12	**0.10**	0.11	0.01	0.48	**0.08**	0.08	0.623	0.060	0.077	0.32	1.63	1.49
MgO	**2.31**	1.41	0.67	4.55	**1.05**	0.72	0.33	3.12	**1.57**	1.23	0.31	5.57	**0.73**	2.20	0.996	0.927	0.937	**3.01**	1.50	1.60
CaO	**17.52**	12.81	3.02	40.60	**3.61**	3.16	1.31	13.90	**4.58**	5.32	1.38	22.33	**1.61**	4.20	0.998	0.735	0.997	**3.68**	0.64	**3.31**
Na_2O	**1.50**	0.46	0.61	2.12	**2.12**	0.48	1.36	2.94	**1.84**	0.45	0.93	2.56	**0.87**	3.90	**0.001**	**0.040**	**0.048**	**3.49**	1.81	1.73
K_2O	**1.72**	0.64	0.43	2.58	**2.34**	0.51	1.59	3.18	**2.26**	0.62	0.83	3.20	**1.95**	3.40	**0.004**	0.179	**0.026**	**2.98**	0.93	**2.06**
P_2O_5	**0.14**	0.14	0.04	0.55	**0.09**	0.10	0.01	0.36	**0.07**	0.04	0.01	0.14	**0.08**	0.16	0.849	0.212	0.940	1.06	0.82	1.68
Ba	**601**	263	237	1,080	**840**	132	648	1,120	**764**	181	370	997	–	550	**0.005**	0.082	**0.039**	**2.93**	1.43	1.87
Ce	**141**	206	28	792	**84**	143	11	654	**147**	145	11	572	–	64	0.796	0.901	0.468	0.85	1.32	0.08
Cr	**73**	54	26	192	**50**	41	11	181	**96**	79	7	356	**115**	35	0.219	**0.041**	0.354	1.27	**2.17**	0.94
Ga	**6**	3	0	10	**8**	5	1	20	**10**	4	0	14	–	17	**0.035**	0.995	**0.048**	**2.22**	0.01	**2.07**
Nb	**16**	16	2	57	**12**	11	3	54	**40**	57	4	242	**16**	25	0.460	0.086	0.156	0.76	1.82	1.48
Ni	**16**	19	3	57	**11**	10	4	46	**13**	7	0	27	**26**	20	0.398	0.606	0.529	0.87	0.52	0.65
Pb	**23**	26	3	103	**14**	3	8	20	**15**	4	9	20	**21**	20	0.308	0.552	0.269	1.07	0.60	1.16
Rb	**43**	14	15	70	**68**	15	44	100	**62**	19	11	84	–	112	**0.000**	0.261	**0.005**	**4.73**	1.15	**3.04**
Sc	**25**	10	10	37	**11**	5	3	24	**16**	10	4	43	**15**	11	**0.000**	0.105	**0.014**	**4.77**	1.69	**2.67**
Sr	**936**	581	319	2266	**371**	90	169	557	**405**	365	54	1,658	**239**	350	**0.007**	0.715	**0.012**	**3.34**	0.37	**2.80**
Th	**22**	14	6	49	**22**	49	3	222	**33**	37	5	156	**13**	11	0.977	0.461	0.268	0.03	0.75	1.14
V	**105**	52	30	193	**84**	75	16	347	**194**	251	11	1,090	**163**	60	0.378	0.100	0.173	0.90	1.73	1.42
Y	**29**	29	8	118	**17**	11	5	39	**26**	21	4	93	**22**	22	0.169	0.111	0.754	1.46	1.66	0.32
Zr	**1,089**	2,226	164	8,123	**460**	847	103	3,914	**1,064**	1,271	107	5,247	**301**	190	0.366	0.109	0.973	0.94	1.66	0.03
As	**7**	4	3	19	**10**	12	2	43	**4**	2	2	9	**4**	5[a]	0.416	**0.047**	**0.029**	0.83	**2.13**	**2.43**
Zn	**49**	38	21	152	**31**	17	9	79	**51**	40	6	181	**57**	71	0.143	0.070	0.920	1.56	1.91	0.10
Cu	**13**	14	2	41	**6**	5	0	23	**6**	4	2	14	**16**	25	0.154	0.751	0.126	1.52	0.32	1.66
Mean GS (phi)	**1.29**	1.39	−0.76	3.43	**1.71**	1.00	0.16	3.47	**1.77**	1.41	−0.95	4.60	–	–	0.372	0.889	0.370	0.92	0.14	0.91
Sorting	**2.08**	0.62	0.41	2.63	**1.64**	0.68	0.30	2.48	**1.51**	0.59	0.81	2.59	–	–	0.076	0.545	**0.021**	1.85	0.61	**2.48**
Ti/Fe	**0.26**	0.13	0.15	0.49	**0.21**	0.09	0.06	0.36	**0.23**	0.07	0.12	0.35	**0.17**	0.11						
Zr/Ti	**0.17**	0.32	0.09	0.63	**0.11**	0.06	0.12	0.30	**0.12**	0.04	0.14	0.17	**0.06**	0.06						

Major oxides in weight percent, trace elements in parts per million; p values less than 0.05, in bold, indicate the null hypothesis is rejected and the three sectors differ in composition. T values, in bold, indicate higher variance where the three sectors differ in composition

LMR lower Mahaweli Rive, UCC upper continental crust

[a] Value from Rudnick and Gao (2005)

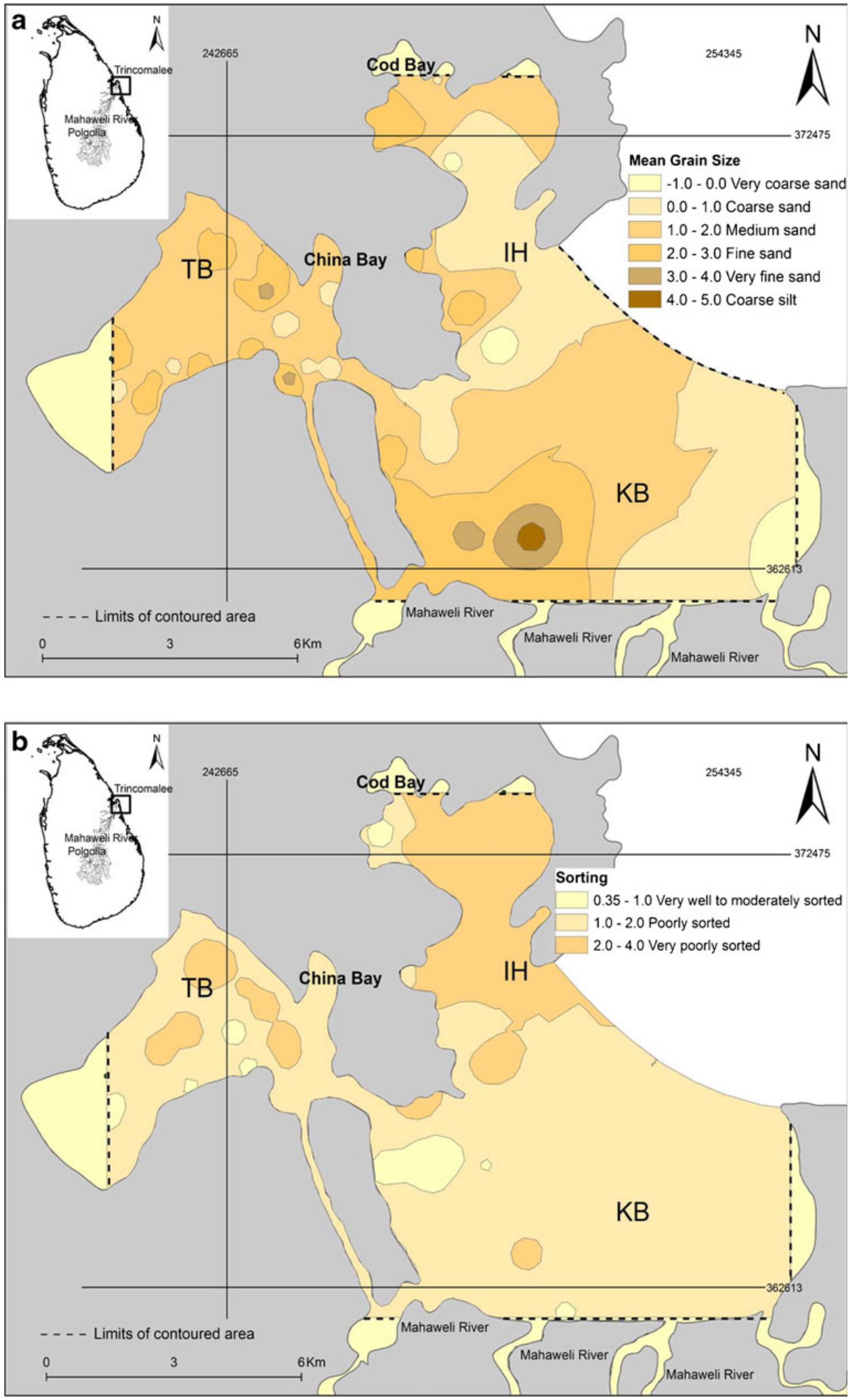


Fig. 3 Geographical information system contour maps showing the spatial variation of **a** mean grain size and **b** sorting in Trincomalee Bay. Grain size and sorting were calculated following Folk and Ward (1957) and units are in ϕ

intermediate between higher levels in UCC and lower levels in the lower Mahaweli sediments. This also tends to be the case for the minor elements MnO and P_2O_5.

The statistical values of σ, p value and the t value for a two sample t test with 95% confidence and the alternative of being not equal are given in Table 1, to test (1) if there is a difference between the means of the three sectors and (2) if there is a difference between the statistical values for the three sectors. The null hypothesis is rejected when the p value is <0.05, where the three sectors differ in composition. Similarity between sectors is indicated by a variance >0.05. In the t test, higher variance indicates that the two means are not equal, and hence, the compositions of the three sectors differ. A lesser variance indicates that the three sectors have similar composition. Statistically, the p values for Ti, Fe, Mn, Mg, Ca and P are much higher (>0.05) for Inner Harbour and Thambalagam Bay, and thus, the null hypothesis that the two data sets are different from each other is rejected. The t values for major elements in Inner Harbour–Thambalagam Bay differ from those in Thambalagam Bay–Koddiyar Bay and Koddiyar Bay–Inner Harbour (Table 1). Therefore, the major element compositions of the three sectors differ.

The major elements were plotted on variation diagrams against Al_2O_3 as a proxy of grain size and clay mineral content. Correlation matrices for all elements are given in the Electronic Supplementary Material 2. SiO_2 shows broad negative correlation with Al_2O_3 in the Koddiyar ($R = -0.58$) and Thambalagam ($R = -0.53$) sectors (Fig. 4a). Correlation is weakest in the Inner Harbour suite ($R = -0.49$), with considerable scatter towards lower values of both SiO_2 and Al_2O_3 (Fig. 4a), consistent with dilution from bioclastic CaO (Fig. 4b). Values of Fe_2O_3, MnO, MgO, Na_2O and K_2O show good correlation ($R > 0.56$) with Al_2O_3 in the Inner Harbour. In Koddiyar Bay, Na_2O, K_2O and P_2O_5 show moderate to strong ($R = 0.58$–0.79) correlations with Al_2O_3. Values of MgO show relatively coherent trends in the Koddiyar and Thambalagam suites, but displacement to higher values in the Inner Harbour, possibly also due to carbonate content (Fig. 4c). Both Fe_2O_3 and TiO_2 show weak correlation with Al_2O_3 in all three suites, with no clear trends, and scatter to high values (Fig. 4d, e). In contrast, K_2O shows relatively strong correlations with Al_2O_3 in all three sectors ($R = 0.69$, 0.63 and 0.58 in the Inner Harbour, Thambalagam Bay and Koddiyar Bay, respectively; Electronic Supplementary Material 2), forming a broad trend coinciding with UCC and the field of the lower Mahaweli River sediments (Fig. 4f). This appears to be a product of positive correlation between Al_2O_3 and the proportion of the <4 Φ (62.5 μm) fraction in each sector ($R = 0.56$, 0.75 and 0.41, respectively).

4.3 Trace elements

Of the 17 trace elements analysed, eight (Ba, Ce, Cr, Sc, Sr, Th, V and Zr) have higher average abundances in all three sectors of Trincomalee Bay than in UCC (Table 1). The most marked enrichment is seen for Zr, with average values of 1, 089, 460 and 1,064 ppm in the Inner Harbour, Koddiyar and Thambalagam, respectively, well above the 190 ppm in UCC. Maximum values of Zr are very high (8,123, 3,914 and 5, 247 ppm, respectively), as are maximums for Ce (792, 654 and 572 ppm, respectively) and Th (49, 222 and 156 ppm, respectively) (Table 1). Strontium is most enriched in the Inner Harbour (average 936 ppm; range 319–2,266 ppm), where CaO is also most abundant. The remaining trace elements are present at levels similar to or less than in UCC or average lower Mahaweli River sediment (Table 1).

Representative trace element–Al_2O_3 variation diagrams show that the mobile elements Ba and Rb show moderate positive correlations with Al_2O_3 (Fig. 5a, b), as does Pb (Fig. 5c). The correlations of Ba and Rb with Al_2O_3 are 0.33 and 0.58, 0.60 and 0.31 and 0.74 and 0.65 in the Inner Harbour, Thambalagam Bay and Koddiyar Bay, respectively. Strontium shows poor correlations with Al_2O_3 (Electronic Supplementary Material 2), with relatively low values (<500 ppm) in both Koddiyar and Thambalagam Bays, but scatter to higher values in the Inner Harbour (Fig. 5d), comparable to the pattern shown for CaO (Fig. 4b). These groupings suggest that Sr may be associated with carbonate; Pb and Ba with plagioclase; and Rb and Ba with K-feldspar and clays. The ferromagnesian trace elements Cr (Fig. 5e), Ni, V and Sc show weak correlations with Al_2O_3, with abundances generally intermediate between UCC and the distribution of lower Mahaweli River sediments. The high field strength elements Th, Ce, Zr (Fig. 5f–h), Nb and Y also show very poor correlations and scatter to very high values, especially in the Inner Harbour. The poor correlations seen in these latter two groups of elements with Al_2O_3 suggest that their abundances in individual samples are not controlled by sorting of common silicate minerals or carbonate dilution.

The p values for Ce and Th for Inner Harbour–Thambalagam Bay are very high (0.796 and 0.977, respectively, Table 1) and the null hypothesis is not rejected. The t values of Inner Harbour–Thambalagam Bay for Rb, Sc and Sr are also very high, indicating that the means for these elements in these two sectors differ significantly.

The PCA analysis of the three sectors is given in the Electronic Supplementary Material 2B. PCA has been widely used in environmental studies where the data sets are large and spatially diverse, which makes the determination of spatial characteristics difficult (Reid and Spencer 2009: Woods et al. 2012). The first two principal components account for 79, 71 and 62% of the total variance in the Koddiyar, Thambalagam and Inner Harbour datasets, respectively. F1 shows the greatest variability (57, 44 and 37%, respectively), whereas F2 is relatively uniform (26, 25 and 22%, respectively). These loadings and differing distributions of the elements on the PCA plots, as outlined in the Electronic Supplementary Material 2, suggest that significant compositional contrasts exist between the three sectors. All three statistical methods (p value, t values and PCA) thus show that the three sectors differ in composition.

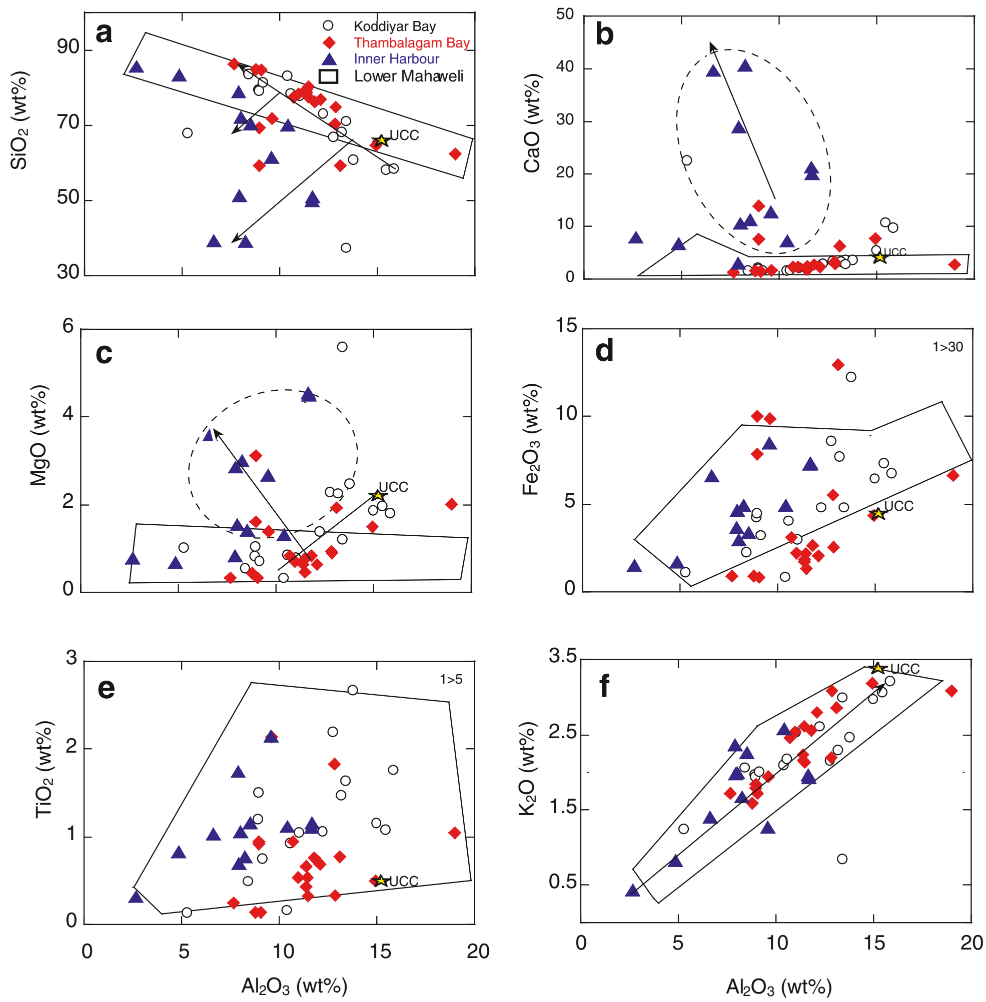


Fig. 4 **a**–**f** Selected major oxides–Al_2O_3 variation diagrams for the Inner Harbour, Thambalagam Bay and Koddiyar Bay surface sediments, compared to upper continental crust (*UCC*; *star*), and fields for lower Mahaweli River sediments. *Lines* indicate possible detrital trends (fitted by eye), *arrows* indicate directions of compositional shift expected from carbonate dilution

5 Discussion

5.1 Upper continental crust-normalized geochemical characteristics

Normalization of average compositions of sediments in the three sectors of Trincomalee Bay and the lower reaches of the Mahaweli River against UCC (Taylor and McLennan 1985) highlights contrasts between the four datasets (Fig. 6). The normalized pattern (UCC_N) for the Mahaweli River sediments is the most regular, although departures from UCC composition are considerable. SiO_2 and TiO_2 are enriched relative to UCC in the Mahaweli River, while the more mobile elements (MgO, CaO, Na_2O and K_2O) are strongly depleted. This reflects derivation from a relatively evolved felsic source, and significant modification of original composition by maturation (relative quartz concentration) and source weathering (Young et al. 2012), by destruction of feldspars and other labile phases. Trace elements in the segment Ba–Th are generally similar to UCC, while Zr and four ferromagnesian trace elements (Cr, V, Sc and Ni) are significantly enriched (Fig. 6). This suggests some zircon concentration in the lower Mahaweli River and also the presence of a significant mafic component in its source.

The UCC_N patterns for the three sectors of Trincomalee Bay show considerably more variability, suggesting modification in the marine environment. The pattern for Koddiyar Bay, the most proximal to the Mahaweli delta, shows the same shape for all major elements, although most are enriched relative to the river sediments, except for SiO_2 (which is depleted), and K_2O and P_2O_5 (which exhibit similar levels). The largest contrasts are for CaO, MgO and Na_2O (Fig. 6), all of which could be contributed from marine sources. Trace element abundances in Koddiyar Bay are generally similar to those in the lower Mahaweli, although Y, Th, Zr and Nb are quite strongly enriched. This grouping of elements, and also relative enrichment of TiO_2 and Fe_2O_3, is suggestive of heavy mineral concentration in Koddiyar Bay as current velocity decreases where the delta meets the sea. The Koddiyar sediments thus carry a strong imprint from the Mahaweli River, as to be expected from their proximal position, along with modification from marine sources (CaO, MgO and Na_2O) and

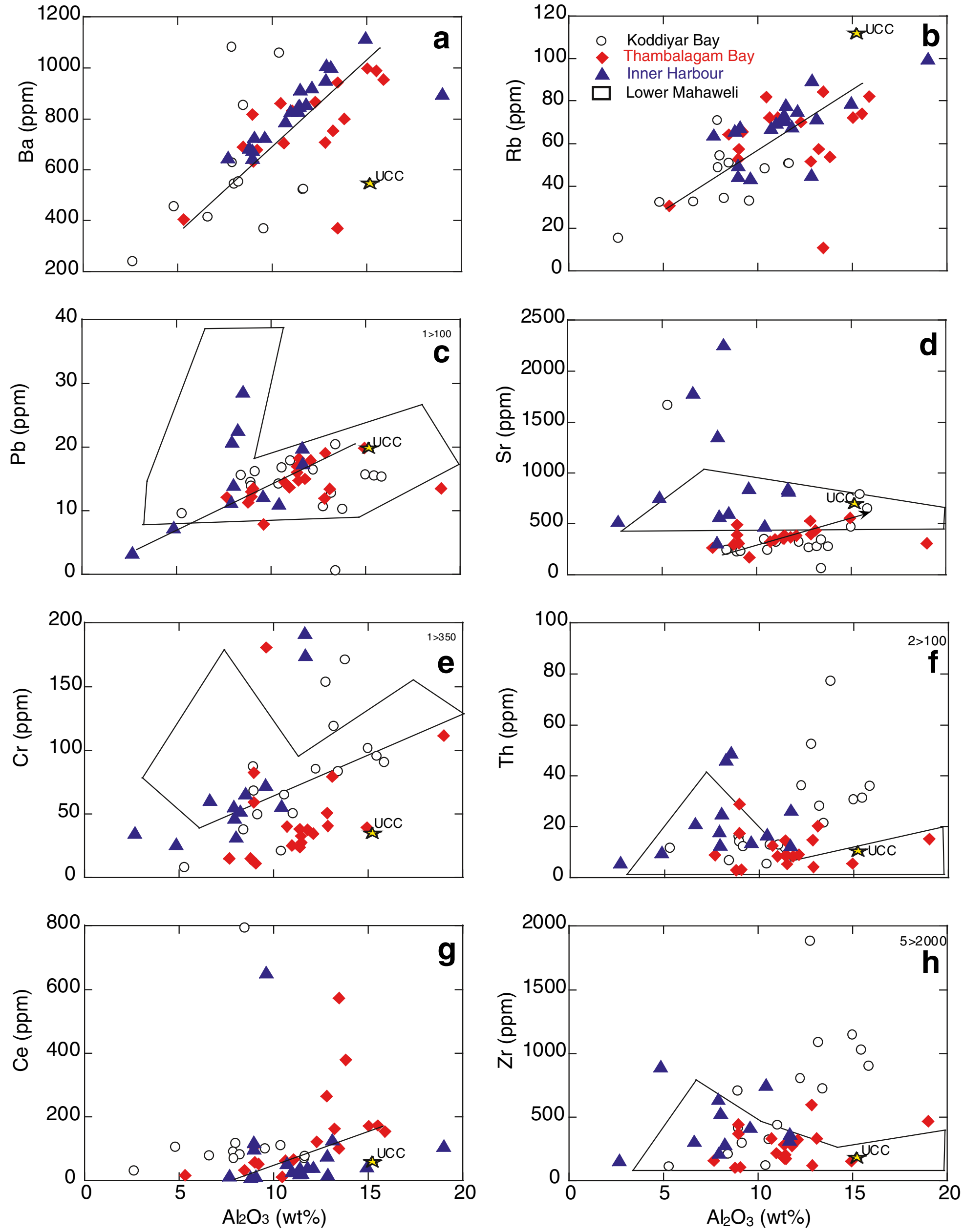


Fig. 5 **a**–**h** Selected trace elements–Al_2O_3 variation diagrams for the Inner Harbour, Thambalagam Bay and Koddiyar Bay surface sediments, compared to upper continental crust (*UCC*; *star*), and fields for lower Mahaweli River sediments. *Lines* indicate possible detrital trends (fitted by eye)

potential heavy mineral concentration (TiO_2, Fe_2O_3, Y, Th, Zr and Nb), as indicated by the PCA analysis.

The Thambalagam Bay UCC_N pattern is similar to that for Koddiyar Bay, with enrichment for TiO_2, Ba, Ce, Th, Zr, Cr and V relative to UCC and depletion for all other elements (Fig. 6). This suggests that the Mahaweli River is also the main source of sediment in Thambalagam Bay, despite its semi-enclosed nature. However, average abundances of TiO_2, Fe_2O_3, Ce, Y, Th, Zr, Nb, Cr and V are all lower than in Koddiyar Bay. This suggests that influence of the Mahaweli River is diminished, and heavy mineral concentration is less of a factor in this more distal setting. In contrast, the UCC_N pattern for the Inner Harbour is quite distinctive. Although the pattern for the major elements in the segment SiO_2–MnO is identical to the other three datasets, MgO, CaO, P_2O_5 and Sr are strongly enriched (Fig. 6). Enrichment of Ca and Sr in sediments is often due to the occurrence of carbonates (Dellwig et al. 2000), and MgO and P_2O_5 are also likely to be associated with bioclastic carbonate or apatite. The Inner Harbour thus shows the greatest marine influence, in keeping with its distal position in relation to the Mahaweli delta, and proximity to the open ocean.

5.2 Source rock signatures

The significant modification of the Mahaweli River and Trincomalee Bay sediments from UCC compositions (Fig. 6)

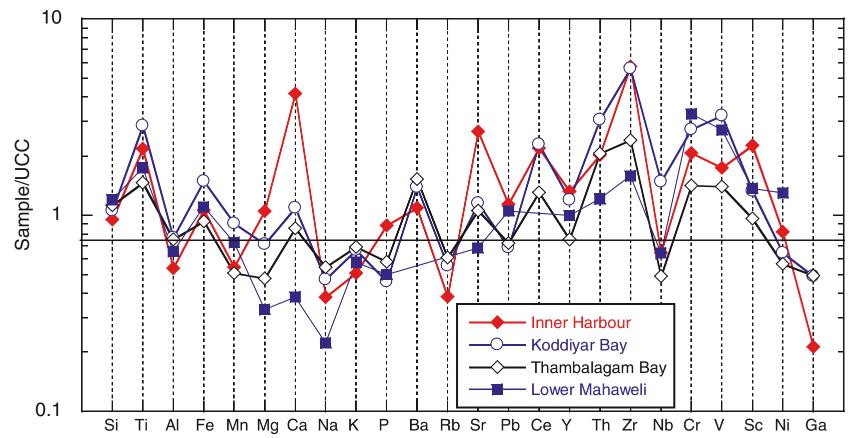


Fig. 6 Upper continental crust (*UCC*)-normalized averages for the Trincomalee Bay sediments, compared to average lower Mahaweli River sediment (data from Young et al. 2012). UCC values from Taylor and McLennan (1985), except for As (from Rudnick and Gao 2005). Major elements are normalized as oxides, trace elements as parts per million

suggests that provenance identification in the three sectors using major element compositions is unlikely to be successful. Elements such as Th, Zr, Ti and Sc are most suited for provenance determination due to their low mobility during sedimentary processes and low residence times in water (Taylor and McLennan 1985; Cullers 1988). Immobile element ratios (e.g. Th/Sc, Zr/Sc; McLennan et al. 1993) have been successfully applied to identify source rock composition. Ratios are inherited directly from source, despite weathering or dilution from quartz or carbonate. Combinations such as Zr/Sc can also be used to identify heavy mineral concentration (McLennan et al. 1993).

A Zr/Sc–Th/Sc ratio plot shows that sediments from the three sectors of Trincomalee Bay all lie on a single trend cutting a model source evolution line near UCC and within the field of lower Mahaweli River sediments (Fig. 7a). This indicates that the bulk of the clastic sediment in Trincomalee Bay is derived from the Mahaweli River, rather than from local or marine sources. A companion Zr/Ti–Th/Ti plot shows an identical pattern (Fig. 7b). The trend across the model source evolution line on both plots reflects zircon concentration, with higher Zr/Sc and Zr/Ti ratios in Koddiyar Bay near the Mahaweli delta and lowest values in the most distal setting of the Inner Harbour. These features suggest that heavy minerals have played an important role in elemental distributions within Trincomalee Bay.

5.3 Hydraulic sorting and heavy minerals

In sediments, Fe_2O_3 and TiO_2 are usually well correlated due to hydraulic sorting effects (Singh 2009), partly due to concentration of heavy mineral phases containing Ti and Fe, such as ilmenite and magnetite, both of which occur in the Trincomalee Bay sediments. As noted above, the Trincomalee Bay sediments are generally very well sorted (Table 1 and Fig. 3). Average Ti/Fe ratios in the Koddiyar Bay, Thambalagam Bay and Inner Harbour sediments (0.23, 0.21 and 0.26, respectively) span the values given by Garcia et al. (2004) for both

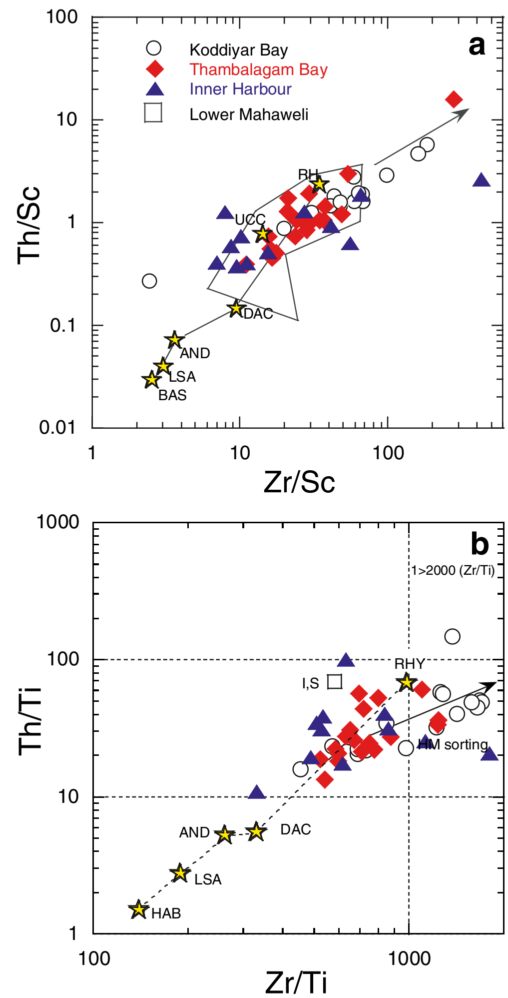


Fig. 7 **a** Zr/Sc–Th/Sc (McLennan et al. 1993) and **b** Zr/Ti–Th/Ti (Roser et al. 2000) for the Trincomalee Bay sediments. *Stars BAS*, *LSA*, *AND*, *DAC*, *RHY*: average basalt, low-silica andesite, andesite, dacite and rhyolite, as plotted by Roser and Korsch (1999), representing a model source evolution trend. *UCC* is upper continental crust (Taylor and McLennan 1985); *square* [*I,S*] spans the average compositions of I- and S-type granite (Whalen et al. 1987). *Arrows* show the trend of zircon concentration. Five samples (three Koddiyar and one each from the Inner Harbour and Thambalagam Bay) plot off scale on (**a**) at Zr/Sc ratios of 101–430. *Arrows* show the trend of zircon concentration

minerals. On cross-plots of Ti and Fe, linear arrays of data points extending towards the origin indicate that heavy minerals in the sediments have been hydraulically fractionated in a similar manner (Singh 2009). Correlation between Fe_2O_3 and TiO_2 is strongest in the Koddiyar samples (R =0.92; Electronic Supplementary Material 2), with some Thambalagam Bay samples (R =0.57) spreading to higher Fe_2O_3 at ~1 wt% TiO_2 (Fig. 8a). However, the broadly similar Ti/Fe ratios in all three sectors suggest that Fe- and Ti-bearing heavy minerals in the sediments were hydraulically fractionated in a similar manner, with elevated contents being produced by winnowing and loss of fines.

Heavy mineral enrichments are often associated with particle sorting effects due to wave action and high current velocities (Dellwig et al. 2000). Since Zr is commonly associated with zircon, enrichments of this element also suggest heavy mineral concentrations in higher depositional energy environment related to modern bar building. Ti and Zr are used as indicators of depositional energy because both elements are concentrated by particle sorting effects (Dellwig et al. 2000). Average Zr/Ti ratios of the lower Mahaweli sediments are 0.058, whereas those for Inner Harbour, Thambalagam Bay and Koddiyar Bay sediments are greater (0.105–0.167) (Table 1). A cross-plot of TiO_2 and Zr (Fig. 8b) shows the spread of Koddiyar Bay samples is broadly similar to that of the Mahaweli sediments, suggesting deposition of both zircons and Ti-bearing heavy minerals in the proximal delta system as current velocity falls. Shift to higher Zr/Ti ratios in Thambalagam Bay may reflect loss of Ti-bearing phases relative to zircons during transport away from the delta and, hence, some decoupling of the heavy mineral assemblages within the bay. However, this could not be confirmed quantitatively by heavy mineral analysis or microscope observation. Nevertheless, these higher ratios and high abundances of elements often linked with heavy minerals (e.g. Zr, Ce, Ti) suggest grain size fractionation, hydraulic sorting and winnowing, circulation and concentration of heavy minerals in high-energy areas within Trincomalee Bay.

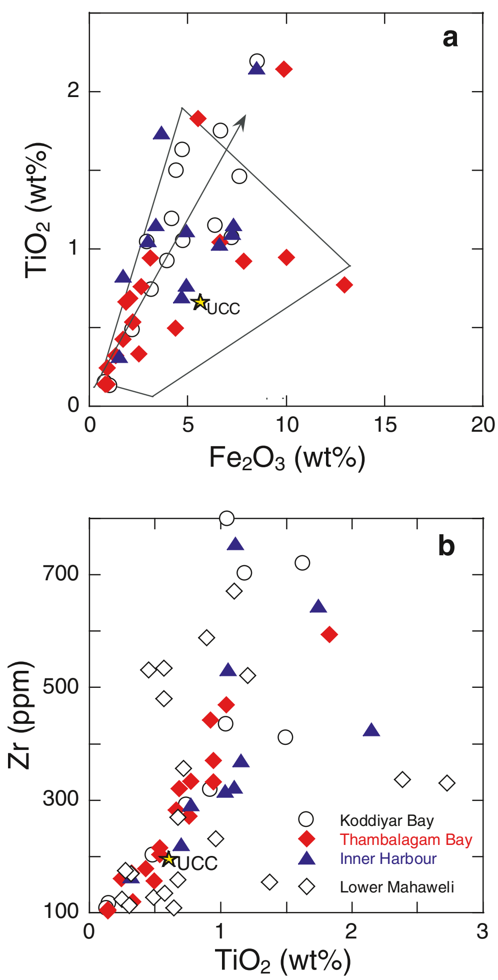


Fig. 8 **a** Fe_2O_3–TiO_2 and **b** TiO_2–Zr plots for the Trincomalee Bay data, illustrating hydraulic fractionation and heavy mineral concentration. *UCC* is upper continental crust (Taylor and McLennan 1985). Field: distribution of lower Mahaweli River sediments. *Arrows* show the broad trend of heavy mineral concentration

5.4 Spatial geochemical variations

GIS contour maps (Electronic Supplementary Material 3) were made to examine the spatial variation of elements within Trincomalee Bay. Al_2O_3 and K_2O were selected to represent the distribution of clay and feldspar components. Both elements show peak values in Koddiyar Bay at the main mouth of the Mahaweli and in the most westerly part of Thambalagam Bay (Electronic Supplementary Material 3A), where grain size is generally finest. The Koddiyar Bay high reflects construction of the Mahaweli delta, whereas the high in Thambalagam Bay is likely due to accumulation of fines in the shallower and calmer waters in that semi-enclosed site.

Four chemically immobile high field strength elements (Th, Nb, Y and Sc; Electronic Supplementary Material 3A) were plotted as representative of provenance-related elements that are unlikely to be contributed from anthropogenic sources (Garcia et al. 1994; Dellwig et al. 2000). Of these, Th, Nb and Y show almost the same spatial distribution, with weak highs in the northwestern part of Koddiyar Bay and lows in Thambalagam Bay and eastern Koddiyar. The relatively uniform distributions of these elements suggest they are mainly associated with clays or very fine-grained heavy minerals. Scandium shows isolated highs in the Inner Harbour and eastern Koddiyar, although these are defined only by a handful of samples.

Six elements which can be associated with both clays and heavy minerals show quite different distributions (Electronic Supplementary Material 3B). Chromium and V GIS maps show similar distributions, with highest concentrations in northwest Koddiyar Bay and lows in Thambalagam Bay. Nickel, Ce, Zr and TiO_2 also show peaks in the same area that correspond to the weaker highs shown by Th, Nb and Y (Electronic Supplementary Material 3A). Isolated highs occur for Zr and Ce (defined by a single sample) and Ni in the Inner Harbour. These may be related to an isolated heavy mineral concentration in the former and contamination from port activity in the latter. Minor highs for all six elements in this group also occur in an arm (China Bay) of eastern Thambalagam Bay (Fig. 1 and Electronic Supplementary Material 3B).

The association of elements enriched in northwest Koddiyar Bay (Cr, V, Th, Sc, Y, Nb, TiO_2, Zr and Ce) strongly suggests association with heavy minerals such as Fe–Ti oxides, zircon, monazite, apatite, garnet, titanite, tourmaline and rutile, all of which occur in the sediments. In coastal depositional systems, bottom current activity can cause winnowing (Schnetger et al. 2000) and thus concentration of heavy minerals. The concentration of elements in northwest Koddiyar Bay corresponds to the area in which strongest current activity was observed during sampling.

The spatial variation maps thus suggest that these heavy minerals were carried along the Mahaweli River and deposited as lags in this high-energy environment in Koddiyar Bay. Except for Ce, Y, Sc and Zr, most other elements are less abundant in the Inner Harbour. The distribution patterns suggest that Mahaweli River sediment entering Koddiyar Bay moves towards the northwest, and heavy mineral-rich sands are deposited in a high-energy zone. Fine sand and clay particles are moved away from Koddiyar Bay by currents into Thambalagam Bay, the Inner Harbour and out to sea.

5.5 Present environmental status

Trace metal concentrations (As, Pb, Zn, Cu, Ni and Cr) in the Trincomalee Bay sediments were compared with four established international standards to evaluate present pollution status for the elements analysed (Table 2). Comparing the data to a single guideline could be misleading. The guidelines used were Coastal Ocean Sediment Database (COSED) and New York State Department of Environmental Conservation (NYSDEC) values of lower effect level (LEL) and severe effect level (SEL), Interim Sediment Quality Guidelines (ISQG) and probable effect level (PEL). The NYSDEC metal criteria are derived from the Ministry of Ontario guidelines and NOAA data that make use of the screening level approach. The LEL for each metal is thus the lowest of either the Persaud et al. (1992) LEL or the Long and Morgan (1990) effect range-low. Similarly, the SEL for each metal is the lowest of either the Persaud et al. (1992) SEL or the Long and Morgan (1990) effect range-moderate. Sediments are considered contaminated if either criterion is exceeded. If both criteria are exceeded, the sediment is considered to be severely impacted. If both the LEL and SEL criteria are exceeded, the metal may severely impact on the health of biota. If only the

Table 2 Average metal contents in the Trincomalee Bay sediments compared to established pollution guidelines and upper continental crust

Element	As	Pb	Zn	Cu	Ni	Cr
IH	7	23	49	13	16	73
TB	10	14	31	6	11	50
KB	4	14	51	6	13	96
LM	4	21	57	16	26	115
EF values (Lower Mahaweli normalized)						
IH	**2.4**	1.0	1.4	1.1	0.7	0.7
TB	**2.3**	0.3	0.6	0.5	0.4	0.4
KB	0.9	0.3	0.6	0.7	0.7	0.4
Environmental guidelines						
UCC	5	20	71	25	20	35
COSED	13	45	135	42	42	125
LEL	6	31	120	16	16	26
SEL	33	110	270	110	50	110
ISQG	7	30	124	19	na	52
PEL	42	112	271	108	na	160

Enrichment factor values were calculated using the lower Mahaweli River data as the background normalizer

UCC upper continental crust, *COSED* Coastal Ocean Sediment Database (NYSDEC 1999), *LEL* lowest effect level, *SEL* severe effect level (NYSDEC 1999), *ISQG* Interim Sediment Quality Guideline (SAIC 2002), *PEL* probable effect level (SAIC 2002)

LEL criterion is exceeded, the metal may moderately impact on biotic health (NYSDEC 1999; Graney and Eriksen 2004). The COSED of chemical concentrations in sediments has been compiled from various electronic sources and contains data for nearly 13,500 US coastal sediment samples (Daskalakis and O'Connor 1995). The COSED values are indicative of metal contamination and are used to quantify the degradation of sediment quality in estuarine and marine ecosystems (Ruiz-Fernandez et al. 2003). The Canadian Council of Ministers of the Environment also developed national ISQG based on co-occurrence of chemical and biological data from the assessment of Great Lakes-contaminated sediments (SAIC 2002). Using guideline values derived from large well-assessed data sets such as those above should result in reasonable results, even though threshold levels may differ between them.

Comparison with the COSED guidelines for As, Pb, Zn, Cu, Ni and Cr show that the Trincomalee Bay sediments are not seriously contaminated. However, average As contents in Thambalagam Bay and the Inner Harbour exceed the LEL, as does Cr in all three sectors (Table 2). However, both elements are below the SEL values. Both As and Cr also exceed the ISQG values and the level in UCC, but fall below the PEL of SAIC (2002). The data thus imply that the sediments in Trincomalee Bay are slightly contaminated by both As and Cr. However, comparison with pollution guidelines can be misleading, if local background values are not taken into account. Consequently, we also examined the data using metal enrichment factors (EF) and GIS maps to identify the spatial distribution of potential contamination. Metal EF values of 0.5–1.5 suggest that the trace metals concerned may be derived entirely from crustal materials or natural weathering processes (Zhang and Liu 2002). Values greater than 1.5 suggest that a significant portion of the trace metal has been delivered from non-natural (anthropogenic) sources (Zhang et al. 2007). The EF values were calculated using the formula given in Zhang et al. (2007):

$$\mathrm{EF} = \frac{(\mathrm{Me}/\mathrm{Al})\ \mathrm{sample}}{(\mathrm{Me}/\mathrm{Al})\ \mathrm{background}}$$

Normalization of element contents against an immobile element is a common practice to accommodate grain size effects and dilution by phases such as quartz and carbonates. Currently, Al is the most frequently used geochemical normalizer in estuarine and coastal sediments, based on the assumption that Al is held exclusively in terrigenous aluminosilicates (Chen and Kandasamy 2007; Karageorgis et al. 2009; Ho et al. 2010). Therefore, in this study, we used Al_2O_3 as the normalizer and the average composition of lower Mahaweli River sediment (Table 1) for the background values.

The average EF values confirm that Pb, Cu, Ni and Cu are present only at natural levels, with EFs ranging from 0.3 to 1.4 (Table 2). However, GIS contour maps of EF values of individual samples show the highest EFs occur within the Inner Harbour (Electronic Supplementary Material 3C). Although all except one sample fall within acceptable limits, there may have been slight contamination of these elements in the port area. The GIS plot for As shows that EFs higher than guideline values occur in both Thambalagam Bay and the Inner Harbour, and thus, some contamination of this element could also have occurred. However, the highs for As also correspond to the highest CaO and Sr contents and clustering in the PCA analysis (Electronic Supplementary Material 2B), suggesting association with biogenic carbonate in the form of shell fragments. This possibility needs to be evaluated by future analysis. Finally, using the lower Mahaweli River sediments as the normalizer, the apparent enrichment in Cr disappears, with average EF in the three sectors ranging only from 0.4 to 0.7 (Table 2) and hence lower than in the Mahaweli River. The GIS map for Cr (Electronic Supplementary Material 3C) shows a relatively uniform EF distribution across the bay, with weak isolated highs in western Koddiyar Bay and Thambalagam Bay corresponding with areas of heavy mineral enrichment and a single sample within the port district of the Inner Harbour. The results thus show that Trincomalee Bay is essentially unpolluted for the elements analysed here when local background levels are taken into account, in contrast to the indication given by the broad-based sediment guidelines. This illustrates the importance of establishing local background values in studies of this type, by determining elemental compositions of fluvial systems entering estuarine or bay environments. These can then be used in conjunction with the sediment guidelines to identify spurious enrichments.

6 Conclusions

Sediments within three sectors of Trincomalee Bay are mostly well-sorted fine- to medium-grained sands, but differ in geochemical composition. Sediments in Koddiyar Bay, closest to the Mahaweli River delta, have geochemical compositions similar those supplied by the river. Sediments in the semi-enclosed and more distal Thambalagam Bay are also mainly derived from the Mahaweli River, but are modified by additions of Ca, Mg and Sr from marine biogenic carbonate sources. This marine component is even greater in the Inner Harbour. Very high concentrations of elements including Ti, Zr, Ce, Nb and Y in Koddiyar Bay are consistent with heavy mineral concentration by winnowing in a high-energy zone, creating heavy mineral lags. Although hydraulic sorting effects among Fe–Ti oxides are similar throughout the three sectors, some fraction of heavy mineral assemblages may occur within the bay.

Evaluation of present-day environmental status using established pollution guidelines (COSED LEL, SEL and PEL) indicates that Zn, Pb, Cu and Ni are present only at natural background levels. However, As contents exceed LEL in the Inner Harbour and Thambalagam Bay, and Cr exceeds LEL in all three sectors, implying that some contamination of these two elements may have occurred. However, a closer evaluation of the data using Al-normalized metal EFs and lower Mahaweli River sediments as background indicators reveals that these apparent enrichments are in fact spurious, and As and Cr are present only at locally higher background levels. This emphasizes the importance of establishing local background levels, to be used in conjunction with more global environmental guidelines.

Acknowledgments We gratefully acknowledge the Japanese government for financial assistance to carry out our study and thank the Sri Lankan Naval Force and Amila Ratnayake for support during sample collection and Toshiaki Irizuki and Tetsuya Sakai for their supervision of the grain size analysis. We also thank the Editor-In-Chief, P.N. Owens, and three anonymous reviewers for their very helpful and constructive comments, which improved the manuscript considerably. The samples were imported via plant protection of the Ministry of Agriculture, Forestry and Fisheries, Japan.

References

Borrego J, Morales JA, De La Torre ML, Grande JA (2002) Geochemical characteristics of heavy metal pollution in surface sediments of the Tinto and Odiel river estuary (southwestern Spain). Environ Geol 41:785–796

Chen CT, Kandasamy S (2007) Evaluation of elemental enrichments in surface sediments off southwestern Taiwan. Environ Geol 54: 1333–1346

Cooray PG (1994) The Precambrian of Sri Lanka, a historical overview. Precambrian Res 66:3–18

Cullers R (1988) Mineralogical and chemical changes of soil and stream sediment formed by intense weathering of the Danburg granite, Georgia, U.S.A. Lithosphere 21:301–314

Daskalakis KD, O'Connor TP (1995) Distribution of chemical concentrations in US coastal and estuarine sediment. Mar Environ Res 40: 381–398

Dellwig O, Hinrichs J, Hild A, Brumsack HJ (2000) Changing sedimentation in tidal flat sediments of the southern North Sea from the Holocene to the present: a geochemical approach. J Sea Res 44: 195–208

Folk RL, Ward WC (1957) Brazos river bar: a study of significance of grain size parameters. J Sed Petrol 27:3–26

Garcia D, Fonteilles M, Moutte J (1994) Sedimentary fractionations between Al, Ti and Zr and the genesis of strongly peraluminous granites. J Geol 102:411–422

Garcia D, Ravenne C, Marechal B, Moutte J (2004) Geochemical variability induced by entrainment sorting: quantified signals for provenance analysis. Sed Geol 171:113–128

Graney JR, Eriksen TM (2004) Metals in pond sediments as archives of anthropogenic activities: a study in response to health concerns. Appl Geochem 19:1177–1188

Hirst DM (1962) The geochemistry of modern sediments from the Gulf of Paria, II. The location and distribution of trace elements. Geochim Cosmochim Acta 26:1147–1187

Ho HH, Swennen R, Damme AV (2010) Distribution and contamination status of heavy metals in estuarine sediments near Cua Ong harbor, Ha Long bay, Vietnam. Geol Belg 2:37–47

Ip CCM, Li XD, Zhang G, Wai OWH, Li YS (2007) Trace metal distribution in sediments of the Pearl River Estuary and the surrounding coastal area, South China. Environ Pollut 147: 311–323

Jayawardena UDS (2005) The stratigraphy and groundwater availability in the delta sediments of river Mahawelli—a study from Sri Lanka. Abstract Volume of the Inter Conf on DELTAS (Mekong venue). January 10–16. Ho Chi Minh City, Vietnam. p40

Karageorgis AP, Katsanevakis S, Kaberi H (2009) Use of enrichment factors for the assessment of heavy metal contamination in the sediments of Koumoundourou Lake, Greece. Water Air Soil Pollut 204:243–258

Kimura J, Yamada Y (1996) Evaluation of major and trace element XRF analyses using a flux to sample ratio of two to one glass beads. J Min Pet Sci 91:62–72

Ladipo MK, Ajibola VO, Oniye SJ, Uzairu A, Agbaji EB (2011) Geochemical partitioning of heavy metals in sediments of some locations of the Lagos lagoon. Jenvscs 1:22–30

Li X, Liu L, Wang Y, Luo G, Chen X, Yang X, Gao B, He X (2012) Integrated assessment of heavy metal contamination in sediments from a coastal industrial basin, NE China. PLoS ONE 7(6):e39690. doi:10.1371/journal.pone.0039690

Lin C, He M, Zhou Y, Guo W, Yang Z (2007) Distribution and contamination assessment of heavy metals in sediment of the Second Songhua River, China. Environ Monit Assess 137: 329–342

Long ER, Morgan LG (1990) The potential for biological effects of sediment-sorbed contaminants tested in the National States and Trends Program. National Oceanic Atmospheric Administration (NOAA) Technical Memorandum No. 5, OMA52, NOAA National Ocean Service, Seattle, Washington, USA

McLennan SM, Hemmings S, McDaniel DK, Hanson GN (1993) Geochemical approaches to sedimentation, provenance and tectonics. Geol Soc Am Spec Pap 284:21–40

Morris AW, Allen JI, Howland RJM, Wood RG (1995) The estuary plume zone: source or sink for land-derived nutrient discharges? Estuar Coast Shelf Sci 40:387–402

NYSDEC (New York State Department of Environmental Conservation) (1999) Technical guidance for screening contaminated sediments. NYSDEC, Division of Fish, Wildlife and Marine Resources, Albany, p 45

Ogasawara M (1987) Trace element analysis of rock samples by X-ray fluorescence spectrometry, using Rh anode tube. Bull Geol Surv Jpn 38(2):57–68

Pattan JN, Rao CM, Higgs NC, Colley S, Parthiban G (1995) Distribution of major, trace and rare-earth elements in surface sediments of the Wharton Basin, Indian Ocean. Chem Geol 121:201–215

Persaud D, Jaagumagi R, Hayton A (1992) Guidelines for the protection and management of aquatic sediment quality in Ontario. Ontario Ministry of the Environment, Ottawa

Reid MK, Spencer KL (2009) Use of principal components analysis (PCA) on estuarine sediment datasets: the effect of data pretreatment. Environ Pollut 157:2275–2281

Roser BP, Korsch RJ (1999) Geochemical characterization, evolution and source of a Mesozoic accretionary wedge: the Torlesse terrane. New Zealand. Geol Mag 136:493–512

Roser BP, Ishiga H, Lee HK (2000) Geochemistry and provenance of Cretaceous sediments from the Euisong block, Gyeongsang basin, Korea. Mem Geol Soc Jpn 57:155–170

Rudnick RL, Gao S (2005) Composition of the continental crust. In: Rudnick RL (ed) The crust. Treatise on geochemistry, vol 3. Elsevier-Pergamon, Oxford, pp 1–64

Ruiz-Fernandez AC, Hillaire-Marcel C, Paez-Osuna F, Ghaleb B, Soto-Jimenez M (2003) Historical trends of metal pollution recorded in the sediments of the Culiacan River Estuary, Northwestern Mexico. Appl Geochem 18:577–588

SAIC (Science Applications International Corporation, Canada) (2002) Compilation and review of Canadian remediation guidelines, standards and regulations (Final report, B187-413, pp 79). Emergencies Engineering Technologies Office (EETO)–Environment Canada, Ottawa, Canada

Schnetger B, Brumsack HJ, Schale H, Hinrichs J, Dittert L (2000) Geochemical characteristics of deep-sea sediments from the Arabian Sea: a high-resolution study. Deep-Sea Res II 47:2735–2768

Singh P (2009) Major, trace and REE geochemistry of the Ganga River sediments: influence of provenance and sedimentary processes. Chem Geol 266:242–255

Taylor SR, McLennan SM (1985) The continental crust: its composition and evolution. Blackwell, Oxford, p 312

Whalen JB, Currie KL, Chappell BW (1987) A-type granites—geochemical characteristics, discrimination and petrogenesis. Contrib Min Pet 95:407–419

Wijayananda NP (1985) Geological setting around the heads of the Trincomalee canyon, Sri Lanka. J Natl Sci Couns Sri Lanka 13: 213–226

Woods AM, Lloyd JM, Zong Y, Brodie CR (2012) Spatial mapping of Pearl River Estuary surface sediment geochemistry: influence of data analysis on environmental interpretation. Estuar Coast Shelf Sci 115:218–233

Young SM, Pitawala A, Ishiga H (2012) Geochemical characteristics of stream sediments, sediment fractions, soils, and basement rocks from the Mahaweli River and its catchment, Sri Lanka. Chem Erde Geochem. doi:10.1016/j.chemer.2012.09.003

Zhang J, Liu CL (2002) Riverine composition and estuarine geochemistry of particulate metals in China—weathering features, anthropogenic impact and chemical fluxes. Estuar Coast Shelf Sci 54:1051–1070

Zhang L, Ye X, Feng H, Jing Y, Ouyang T, Yu X, Liang R, Gao C, Chen W (2007) Heavy metal contamination in western Xiamen Bay sediments and its vicinity, China. Mar Pollut Bull 54:974–982

Electronic Supplementary Material One: XRF data

(A) Individual XRF analyses and texture of sediments from Trincomalee Bay, Sri Lanka.

OR1: Individual XRF analyses and texture of sediments from Trincomalee Bay, Sri Lanka

	Major elements (wt%)										Trace Elements (ppm)																	Texture			
Sample No	SiO_2	TiO_2	Al_2O_3	$Fe_2O_3^*$	MnO	MgO	CaO	Na_2O	K_2O	P_2O_5	Ba	Ce	Cr	Ga	Nb	Ni	Pb	Rb	Sc	Sr	Th	V	Y	Zr	As	Zn	Cu	Mean GS	Sorting	<4ϕ wt%	LOI
Inner Harbour																															
TR1	83.36	0.83	4.86	1.70	0.03	0.67	6.79	0.90	0.82	0.04	453	103	26	6	11	5	7	32	16	764	10	54	11	899	3	27	6	1.22	2.49	7.05	6.79
TR2	61.41	2.15	9.58	8.49	0.13	2.67	12.79	1.40	1.28	0.10	366	97	73	10	18	16	12	33	27	851	14	193	30	425	5	62	7	0.98	2.59	8.93	8.14
TR3	39.23	1.03	6.64	6.61	0.06	3.60	39.65	1.23	1.40	0.55	411	76	61	1	7	16	103	32	36	1790	21	89	118	315	19	152	41	2.75	0.41	4.99	44.33
TR4 Top	49.87	1.10	11.65	7.27	0.09	4.55	21.21	2.12	1.97	0.19	520	67	192	10	9	57	20	50	34	847	13	129	28	324	8	80	33	3.43	1.87	13.41	12.48
TR4 Bott	50.97	1.15	11.70	7.34	0.08	4.50	20.03	2.11	1.93	0.19	521	74	175	1	10	54	17	50	36	826	27	132	26	370	8	76	34	0.79	2.37	13.41	11.75
TR5	70.35	1.16	8.52	3.39	0.05	1.42	11.24	1.57	2.26	0.05	849	792	66	6	38	7	29	51	19	614	49	165	31	8123	10	34	5	0.79	2.37	6.95	8.21
TR6	72.13	1.06	8.03	2.97	0.07	1.55	10.60	1.54	1.99	0.07	542	115	32	7	14	6	14	54	20	579	25	70	26	532	4	22	3	-0.29	2.00	2.68	7.41
TR7	78.92	1.74	7.90	3.66	0.04	0.83	3.02	1.46	2.36	0.06	1080	88	56	7	18	5	11	70	10	319	18	120	13	645	4	23	4	0.08	2.57	5.51	1.62
TR8	70.16	1.11	10.41	4.92	0.06	1.30	7.32	2.05	2.58	0.08	1054	109	56	9	57	8	11	48	18	486	17	159	18	756	8	26	2	0.59	2.63	11.59	4.49
TR9	39.04	0.77	8.25	4.92	0.04	3.01	40.60	1.49	1.68	0.20	551	79	53	nd	2	11	23	34	37	2266	46	58	21	292	9	39	7	3.00	1.81	16.05	24.72
TR10	51.24	0.70	7.92	4.67	0.04	2.85	29.00	1.46	1.98	0.13	625	67	47	4	5	9	21	48	32	1361	13	58	21	221	9	30	5	2.86	1.62	12.15	18.83
TR11	85.65	0.32	2.67	1.52	0.02	0.78	7.94	0.61	0.43	0.05	237	28	35	0	4	3	3	15	15	531	6	30	8	164	3	21	4	-0.76	2.24	5.92	7.13
Average IH	62.69	1.09	8.18	4.79	0.06	2.31	17.52	1.50	1.72	0.14	601	141	73	6	16	16	23	43	25	936	22	105	29	1089	7	49	13	1.29	2.08	9.05	12.99
STDEV	16.42	0.48	2.62	2.27	0.03	1.41	12.81	0.46	0.64	0.14	263	206	54	3	16	19	26	14	10	581	14	52	29	2226	4	38	14	1.39	0.62	4.17	11.71
Thambalagam Bay																															
TR13	77.50	0.94	10.72	3.11	0.05	0.83	2.29	2.03	2.46	0.05	791	55	40	8	14	8	14	67	9	324	13	82	14	332	7	27	3	0.82	1.83	1.35	1.44
TR14	74.80	0.33	12.87	2.53	0.02	0.90	2.88	2.51	3.09	0.06	1011	19	41	12	5	12	19	90	7	396	4	37	10	119	6	33	9	1.11	2.20	3.68	3.73
TR15	86.30	0.24	7.68	0.90	0.02	0.33	1.31	1.48	1.72	0.02	650	16	15	3	5	4	12	64	3	264	9	20	6	160	3	14	4	0.16	2.34	1.91	0.79
TR16	71.83	2.14	9.62	9.90	0.11	1.39	1.61	1.36	1.95	0.10	729	654	181	8	54	18	8	44	14	169	222	347	39	3914	8	55	8	0.82	1.92	2.83	1.16
TR17	59.28	0.77	13.10	12.97	0.12	1.93	6.24	2.39	2.86	0.36	1005	129	79	6	13	19	13	72	16	434	20	132	38	333	34	48	7	3.47	2.24	22.93	6.46
TR18	59.25	0.95	8.96	10.01	0.12	3.12	13.90	1.62	1.79	0.28	648	100	59	6	14	15	13	45	24	488	17	130	32	370	43	34	5	1.90	2.05	1.79	10.67
TR19	69.28	0.92	8.97	7.86	0.10	1.61	7.58	1.61	1.85	0.22	679	121	82	nd	13	12	12	50	15	390	29	117	27	442	26	31	5	2.09	2.24	9.69	6.63
TR20	84.78	0.14	9.06	0.82	0.01	0.33	1.43	1.69	1.72	0.02	729	15	11	8	3	4	13	68	6	311	3	16	5	105	4	9	3	1.86	0.39	1.74	1.17
TR21	79.66	0.43	11.39	1.72	0.03	0.63	1.91	2.04	2.16	0.03	832	24	38	3	8	5	16	74	8	358	14	51	10	178	6	20	2	1.31	2.41	1.97	0.82
TR22	78.80	0.66	11.40	1.86	0.04	0.63	2.19	2.16	2.23	0.03	851	42	24	11	12	7	17	71	10	375	9	62	11	282	4	25	5	1.80	2.48	10.12	1.33
TR23	64.69	0.49	14.95	4.37	0.07	1.49	7.70	2.94	3.18	0.12	1120	44	39	15	7	14	20	79	14	557	6	58	18	156	15	33	6	2.79	1.91	10.07	5.52
TR24	62.35	1.04	19.00	6.64	0.08	2.01	2.71	2.92	3.08	0.15	898	109	111	20	15	46	14	100	16	311	15	123	31	469	10	79	23	0.34	0.30	66.44	8.76
TR25	80.27	0.32	11.48	1.33	0.02	0.47	1.93	2.02	2.13	0.02	915	25	27	11	7	5	18	78	7	387	5	37	8	170	3	19	4	2.45	1.47	7.82	1.42
TR26	78.45	0.53	10.99	2.20	0.04	0.70	2.38	2.14	2.54	0.03	831	31	25	7	8	7	14	70	8	345	8	46	10	215	3	21	3	0.49	1.39	3.49	1.94
TR27	76.25	0.76	11.81	2.64	0.04	0.84	2.75	2.31	2.56	0.03	859	43	38	10	11	8	15	68	8	368	8	67	12	272	4	38	5	2.19	1.13	0.24	2.09
TR28	77.62	0.53	11.44	2.19	0.03	0.75	2.45	2.33	2.61	0.03	853	30	33	9	9	7	15	71	8	356	9	52	10	203	3	23	5	2.52	0.86	5.23	1.76
TR29	76.85	0.69	12.10	2.05	0.03	0.64	2.37	2.45	2.80	0.03	924	42	34	10	11	4	18	76	9	385	9	59	10	321	3	19	4	2.28	0.72	0.24	1.31
TR30	70.36	1.83	12.85	5.51	0.10	0.93	3.29	2.75	2.19	0.17	954	80	51	6	17	15	12	45	12	530	15	140	16	594	2	50	14	3.41	1.59	0.24	1.89
TR31	84.93	0.14	8.80	0.90	0.02	0.43	1.56	1.62	1.59	0.01	687	11	15	7	4	5	11	66	6	298	3	25	7	103	5	9	0	0.69	1.68	1.72	1.47
Average TB	74.38	0.73	11.43	4.19	0.06	1.05	3.61	2.12	2.34	0.09	840	84	50	9	12	11	14	68	11	371	22	84	17	460	10	31	6	1.71	1.64	8.08	3.18
STDEV	8.28	0.52	2.58	3.62	0.04	0.72	3.16	0.48	0.51	0.10	132	143	41	4	11	10	3	15	5	90	49	75	11	847	12	17	5	1.00	0.68	15.16	2.96
Koddiyar Bay																															
TR12	79.14	1.19	8.98	4.21	0.04	0.81	1.96	1.65	1.96	0.06	817	106	87	9	21	9	14	52	10	251	16	109	12	702	4	29	8	0.43	2.59	5.90	1.47
TR32	37.06	5.18	13.46	32.91	0.48	5.57	3.43	0.93	0.83	0.14	370	572	356	nd	242	21	0	11	28	54	156	1090	93	5247	4	181	4	2.37	0.81	0.00	-1.01
TR33	66.70	2.19	12.81	8.58	0.14	2.26	3.19	1.90	2.14	0.10	707	265	153	12	52	16	11	52	19	258	52	275	42	1876	4	63	2	2.37	0.81	0.00	0.70
TR34	60.58	2.66	13.83	12.21	0.18	2.46	3.46	2.04	2.46	0.12	799	380	170	13	81	16	10	54	17	271	77	417	48	2735	6	81	3	1.79	0.98	3.64	0.95
TR35	64.64	1.15	15.04	6.41	0.09	1.85	5.32	2.43	2.96	0.10	997	171	101	14	29	16	15	72	17	464	30	169	29	1141	6	58	5	1.79	1.51	10.46	3.28
TR36	72.94	1.05	12.27	4.76	0.08	1.37	2.74	2.12	2.60	0.07	865	121	85	0	23	10	16	70	13	313	36	132	23	799	4	41	2	2.11	1.46	1.32	0.83
TR37	57.90	1.07	15.50	7.26	0.09	1.94	10.63	2.42	3.05	0.12	988	173	95	14	29	21	15	74	22	780	31	171	30	1023	9	72	11	3.34	1.11	17.09	7.68
TR38	67.90	1.46	13.24	7.66	0.14	2.24	3.11	1.90	2.28	0.08	753	162	118	14	32	13	13	57	18	269	28	201	41	1078	4	63	4	2.15	1.27	1.25	0.56
TR39	58.30	1.75	15.89	6.69	0.08	1.79	9.62	2.56	3.20	0.12	953	153	90	7	22	27	15	82	20	646	36	145	26	896	8	65	14	4.60	2.34	39.81	7.93
TR40A	82.87	0.15	10.45	0.80	0.01	0.31	1.39	1.92	2.08	0.01	862	11	20	7	4	4	14	82	6	344	5	19	4	116	4	12	2	3.22	0.93	9.64	1.10
TR40B	77.66	1.04	11.07	2.93	0.04	0.77	1.99	1.93	2.53	0.04	832	64	50	10	15	8	18	72	9	316	13	83	14	434	3	27	4	2.56	1.12	0.00	1.03
TR41	70.96	1.63	13.46	4.75	0.07	1.19	2.64	2.25	2.98	0.07	942	101	83	13	25	15	20	84	11	334	21	136	19	720	3	41	5	2.55	0.90	0.00	0.99
TR42A	78.94	1.50	8.99	4.42	0.07	1.02	1.72	1.38	1.93	0.04	632	57	67	7	23	9	14	57	10	221	14	125	19	410	2	36	4	0.45	1.71	3.69	0.54
TR42B	83.37	0.48	8.46	2.20	0.04	0.53	1.38	1.46	2.05	0.03	688	32	37	7	9	5	15	64	4	236	6	48	9	201	2	20	5	0.31	1.90	2.39	0.79
TR42C	78.22	0.92	10.62	3.99	0.07	0.83	1.55	1.58	2.17	0.05	706	62	64	9	15	16	17	72	10	237	13	91	16	318	2	38	11	1.11	2.43	15.84	2.00
TR42D	81.25	0.74	9.21	3.17	0.05	0.68	1.40	1.46	2.00	0.04	677	51	49	7	12	11	16	65	nd	225	12	72	13	291	2	31	8	-0.13	1.96	2.63	1.59
TR43	67.58	0.13	5.32	1.05	0.03	0.99	22.33	1.28	1.24	0.04	405	17	7	nd	nd	0	9	31	43	1658	11	11	6	107	4	6	3	-0.95	1.84	2.84	15.29
Average KB	69.76	1.43	11.68	6.71	0.10	1.57	4.58	1.84	2.26	0.07	764	147	96	10	40	13	14	62	16	405	33	194	26	1064	4	51	6	1.77	1.51	6.85	2.69
STDEV	11.93	1.17	2.88	7.34	0.11	1.23	5.32	0.45	0.62	0.04	181	145	79	4	57	7	4	19	10	365	37	251	21	1271	2	40	4	1.41	0.59	10.05	4.03

nd - not detected

Electronic Supplementary Material One

Part B: XRF analysis

Glass fusion beads for X-ray fluorescence (XRF) analysis (anhydrous basis) were prepared with an alkali flux, following the method described in detail in Kimura and Yamada (1996). The flux used comprised 80 % lithium tetraborate (Merck Spectromelt®A10) and 20 % lithium metaborate (Merck Spectromelt®A20). Both components were dried for at least 24 h at 110 °C before mixing. The beads contained 1.8 g of the anhydrous sample from the LOI determinations and 3.6 g of flux, giving a sample to flux ratio of 1:2. Abundances of the major elements and 14 trace elements were determined from these fusion beads using a Rigaku RIX-2000 XRF spectrometer equipped with an Rh-anode tube. The instrument conditions, interference corrections, and calibration used were those described by Kimura and Yamada (1996). Primary calibration was made using the same beads from that study, including both international rock standards, synthetic mixes, and standards with elemental ranges extended by standard addition. These standards thus had elemental ranges spanning that expected in most geological situations. Major element matrix corrections were made as described by Kimura and Yamada (1996). Overlap corrections were applied for significant spectral interferences among the trace elements, as specified by Kimura and Yamada (1996).

During routine analysis, the primary calibration was verified by analysis and cross-calibration of nine Geological Survey of Japan rock standards spanning the compositional range from gabbro to granite. Average results, standard deviations, and two-sigma coefficients of variation for repeat analyses (n=6) of these standards during normal operation are listed in the Table OR2. These data show that average precision of the major elements ranges from ±0.29 wt% of the amount present (SiO_2) to ±4.72 wt% (Na_2O). Among the 14 trace elements analyzed by this method the two-sigma values range from a low of 0.6 % relative (Zr) to 26.5 % (Th). The trace element two-sigma CVs are, however, influenced by higher values when abundances are <10 ppm, even though the disparity between the observed and recommended values may only be a few ppm. When values where abundances are <10 ppm are excluded, the range of two-sigma values for the trace elements falls to a maximum of 12.7 % relative (Ce), and for half of the analyzed elements (Nb. Ni, Pb, Rb, Sr, Y, Zr) the precision is better than 5 %.

Abundances of three additional trace elements (As, Cu, Zn) were determined from pressed powder briquettes (sample weight 3.0-3.5 g), prepared using a force of 200KN for 60

s. The pressed powder analysis followed Ogasawara (1987), using conventional peak over background (Ip/Ib) method, with calibration against recommended or preferred values for seven GSJ rock standards (Table OR3). Arsenic values were also corrected for Pb peak overlap. Precision was estimated as for the glass bead data, but based on 5 analyses of the seven calibration standards during normal operation. Average 2-sigma coefficients of variation for the three elements range from 3.5-6.7 % relative at concentrations of > 5 ppm. This was confirmed by repeat analysis (n=5) of seven samples from this study, yielding similar results.

(B) XRF analysis methods, standard data and precision

Table OR2: Mean concentrations from repeat analyses (n=6) of GSJ rock standards using the glass bead method.

RV - recommended or preferred values, recalulated on an anhydrous basis, from Gelogical Survey of Japan data, available at https://gbank.gsj.jp/geostandards/welcome.html
SDp - Standard deviation; CV% - 2-sigma coefficient of variation. N/A - not available. Dash (-) not detected. Analyst: BPR.

Std	SiO2	TiO2	Al2O3	Fe2O3	MnO	MgO	CaO	Na2O	K2O	P2O5	Sum	Ba	Ce	Cr	Ga	Nb	Ni	Pb	Rb	Sc	Sr	Th	V	Y	Zr
Standards run (n=6 each																									
JG-1a (granite)																									
RV	**72.65**	**0.25**	**14.31**	**2.06**	**0.06**	**0.69**	**2.14**	**3.43**	**4.04**	**0.08**	**99.72**	**460.9**	**47.4**	**18.7**	**17.1**	**12.1**	**6.4**	**27.2**	**181.1**	**6.2**	**186.2**	**12.2**	**23.1**	**32.2**	**115.7**
Mean	**72.47**	**0.24**	**14.47**	**2.03**	**0.06**	**0.76**	**2.17**	**3.51**	**3.98**	**0.08**	**99.77**	**471.5**	**41.9**	**9.6**	**17.9**	**11.5**	**6.2**	**26.5**	**183.1**	**8.5**	**187.6**	**12.7**	**20.7**	**27.8**	**124.9**
SDp	0.12	0.01	0.05	0.03	0.00	0.01	0.01	0.03	0.02	0.00	0.09	15.9	2.8	2.9	0.9	0.2	0.5	0.2	0.8	0.9	0.9	0.4	2.7	0.3	0.4
CV%	0.33	4.96	0.69	2.68	2.39	2.17	1.07	1.79	0.85	11.89	0.19	6.7	13.6	60.3	10.2	3.6	15.4	1.9	0.9	22.1	1.0	5.8	25.9	2.0	0.6
JG-2 (granite)																									
RV	**77.09**	**0.04**	**12.51**	**0.97**	**0.02**	**0.04**	**0.70**	**3.55**	**4.73**	**0.00**	**99.65**	**81.3**	**48.5**	**6.4**	**18.7**	**14.7**	**4.4**	**31.6**	**302.0**	**2.4**	**18.0**	**31.7**	**3.8**	**86.8**	**97.9**
Mean	**76.87**	**0.03**	**12.89**	**1.00**	**0.01**	**0.16**	**0.69**	**3.67**	**4.60**	**0.00**	**99.92**	**87.4**	**50.5**	**1.8**	**19.7**	**16.5**	**6.6**	**30.2**	**300.9**	**3.7**	**16.4**	**31.1**	**n.d.**	**79.0**	**109.0**
SDp	0.10	0.00	0.04	0.00	0.00	0.00	0.00	0.06	0.02	0.00	0.08	6.3	2.6	4.4	0.9	0.2	0.4	0.7	1.2	0.8	0.3	0.3	2.4	0.6	0.2
CV%	0.25	9.93	0.57	0.22	0.24	2.56	0.24	3.25	0.66	-	0.16	14.4	10.1	483.8	9.3	2.0	10.9	4.5	0.8	41.1	3.3	2.0	-	1.6	0.5
JA-2 (andesite)																									
RV	**57.40**	**0.68**	**15.65**	**6.27**	**0.11**	**7.85**	**6.62**	**3.15**	**1.84**	**0.15**	**99.73**	**323.9**	**33.7**	**475.1**	**16.8**	**14.3**	**142.0**	**19.3**	**68.0**	**20.0**	**257.5**	**4.8**	**132.8**	**15.6**	**121.6**
Mean	**57.50**	**0.68**	**15.79**	**6.40**	**0.11**	**7.19**	**6.45**	**3.10**	**1.90**	**0.16**	**99.29**	**324.9**	**30.7**	**447.7**	**17.3**	**9.7**	**139.1**	**20.4**	**73.7**	**21.0**	**256.8**	**4.8**	**128.0**	**16.7**	**117.1**
SDp	0.06	0.01	0.07	0.05	0.00	0.05	0.01	0.03	0.02	0.00	0.07	8.2	1.4	7.4	1.1	0.2	2.0	0.6	0.4	0.7	1.7	0.3	8.8	0.6	0.3
CV%	0.19	1.87	0.83	1.64	0.80	1.50	0.42	1.87	2.55	1.86	0.13	5.0	9.4	3.3	12.6	3.9	2.8	5.6	1.2	6.7	1.3	13.7	13.8	6.8	0.6
JA-3 (andesite)																									
RV	**62.39**	**0.70**	**15.59**	**6.61**	**0.10**	**3.73**	**6.25**	**3.20**	**1.41**	**0.12**	**100.11**	**324.0**	**23.0**	**66.3**	**16.3**	**3.4**	**32.3**	**7.7**	**36.8**	**22.0**	**287.6**	**3.3**	**169.3**	**21.2**	**118.2**
Mean	**61.98**	**0.68**	**15.67**	**6.63**	**0.11**	**3.66**	**6.33**	**3.18**	**1.34**	**0.11**	**99.70**	**324.8**	**25.3**	**68.6**	**17.7**	**4.5**	**32.3**	**7.4**	**35.7**	**22.8**	**289.5**	**1.6**	**171.1**	**18.9**	**113.8**
SDp	0.10	0.01	0.05	0.06	0.00	0.04	0.01	0.02	0.03	0.00	0.13	18.1	1.5	3.5	1.0	0.2	1.2	0.4	0.3	1.3	1.8	0.4	11.0	0.4	0.3
CV%	0.33	1.55	0.58	1.91	1.20	2.43	0.24	1.56	3.94	3.54	0.26	11.2	11.7	10.1	10.8	9.4	7.6	10.9	1.6	11.3	1.2	51.4	12.8	4.2	0.5
JB-1b (basalt)																									
RV	**51.91**	**1.28**	**14.60**	**9.16**	**0.15**	**8.27**	**9.75**	**2.67**	**1.34**	**0.26**	**99.40**	**N/A**	**N/A**	**445.9**	**N/A**	**N/A**	**150.3**	**6.9**	**39.7**	**29.0**	**445.9**	**N/A**	**217.3**	**N/A**	**N/A**
Mean	**51.87**	**1.27**	**14.07**	**9.24**	**0.15**	**8.53**	**9.87**	**2.60**	**1.30**	**0.26**	**99.17**	**515.5**	**55.4**	**479.6**	**17.9**	**23.4**	**155.3**	**6.0**	**34.9**	**30.9**	**450.7**	**9.0**	**227.1**	**20.7**	**128.4**
SDp	0.05	0.00	0.03	0.08	0.00	0.08	0.03	0.07	0.03	0.00	0.15	15.8	2.9	10.4	1.1	0.9	1.3	0.4	0.6	1.6	2.6	0.5	8.5	0.4	0.2
CV%	0.20	0.60	0.49	1.77	0.63	1.79	0.56	5.21	4.31	1.29	0.31	6.1	10.6	4.3	12.3	7.9	1.7	12.6	3.7	10.6	1.2	10.6	7.5	4.2	0.3
JB-3 (basalt)																									
RV	**51.05**	**1.44**	**17.23**	**11.84**	**0.18**	**5.20**	**9.81**	**2.73**	**0.78**	**0.29**	**100.56**	**245.5**	**21.5**	**58.2**	**19.8**	**2.5**	**36.3**	**5.6**	**15.1**	**33.9**	**403.7**	**1.3**	**372.7**	**26.9**	**98.0**
Mean	**50.76**	**1.43**	**16.86**	**11.85**	**0.18**	**5.26**	**9.78**	**2.70**	**0.67**	**0.29**	**99.85**	**232.0**	**20.2**	**67.5**	**20.1**	**3.3**	**35.6**	**5.0**	**13.9**	**33.0**	**405.4**	**0.8**	**396.4**	**24.0**	**93.9**
SDp	0.05	0.00	0.03	0.01	0.00	0.02	0.01	0.04	0.03	0.00	0.20	6.7	2.9	2.7	1.0	0.2	0.7	0.5	0.5	0.6	2.4	0.4	15.5	0.4	0.3
CV%	0.21	0.36	0.34	0.21	0.51	0.69	0.29	3.30	9.37	1.26	0.40	5.8	28.5	7.9	9.5	9.9	3.7	20.5	7.1	3.7	1.2	84.6	7.8	3.6	0.6
JGb-1 (gabbro)																									
RV	**44.22**	**1.62**	**17.72**	**15.25**	**0.19**	**7.95**	**12.05**	**1.22**	**0.24**	**0.06**	**100.53**	**65.1**	**8.3**	**58.5**	**18.1**	**3.4**	**25.7**	**1.9**	**7.0**	**36.3**	**331.2**	**0.5**	**643.2**	**10.5**	**33.2**
Mean	**44.22**	**1.61**	**17.24**	**15.25**	**0.19**	**8.26**	**12.01**	**1.14**	**0.28**	**0.05**	**100.24**	**56.5**	**7.5**	**73.5**	**18.8**	**3.2**	**22.1**	**2.2**	**7.8**	**35.9**	**325.9**	**1.5**	**648.1**	**9.3**	**31.0**
SDp	0.09	0.01	0.03	0.01	0.00	0.03	0.01	0.08	0.01	0.00	0.11	8.9	1.7	7.3	0.9	0.3	0.7	0.6	0.3	1.8	1.4	0.4	13.3	0.3	0.2
CV%	0.40	0.72	0.35	0.19	0.66	0.74	0.22	13.65	4.85	1.76	0.22	31.4	44.2	20.0	9.8	18.4	6.5	55.8	7.1	10.0	0.9	52.1	4.1	7.5	1.1
JSL-1 (shale)																									
RV	**62.86**	**0.77**	**18.60**	**7.29**	**0.06**	**2.55**	**1.56**	**2.31**	**3.01**	**0.21**	**99.22**	**322.4**	**64.0**	**64.4**	**21.9**	**10.0**	**39.7**	**18.4**	**123.7**	**17.7**	**204.0**	**10.5**	**138.5**	**31.7**	**183.9**
Mean	**63.42**	**0.76**	**18.85**	**7.10**	**0.06**	**2.51**	**1.59**	**2.49**	**3.20**	**0.21**	**100.19**	**342.7**	**61.2**	**62.6**	**23.2**	**10.9**	**41.8**	**20.5**	**125.5**	**14.3**	**207.8**	**9.8**	**154.5**	**28.7**	**179.7**
SDp	0.12	0.00	0.03	0.01	0.00	0.01	0.00	0.06	0.00	0.00	0.17	9.2	3.7	2.1	0.8	0.2	0.9	0.6	0.8	0.6	1.4	0.4	8.0	0.7	0.7
CV%	0.38	0.49	0.33	0.22	1.86	0.75	0.26	5.00	0.09	0.70	0.33	5.3	12.1	6.6	6.8	3.5	4.3	5.9	1.2	9.1	1.3	8.0	10.4	4.9	0.8
JSL-2 (shale)																									
RV	**62.87**	**0.68**	**19.22**	**7.03**	**0.08**	**2.52**	**1.99**	**1.42**	**3.18**	**0.17**	**99.18**	**319.9**	**73.7**	**68.5**	**24.2**	**13.0**	**43.0**	**20.9**	**125.0**	**17.8**	**243.7**	**12.2**	**129.2**	**33.2**	**202.3**
Mean	**63.51**	**0.79**	**19.44**	**6.93**	**0.09**	**2.48**	**1.98**	**1.64**	**3.27**	**0.18**	**100.31**	**339.5**	**71.9**	**64.7**	**24.5**	**13.1**	**46.5**	**23.0**	**126.6**	**15.3**	**250.2**	**12.5**	**144.9**	**30.8**	**202.8**
SDp	0.10	0.00	0.04	0.01	0.00	0.01	0.00	0.06	0.00	0.00	0.14	8.4	2.0	4.0	0.9	0.3	1.2	0.5	0.6	0.6	1.4	0.7	7.0	0.5	0.8
CV%	0.33	1.14	0.37	0.38	1.30	0.69	0.50	6.83	0.27	1.90	0.27	5.0	5.7	12.2	7.3	5.0	5.2	4.0	0.9	8.3	1.1	10.7	9.7	3.5	0.8
Average CV%	**0.29**	**2.40**	**0.51**	**1.02**	**1.06**	**1.48**	**0.42**	**4.72**	**2.99**	**3.03**	**0.25**	**10.1**	**16.2**	**67.6**	**9.8**	**7.1**	**6.4**	**13.5**	**2.7**	**13.7**	**1.4**	**26.5**	**10.2**	**4.3**	**0.6**
Standards >10 ppm												**10.1**	**12.7**	**9.2**	**9.8**	**4.3**	**4.5**	**4.4**	**2.2**	**8.5**	**1.4**	**7.4**	**11.5**	**3.8**	**0.6**

Electronic Supplementary Material Table OR3: Press powder standard analyses

Table OR3: Pressed powder standard analyses (n=5)

RV- Recommended or preferred values, source as in Table OR2.
SD- Standard deviation, CV% - 2 sigma coefficient of variation
n.d. - not detected

Standard	As	Zn	Cu
JA-2 RV	**0.9**	**64.7**	**29.7**
Mean	**1.0**	**70.9**	**28.4**
SD	0.4	1.0	1.0
CV%	38.5	1.4	3.5
JA-3 RV	**4.7**	**67.7**	**43.4**
Mean	**3.9**	**71.2**	**47.4**
SD	0.3	1.3	2.4
CV%	14.9	3.6	10.1
JB-3 RV	**1.8**	**100.0**	**194.0**
Mean	**1.1**	**91.0**	**182.1**
SD	0.3	3.4	4.2
CV%	47.7	7.5	4.6
JG-2 RV	**0.7**	**13.6**	**0.5**
Mean	**1.6**	**10.0**	**n.d.**
SD	0.2	1.4	-
CV%	28.9	28.5	-
JLk-1 RV	**26.8**	**152.0**	**62.9**
Mean	**28.2**	**161.8**	**72.6**
SD	0.3	1.9	1.7
CV%	2.4	2.4	4.7
JR-3 RV	**1.1**	**209.0**	**2.9**
Mean	**2.7**	**200.7**	**n.d.**
SD	0.2	2.0	-
CV%	12.1	2.0	-
JSL-1 RV	**14.9**	**108.0**	**40.8**
Mean	**12.9**	**118.3**	**41.3**
SD	0.3	1.4	0.7
CV%	2.3	1.2	1.7
Average CV%	21.0	6.7	4.1
Average >5 ppm	3.5	6.7	4.1

Electronic Supplementary Material Two: Statistical Analyses

(A) Correlation matrices for the Inner Harbour, Thambalagam Bay and Koddiyar Bay datasets. Strong positive correlations are indicated in bold; negative correlations in red.

Online Resource Two : Correlation matrix for Inner Harbour, Thambalagam Bay and the Koddiyar Bay

Inner Harbour

	SiO_2	TiO_2	Al_2O_3	Fe_2O_3*	MnO	MgO	CaO	Na_2O	K_2O	P_2O_5	Ba	Ce	Cr	Ga	Nb	Ni	Pb	Rb	Sc	Sr	Th	V	Y	Zr	As	Zn
TiO_2	-0.09																									
Al_2O_3	-0.49	0.45																								
Fe_2O_3*	-0.75	0.44	**0.72**																							
MnO	-0.34	0.53	**0.72**	**0.78**																						
MgO	-0.84	0.07	**0.56**	**0.81**	**0.55**																					
CaO	-0.92	-0.13	0.12	0.49	0.03	**0.69**																				
Na_2O	0.00	-0.14	**0.63**	0.07	0.32	0.11	-0.25																			
K_2O	-0.25	0.30	**0.69**	0.19	0.14	0.05	0.01	**0.61**																		
P_2O_5	-0.76	-0.04	0.11	**0.58**	0.15	**0.66**	**0.78**	-0.17	-0.12																	
Ba	0.18	0.41	0.33	-0.12	-0.16	-0.41	-0.34	0.32	**0.78**	-0.28																
Ce	0.15	0.01	0.12	-0.27	-0.06	-0.33	-0.19	0.39	0.19	-0.22	0.34															
Cr	-0.44	0.07	**0.77**	**0.64**	**0.53**	0.73	0.16	**0.52**	0.25	0.23	-0.06	-0.06														
Ga	0.28	0.55	0.45	0.15	**0.54**	-0.09	-0.53	0.35	0.38	-0.40	0.39	0.14	0.14													
Nb	0.32	0.18	0.30	-0.08	0.12	-0.48	-0.50	**0.52**	**0.56**	-0.32	**0.71**	0.48	-0.09	0.53												
Ni	-0.50	0.02	**0.72**	**0.65**	**0.53**	**0.80**	0.24	0.47	0.19	0.30	-0.19	-0.18	**0.98**	0.07	-0.21											
Pb	-0.60	-0.02	-0.01	0.39	0.05	0.44	**0.66**	-0.15	-0.12	**0.93**	-0.15	0.07	0.02	-0.33	-0.15	0.07										
Rb	0.01	**0.55**	**0.58**	0.09	0.14	-0.01	-0.25	0.46	**0.76**	-0.19	**0.78**	0.22	0.27	0.46	0.34	0.18	-0.13									
Sc	-0.95	-0.05	0.48	**0.74**	0.40	**0.90**	**0.87**	0.04	0.11	**0.69**	-0.40	-0.22	**0.54**	-0.32	-0.42	**0.62**	0.49	-0.16								
Sr	-0.82	-0.09	-0.03	0.36	-0.07	0.53	**0.96**	-0.40	-0.05	**0.67**	-0.34	-0.19	-0.03	-0.54	-0.49	0.06	**0.56**	-0.35	**0.77**							
Th	-0.35	0.06	0.26	-0.03	-0.05	-0.01	0.34	0.29	0.40	0.09	0.28	**0.65**	0.02	-0.25	0.17	-0.04	0.20	0.23	0.23	0.37						
V	-0.08	**0.60**	**0.73**	**0.54**	**0.72**	0.10	-0.26	0.44	0.41	-0.07	0.42	0.40	0.42	**0.62**	**0.65**	0.31	-0.02	0.40	0.03	-0.33	0.19					
Y	-0.57	0.04	0.04	0.47	0.20	0.47	**0.60**	-0.11	-0.16	**0.92**	-0.22	0.02	0.06	-0.24	-0.13	0.12	**0.98**	-0.15	0.48	0.48	0.12	0.07				
Zr	0.19	-0.01	0.08	-0.31	-0.10	-0.36	-0.22	0.37	0.17	-0.24	0.35	**1.00**	-0.07	0.13	0.48	-0.19	0.05	0.21	-0.25	-0.22	**0.63**	0.38	-0.01			
As	-0.75	-0.06	0.21	0.49	0.08	0.51	**0.74**	0.02	0.13	**0.88**	0.00	0.17	0.18	-0.32	0.00	0.19	**0.93**	-0.05	**0.63**	**0.62**	0.34	0.12	**0.88**	0.14		
Zn	-0.68	0.07	0.27	**0.70**	0.40	**0.73**	**0.62**	-0.04	-0.18	**0.93**	-0.35	-0.14	0.44	-0.20	-0.26	0.50	**0.85**	-0.18	**0.67**	0.47	0.00	0.18	**0.90**	-0.16	**0.80**	
Cu	-0.64	-0.07	0.39	**0.65**	0.34	**0.81**	0.53	0.17	-0.08	**0.80**	-0.33	-0.19	**0.71**	-0.23	-0.33	**0.77**	**0.65**	-0.04	**0.69**	0.33	-0.03	0.11	**0.68**	-0.20	**0.65**	**0.90**

Thambalagam Bay

	SiO_2	TiO_2	Al_2O_3	Fe_2O_3*	MnO	MgO	CaO	Na_2O	K_2O	P_2O_5	Ba	Ce	Cr	Ga	Nb	Ni	Pb	Rb	Sc	Sr	Th	V	Y	Zr	As	Zn
TiO_2	-0.43																									
Al_2O_3	-0.53	0.14																								
Fe_2O_3*	-0.86	**0.57**	0.20																							
MnO	-0.87	**0.67**	0.21	**0.95**																						
MgO	-0.87	0.47	0.30	**0.78**	**0.78**																					
CaO	-0.76	0.10	0.01	**0.62**	**0.67**	**0.78**																				
Na_2O	-0.41	-0.07	**0.74**	0.01	0.08	0.24	0.21																			
K_2O	-0.33	0.02	**0.63**	0.06	-0.04	0.22	0.01	0.42																		
P_2O_5	-0.89	0.38	0.21	**0.92**	**0.89**	**0.80**	**0.75**	0.19	0.08																	
Ba	-0.34	-0.04	**0.74**	0.03	0.02	0.03	-0.04	**0.69**	**0.65**	0.11																
Ce	-0.29	**0.59**	-0.04	**0.59**	**0.57**	0.20	0.05	-0.40	-0.17	0.25	-0.18															
Cr	-0.57	0.62	0.27	**0.76**	**0.72**	0.48	0.20	-0.13	0.01	0.48	-0.04	**0.90**														
Ga	-0.25	-0.05	**0.79**	-0.09	-0.10	0.03	-0.10	**0.56**	**0.53**	-0.14	**0.57**	-0.03	0.12													
Nb	-0.31	**0.72**	0.01	**0.58**	**0.59**	0.25	0.03	-0.35	-0.18	0.24	-0.15	**0.97**	**0.89**	-0.01												
Ni	-0.72	0.36	**0.75**	**0.61**	**0.58**	**0.57**	0.26	0.43	0.30	**0.53**	0.22	0.33	**0.66**	0.55	0.35											
Pb	0.02	-0.48	0.40	-0.43	-0.43	-0.08	0.01	**0.52**	0.46	-0.26	**0.69**	-0.57	-0.48	0.48	-0.54	-0.17										
Rb	0.06	-0.51	**0.65**	-0.36	-0.49	-0.16	-0.32	0.47	**0.60**	-0.29	**0.55**	-0.45	-0.24	**0.70**	-0.47	0.27	**0.66**									
Sc	-0.92	0.46	0.29	**0.85**	**0.89**	**0.90**	0.84	0.24	0.05	**0.84**	0.04	0.38	**0.59**	0.11	0.40	**0.63**	-0.17	-0.28								
Sr	-0.51	-0.02	0.31	0.18	0.30	0.38	**0.60**	**0.67**	0.22	0.45	**0.56**	-0.44	-0.29	0.09	-0.38	0.03	**0.51**	-0.01	0.41							
Th	-0.15	**0.53**	-0.13	0.47	0.45	0.08	-0.05	-0.47	-0.22	0.12	-0.23	**0.99**	**0.84**	-0.08	**0.96**	0.22	-0.56	-0.45	0.26	-0.51						
V	-0.51	**0.75**	0.09	**0.76**	**0.77**	0.43	0.21	-0.23	-0.15	0.47	-0.11	**0.95**	**0.94**	-0.03	**0.97**	0.48	-0.57	-0.50	**0.58**	-0.23	**0.90**					
Y	-0.85	**0.57**	0.27	**0.97**	**0.92**	**0.76**	**0.57**	-0.03	0.07	**0.83**	0.00	**0.69**	**0.86**	0.05	**0.67**	**0.70**	-0.42	-0.28	**0.85**	0.04	**0.58**	**0.82**				
Zr	-0.16	**0.58**	-0.08	0.47	0.46	0.08	-0.07	-0.42	-0.21	0.11	-0.20	**0.99**	**0.84**	-0.03	**0.97**	0.25	-0.55	-0.45	0.26	-0.49	**0.99**	**0.91**	**0.57**			
As	-0.77	0.13	-0.04	**0.79**	**0.74**	**0.80**	**0.90**	0.02	-0.02	**0.88**	-0.12	0.16	0.32	-0.21	0.10	0.32	-0.18	-0.30	**0.83**	0.39	0.05	0.31	**0.72**	0.01		
Zn	-0.75	**0.60**	**0.72**	**0.70**	**0.70**	**0.59**	0.23	0.36	0.29	**0.56**	0.31	0.50	**0.78**	0.45	**0.56**	**0.92**	-0.20	0.08	**0.63**	0.08	0.39	**0.67**	**0.76**	0.44	0.28	
Cu	-0.57	0.41	**0.79**	0.42	0.43	0.39	0.06	**0.54**	0.29	0.37	0.35	0.23	**0.53**	**0.58**	0.28	**0.90**	-0.06	0.28	0.43	0.11	0.13	0.38	0.47	0.19	0.05	**0.89**

Koddiyar Bay

	SiO_2	TiO_2	Al_2O_3	Fe_2O_3*	MnO	MgO	CaO	Na_2O	K_2O	P_2O_5	Ba	Ce	Cr	Ga	Nb	Ni	Pb	Rb	Sc	Sr	Th	V	Y	Zr	As	Zn
TiO_2	-0.81																									
Al_2O_3	-0.58	0.52																								
Fe_2O_3*	-0.86	**0.92**	0.41																							
MnO	-0.84	**0.90**	0.37	**0.99**																						
MgO	-0.90	**0.86**	0.43	**0.97**	**0.96**																					
CaO	-0.33	-0.17	-0.15	-0.10	-0.11	0.03																				
Na_2O	-0.10	0.04	**0.69**	-0.14	-0.20	-0.14	-0.02																			
K_2O	0.15	-0.19	**0.58**	-0.36	-0.40	-0.32	-0.16	**0.66**																		
P_2O_5	-0.90	**0.77**	**0.79**	0.73	**0.70**	**0.77**	0.16	0.35	0.12																	
Ba	0.19	-0.24	**0.60**	-0.40	-0.46	-0.40	-0.20	**0.76**	**0.91**	0.12																
Ce	-0.86	**0.93**	**0.54**	**0.95**	**0.94**	**0.91**	-0.10	0.01	-0.26	**0.84**	-0.25															
Cr	-0.83	**0.94**	0.49	**0.98**	0.98	0.94	-0.19	-0.06	-0.29	**0.77**	-0.31	**0.97**														
Ga	0.10	-0.07	0.51	-0.20	-0.21	-0.17	-0.26	0.45	0.47	0.20	**0.63**	-0.02	-0.08													
Nb	-0.80	**0.91**	0.32	**0.99**	**0.99**	**0.94**	-0.14	-0.23	-0.42	**0.65**	-0.46	**0.93**	**0.97**	-0.26												
Ni	-0.69	**0.66**	**0.88**	0.55	0.50	**0.59**	-0.04	0.52	0.34	**0.85**	0.32	**0.60**	**0.59**	0.32	0.45											
Pb	**0.70**	-0.62	0.03	-0.80	-0.81	-0.78	-0.22	0.39	**0.75**	-0.46	**0.71**	-0.75	-0.75	0.43	-0.82	-0.13										
Rb	0.51	-0.48	0.31	-0.65	-0.68	-0.66	-0.24	**0.60**	**0.82**	-0.27	**0.86**	-0.58	-0.61	0.48	-0.69	0.10	**0.90**									
Sc	-0.67	0.26	0.04	0.37	0.38	0.46	**0.84**	-0.05	-0.36	0.47	-0.40	0.38	0.31	-0.29	0.34	0.14	-0.60	-0.58								
Sr	-0.10	-0.38	-0.29	-0.32	-0.32	-0.19	**0.97**	-0.04	-0.12	-0.06	-0.14	-0.30	-0.40	-0.23	-0.33	-0.24	-0.06	-0.11	**0.72**							
Th	-0.87	**0.93**	0.43	**0.98**	**0.97**	**0.94**	-0.06	-0.10	-0.34	**0.76**	-0.38	**0.97**	**0.97**	-0.23	**0.97**	0.53	-0.81	-0.65	0.41	-0.27						
V	-0.83	**0.92**	0.37	**1.00**	**0.99**	**0.95**	-0.13	-0.19	-0.39	**0.69**	-0.43	**0.95**	**0.98**	-0.21	**1.00**	0.49	-0.81	-0.68	0.35	-0.33	**0.98**					
Y	-0.87	**0.90**	0.53	**0.97**	**0.97**	**0.95**	-0.11	-0.05	-0.27	**0.81**	-0.31	**0.97**	**0.98**	-0.04	**0.94**	**0.61**	-0.75	-0.60	0.38	-0.33	**0.96**	**0.96**				
Zr	-0.85	**0.93**	0.44	**0.98**	**0.97**	**0.93**	-0.11	-0.10	-0.34	**0.76**	-0.35	**0.99**	**0.98**	-0.13	**0.97**	**0.53**	-0.80	-0.65	0.37	-0.31	**0.99**	**0.98**	**0.97**			
As	-0.59	0.20	**0.68**	0.19	0.13	0.27	0.46	**0.58**	0.38	**0.70**	0.49	0.33	0.20	0.28	0.10	**0.60**	-0.12	0.15	0.45	0.36	0.24	0.14	0.26	0.23		
Zn	-0.90	**0.92**	**0.58**	**0.98**	**0.96**	**0.97**	-0.09	-0.02	-0.20	**0.83**	-0.25	**0.95**	**0.97**	-0.07	**0.94**	**0.69**	-0.71	-0.53	0.35	-0.32	**0.95**	**0.96**	**0.98**	**0.95**	0.33	
Cu	-0.10	-0.01	0.30	-0.09	-0.15	0.02	0.17	0.38	0.31	0.24	0.32	-0.13	-0.11	0.18	-0.16	**0.58**	0.29	0.34	-0.07	0.09	-0.16	-0.15	-0.13	-0.18	0.39	0.04

Electronic Supplementary Material 2B: Principal Component Analysis

Principal component plots and loadings of individual elements in the three sectors are given on the following pages. The plots show clear contrast between the sectors.

(a) Inner Harbour

Scattering of the elements within the three sectors is greatest in the Inner Harbour dataset, with a high positive loading on F1 for SiO_2. Most other elements are scattered, with negative F1 loadings and positive F2. A number of elements (CaO, P_2O_5, Pb, Y, Sr) cluster together with negative loadings for both F1 and F2, suggesting association with carbonates in the Inner Harbour. A broad grouping of elements with positive F2 scores (Al_2O_3, Na_2O, K_2O, TiO_2, Rb, Ga, Ba) implies association with both feldspars and clays, while a cluster of Fe_2O_3, Cr, Ni and MgO at negative F1 suggests influence of ferromagnesian and Fe-oxide minerals.

(b) Thambalagam Bay

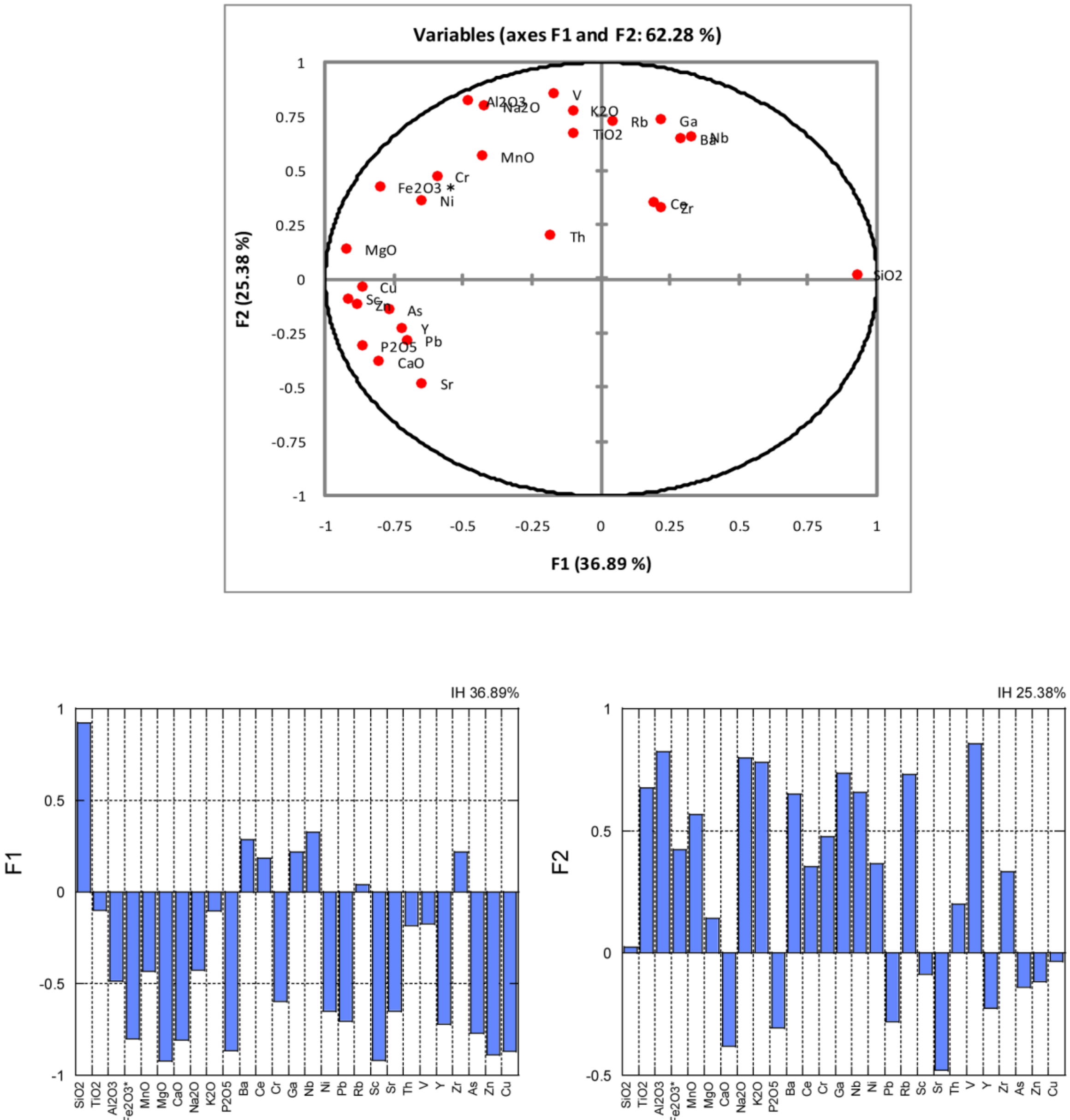
Elements show a differing distribution to those in the Inner Harbour, with negative loading for both F1 and F2 for SiO_2 (quartz), whereas another group (Al_2O_3, Na_2O, K_2O, Ba, Ga, Rb, Pb, Sr) are characterized by positive F2 loading, suggesting association with both plagioclase and K-feldspar. The remaining elements have high F1 loadings, with both positive and negative F2. These groups suggest greater influence of clays and heavy minerals in this sector.

(c) Koddiyar Bay

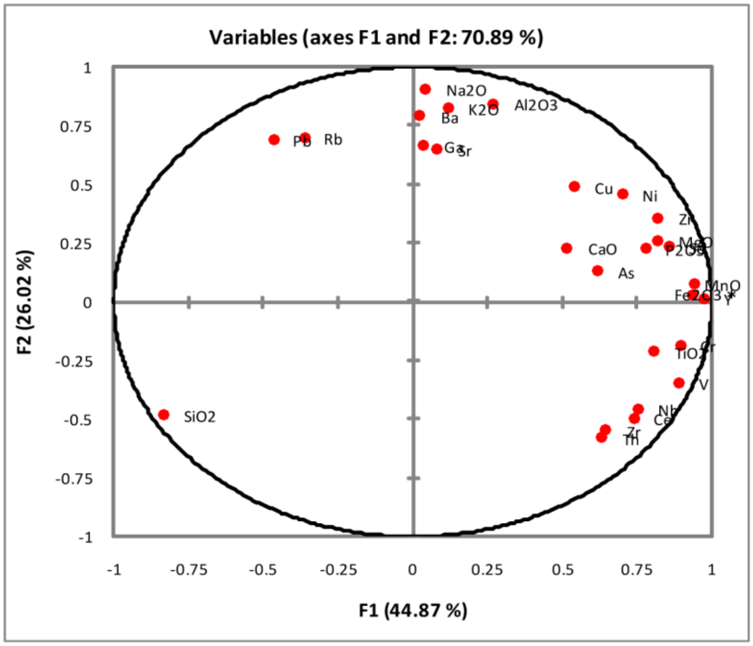
Distribution are different again, with negative loading for both F1 and F2 for SiO_2 as in Thambalagam Bay, and positive F2 and negative F1 loadings for Na_2O, K_2O, Ba, Ga, Rb, Pb), again suggesting association with feldspars. Another group of elements (Fe_2O_3, TiO_2, MnO, MgO, Ce, Cr, Nb, Th, V, Y, Zr) show strong association, all with high F1 scores. This grouping of elements is consistent with stronger influence in this sector of Trincomalee Bay from ferromagnesian phases, Fe-Ti oxide minerals, and heavy minerals, including zircon.

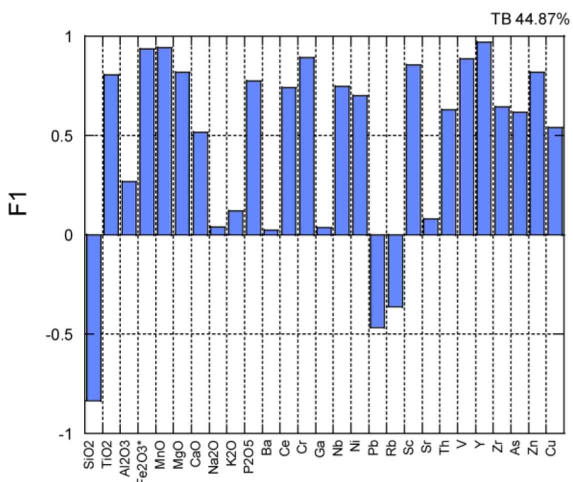
Principal Component Analysis. PCA plots for all data analyzed and factor 1 and 2 loadings for (a) Inner Harbour (b) Thambalagam Bay (c) Koddiyar Bay.

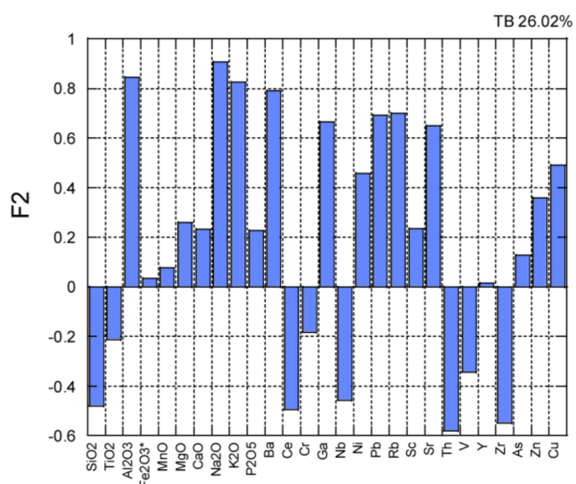
(a) Inner Harbour



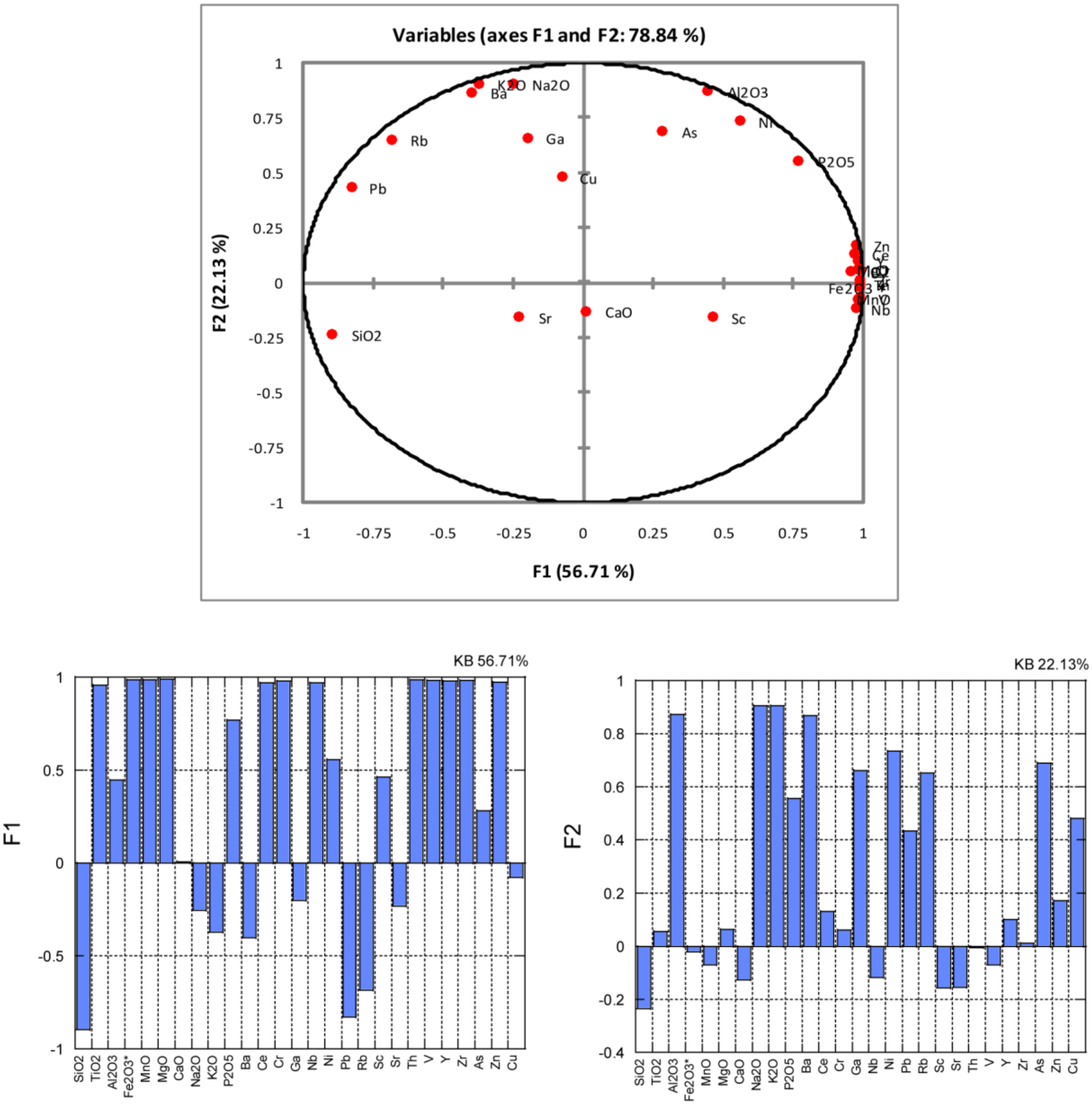
(b) Thambalagam Bay







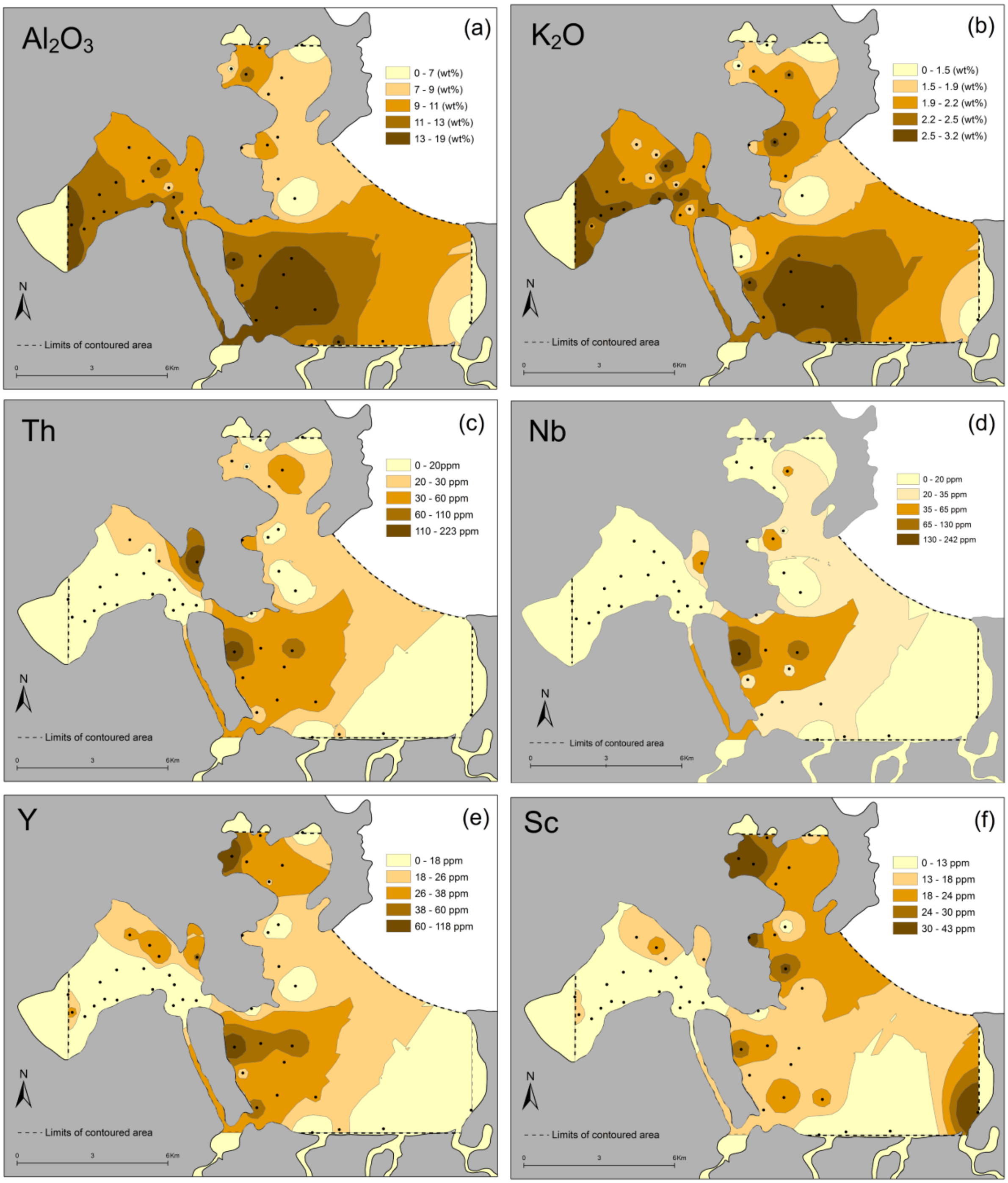
(c) Koddiyar Bay



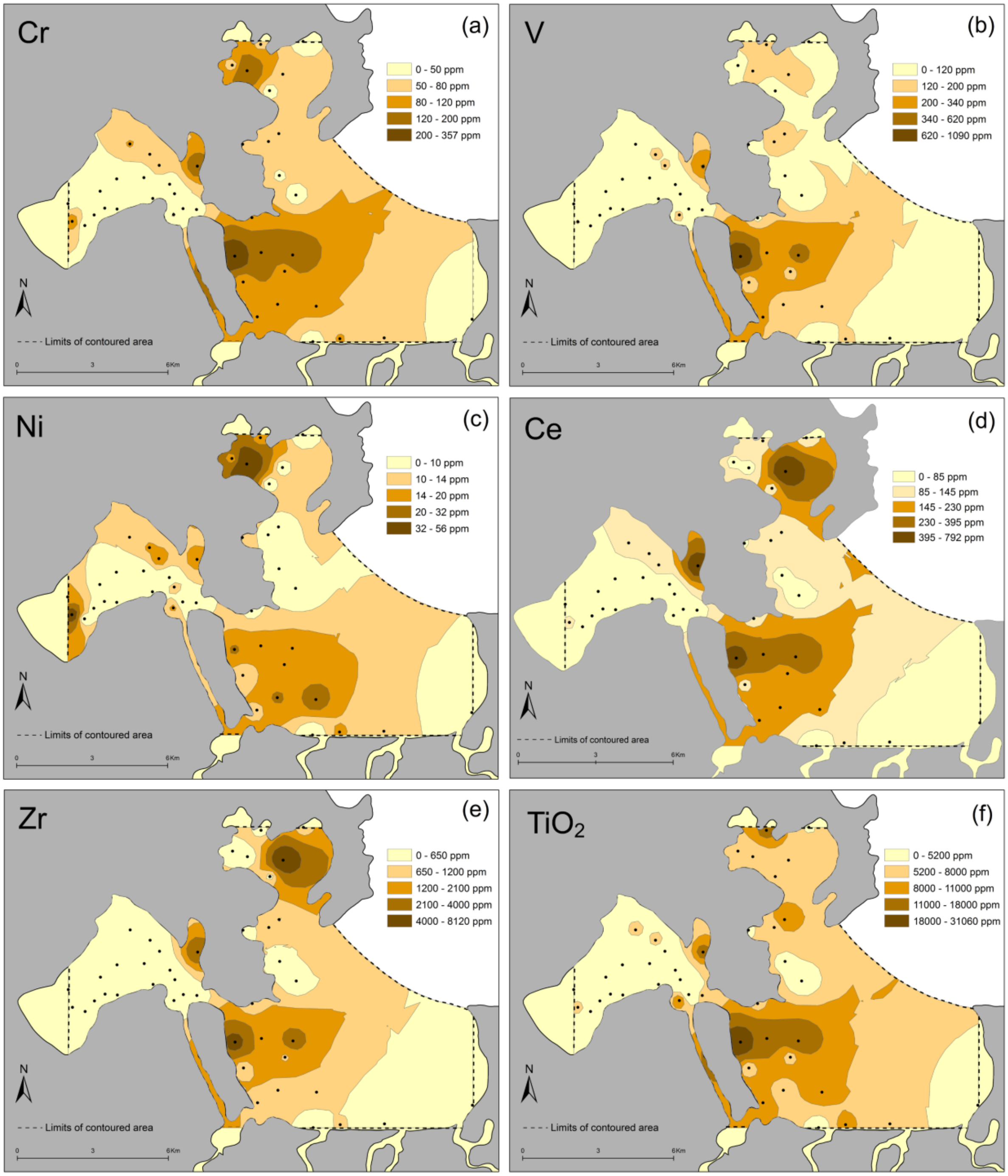
Electronic Supplementary Material Three: GIS maps of element distributions.

The maps were generated using the nearest neighbor method with inverse distance weighted (IDW) interpolation, with contours in five classes. IDW interpolation explicitly implements the assumption that sites that are close to one another are more alike than those that are farther apart. To predict a value for any unmeasured location, IDW will use the measured values surrounding the prediction location. Those measured values closest to the prediction location will have more influence on the predicted value than those farther away. IDW thus assumes that each measured point has a local influence that diminishes with distance. Points closer to the prediction location are given greater weighting than those farther away. The optimal power (p) value is determined by minimizing the root mean square prediction error (RMSPE). The RMSPE is the statistic that is calculated from cross-validation, in which each measured point is removed and compared to the predicted value for that location. The RMSPE is a summary statistic quantifying the error of the prediction surface. Geostatistical Analyst tries several different powers for IDW to identify the power that produces the minimum RMSPE. The error for generating the maps is less than ±7 % (Text based on the ArcGIS 9.2 software manual).

(A) GIS contour maps for (a) Al_2O_3, (b) K_2O, (c) Th, (d) Nb, (e) Y and (f) Sc showing spatial elemental distribution within Trincomalee Bay



(B) GIS contour maps for (a) Cr, (b) V, (c) Ni, (d) Ce, (e) Zr and (f) TiO_2 showing spatial elemental distribution within Trincomalee Bay



(C) GIS contour maps for Enrichment Factor (EF) for (a) As, (b) Zn, (c) Pb, (d) Cu, (e) Ni, and (f) Cr showing spatial distribution within Trincomalee Bay