

Occurrence and distribution of selected pharmaceuticals in fresh fish along the Kenyan coast and assessment of potential human health risks

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S1. Analysis using the UPLC-QTOF

UPLC- QTOF chromatographic conditions

The column used for compound separation was a Kinetex® 1.7 µm EVO C18 100 Å column (2.1 mm ID x 100 mm length). To elute the compounds, the initial solvent consisting of a mixture of 5% methanol (0.1% formic acid) was transitioned to 100% methanol (0.1% formic acid). The formic acid was not only used as a buffer but also as a proton source for ionisation and as a preservative. Initially, an isocratic flow (0.1 min) was used to start the gradient elution, and then a linear increase to 100% methanol. After each run, the column was washed for 1 minute, the initial conditions were re-established, and the column was allowed to re-equilibrate before starting the next run. Throughout the entire run, the column temperature was maintained at 40 °C, and the flow rate was set at 0.4 mL/min, resulting in a total run time of 20 minutes and injection volumes were set at 5 µL. To ensure unbiased analysis, the samples were analyzed separately in both ESI positive and ESI negative ionisation modes.

UPLC- QTOF instrumentation and MS conditions

The sample was analyzed using a Waters® Synapt G2 high-definition mass spectrometry (HDMS) system (Waters Inc., Milford, Massachusetts, USA) coupled to an Acquity UPLC. MassLynx™ software (version 4.1) from Waters Inc. was used to operate the system for data acquisition and processing. The Intellistart feature and sodium formate clusters were used to calibrate the instrument over a mass range of 112.936 to 1,132.688 Da. The mass error was less than 0.4 mDa

with a resolution of 20,000 at m/z 200 FWHM (full width at half maximum). For the ESI source in positive mode ionization, the voltage was set at 2.6 kV, and for negative mode ionization, the voltage was set at 2.0 kV. The source temperature was set at 120 °C, the sampling cone voltage was 25 V, and the extraction cone voltage was 4.0 V. Nitrogen gas was used for the cone at a flow rate of 10.0 L/min, and desolvation occurred at 350°C with a nitrogen gas flow rate of 600.0 L/min.

Data acquisition for the UPLC- QTOF analysis

Two simultaneous acquisition functions with low and high collision energy (MSE approach) on the QTOF instrument were used for quantitative data-independent acquisition. The high-energy mass spectral scan was time-aligned with the low-energy scan, enabling the prediction of fragment ions from precursor ions and the acquisition of the full mass spectrum. Fragmentation patterns were used for qualitative confirmation via high-energy collision-induced dissociation. For the fragmentation energy, the collision energy was set at 3V and the trap was set at 2 V. A ramp from 3 to 4 V was used for the trap, and a ramp of 20 to 40 V for the transfer of collision energy. Mass spectral scans were collected every 0.3 seconds, covering mass-to-charge ratios (m/z) between 50 and 1,200 Da.

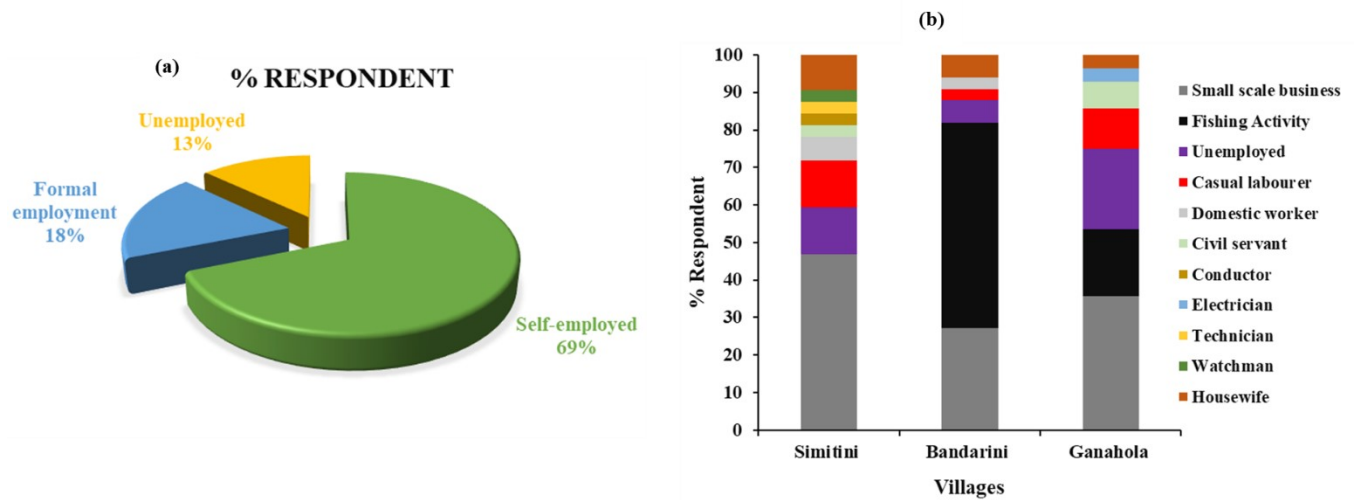


Figure S1: (a) Occupation categories of the respondents from Ganahola, Simitini, and Bandarini and (b) the occupation of respondents of Ganahola, Simitini, and Bandarini.

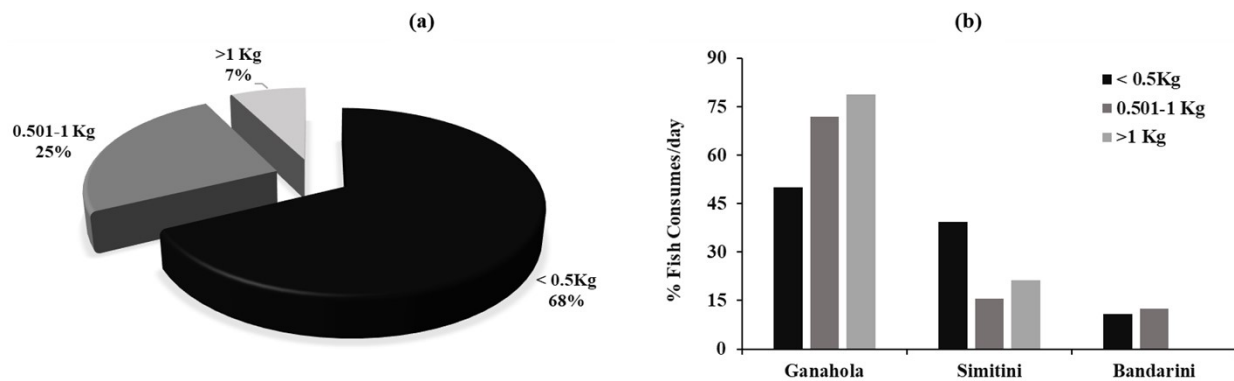


Figure S2: (a) Average daily fish consumption in Tudor creek and (b) Average amount of fish consumed per household in Ganahola, Simitini, and Bandarini.

Table S1: Household [HH] Fish Consumption Survey Questionnaire

Date _____ County _____ Location _____ ID No. _____

(A) Demographic data	
(1) Name of respondent: _____	
(2) Gender of HH head: i) M _____ (ii) F _____	(3) Age (years) _____
(4) Marital Status: (i) Single _____ (ii) Married _____ (iii) Separated _____ (iv) Divorced _____ (v) Widow/er _____	
(5) HH size _____	
(6) Educational level: (i) Madrassa _____ (ii) Incomplete primary _____ (iii) Completed primary _____ (iv) Incomplete secondary _____ (v) Completed secondary _____ (vi) Tertiary _____ (vii) None _____	
(7) Number of Children you have? _____	
(8) How many children <18 years live with you? _____	
(9) Are any children in school? (i) Y _____ (ii) N _____ If Yes, how many? _____ Number in Primary _____ Secondary _____	
(10) Occupation Primary occupation _____ Secondary occupation: _____	
(B) Household Fish Consumption	
(11) When do you consume fish most?	
(i) During certain periods of the year _____	
(ii) Throughout the year _____	
If (i), when? Why? _____	
(12) How often do you consume fish?	
(i) Daily _____	
(ii) < thrice/week _____	
(iii) 3-6 times/week _____	
(iv) Rarely _____	
(13) On average, what quantity of fish does your HH consume/meal?	
(i) <0.5 kg _____	
(ii) 0.5-1 kg _____	
(iii) > 1 kg _____	
(14) Three most preferred species (order of preference)?	
(i) _____	
(ii) _____	
(iii) _____	
Reason for preference? _____	
(14) Source of fish? (i) Local landing site _____ (ii) Local mkt _____ (iii) Local fish shop _____	
(iv) Other _____	
(15) How do you buy your fish? (i) Fresh _____ (ii) Frozen _____ (iii) Deep-fried _____ (iv) Smoked _____ (v) Other _____	

THANK YOU FOR YOUR TIME