Electronic Supplementary Material (ESI) for RSC Advances.

Chemical Fingerprinting and quantitative analysis of the doping drugs bambuterol and terbutaline in human urine samples using ATR-FTIR coupled with chemometric tools.

Supplementary Figures

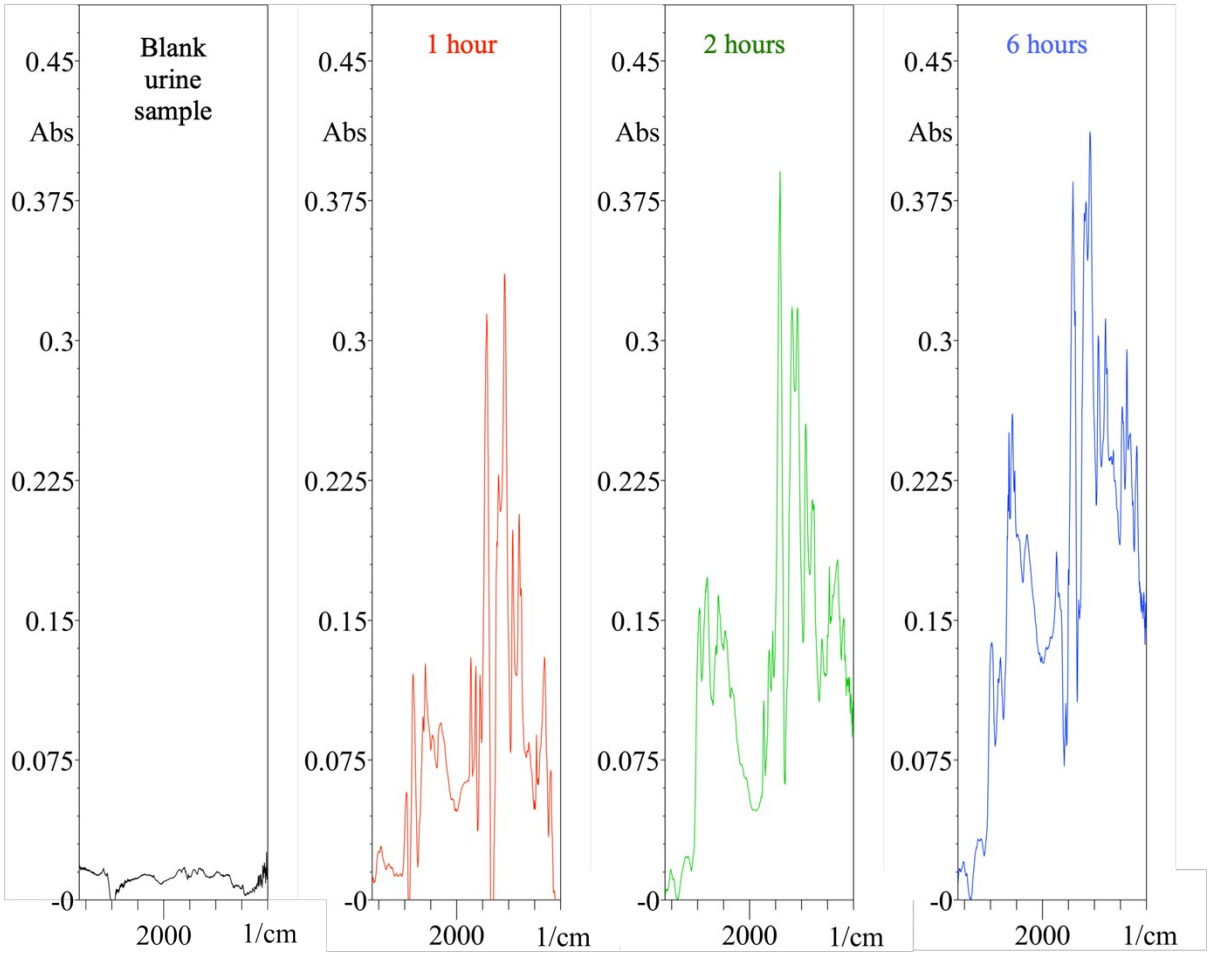
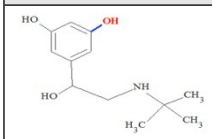
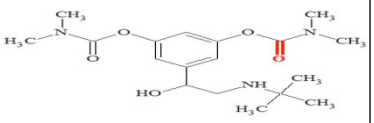
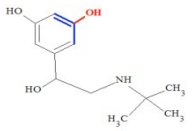
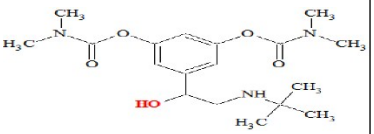
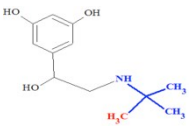
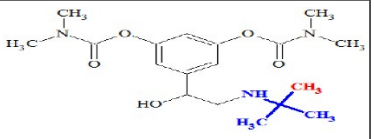
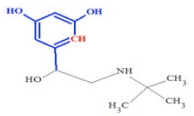
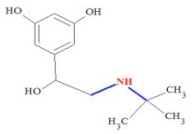
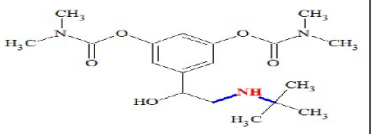
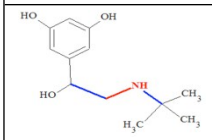
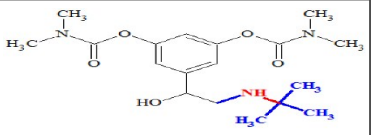
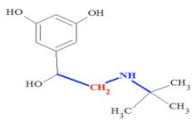
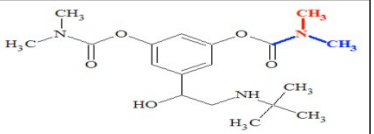
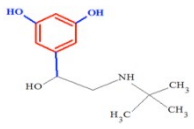


Figure (1S): Typical ATR-FTIR spectra of bank urine sample side by side to the urine samples obtained from volunteers at various times (1, 2 and 6 hours) after a single oral dose of 20 mg bambuterol tablet. All the samples were measured against urine sample background spectrum that contain all unit components of urine without the under investigation drug or its metabolites.

Supplementary Tables

Table (1S): Characteristic groups and spectrum peaks differences between BAM and TER

Terbutaline		***Bambuterol***	
	O-H and C-O combination band at 1195.87 – 1236.46 -1342 – 1381 - 1394 cm^{-1} and O-H stretching in range of 3100 – 3600 cm^{-1}	Characteristic carbonyl shows C=O stretching at 1720 cm^{-1}	
	C-O stretching at 1195.87 – 1236.46 cm^{-1}	Hydroxyl [OH] group shows stretching in its characteristic region nearly from 3150 to 3600 cm^{-1}	
	Tertiary butyl CH_3 vibration at 1381.03 cm^{-1}	Tertiary butyl CH_3 vibration at 1384.8 cm^{-1}	
	Aromatic 1,3,5-tri substituted benzene C-H out of plane at regions [700.16 – 846.75 cm^{-1}] also C-H stretching 3113.1 cm^{-1}	Aromatic 1,3,5-tri substituted benzene C-H out of plane at regions [651.9 - 692.4 – 810 – 850.3 cm^{-1}] also C-H stretching 3053 – 3113.1 cm^{-1}	
	Amino [NH] group shows stretching in its characteristic region nearly from 3275 to 3350 cm^{-1}	Amino [NH] group shows stretching in its characteristic region nearly from 3275 to 3350 cm^{-1}	
	Secondary di alkyl amine C-N stretching at 1122.57 cm^{-1}	Secondary di alkyl amine C-N stretching at 1150 cm^{-1}	
	CH_2 at 1467.83 cm^{-1}	Tertiary amine C-N stretching show peak at 1166.93 cm^{-1}	
		N,N-di alkyl Carbamate shows C-N stretching at 1295.3 and 1292.31 cm^{-1}	
	Aromatic 1,3,5-tri substituted benzene ring stretching at [1604.78 – 1481.33 – 1467.83 cm^{-1}] and ring out of plane pending at 730 cm^{-1}]	Aromatic 1,3,5-tri substituted benzene ring stretching at [1442.75 – 1483.26 – 1622.13 cm^{-1}] and ring out of plane pending at 692.43 - 756 cm^{-1}]