Sodium hexametaphosphate-treated halloysite based solid-phase extraction of biguanides from dietary supplements

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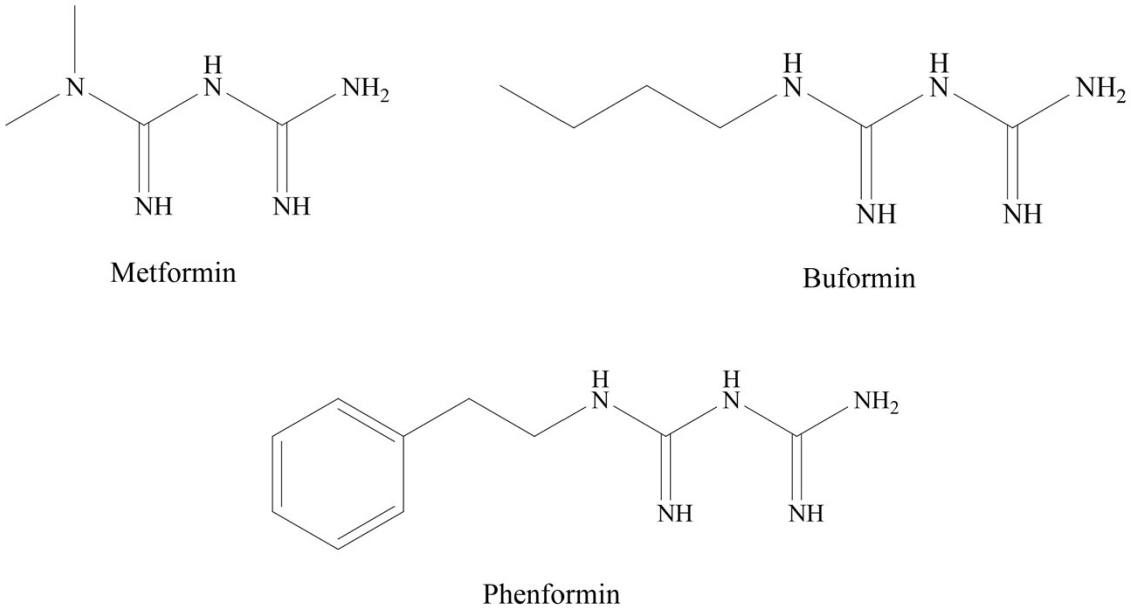

Fig. S1 Chemical structures of metformin, buformin, and phenformin.

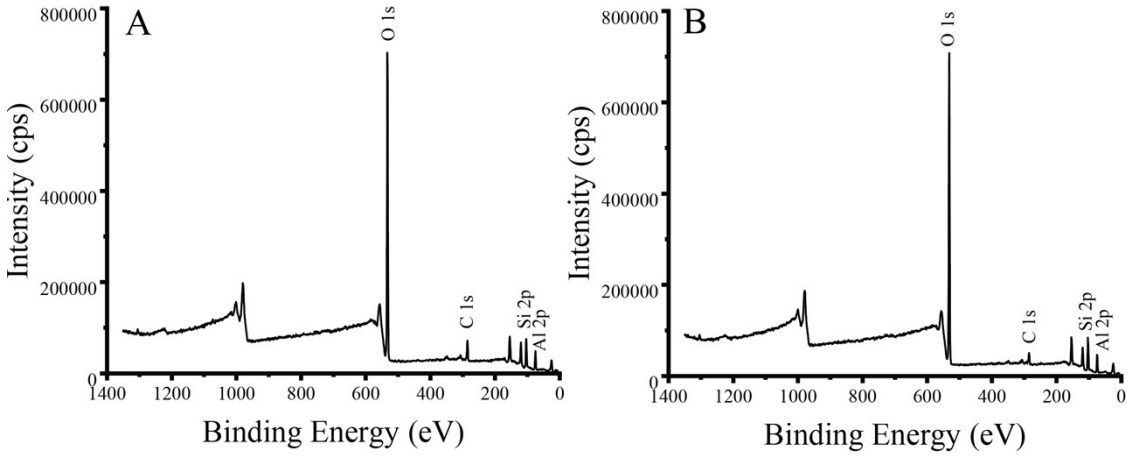

Fig. S2 XPS survey of the raw halloysite (A) and the purified halloysite (B).

Table S1 The pK_{a1}, pK_{a2}, and log P values of metformin, buformin, and phenformin.

Compound	pK_{a1} [a]	pK_{a2} [b]	log P [b]
Metformin	2.95	12.27	-1.43
Buformin	2.92	12.27	-1.20
Phenformin	2.86	12.15	-0.64

[a] Calculated using Advanced Chemistry Development (ACD/Labs) Software V6.0.

[b] From ref. 25.

Table S2 MRM parameters for metformin, buformin, and phenformin analyzed by RPLC-MS/MS.

Analyte	Retention time (min)	Precursor ion (*m/z*)	Product ions (*m/z*)	Declustering potential (V)	Collision energy (V)
Metformin	1.9	130.3	60.3*/71.4	45	19/31
Buformin	3.7	158.3	60.1*/116.	55	23/22
Phenformin	4.9	206.0	60.2*/105.0	80	31/36

* Quantitation ion.

Table S3 XPS atomic content (at.%) for the raw halloysite and the purified halloysite.

Material	Surface concentration (at. %)			
	Al	Si	O	C
Raw halloysite	13.17	14.41	61.86	10.56
Purified halloysite	14.04	15.43	63.74	6.79