In-silico pharmacokinetic properties study of alpha-mangostin and its derivatives via ADMET predictor

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Abstract: Alpha- and beta-mangostins (1) and (2) were evaluated for their anti-bacterial activity against MRSA and P. aureginosa. Only compound 1 showed strong activity against MRSA and P. aureginosa with MIC value of 2.34 µg/mL. Moreover, compound 1 was further predicted for their pharmacokinetic (PK) properties via ADMET predictor™ software. The result revealed that 1 has a problem with its PK properties including, mutagenicity (mu) and low fraction unbound (fu). Therefore, the modification of compound 1, 3-isomangostin (1a), 3-isomangostin hydrate (1b) and 1-isomangostin hydrate (1c) led to improve its PK properties. Surprisingly, compounds 1b and 1c have no problem with their pharmacokinetic properties and showed activity against MRSA and P. aureginosa.

Keywords: Alpha-mangostins; Pharmacokinetic properties; ADMET predictor; Anti-bacterial activity