SUPPLEMENTARY MATERIAL

CHARACTERIZATION OF TEAGHRELIN-LIKE COMPOUNDS FROM TEA CULTIVARS IN THAILAND AND *IN SILICO* STUDY OF THEIR BIOACTIVITY

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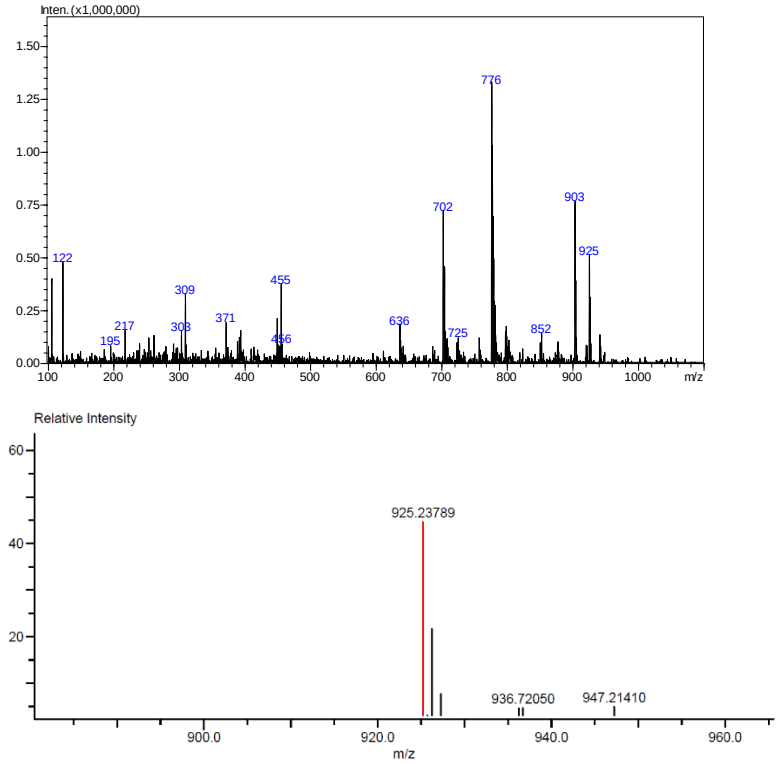
Abstract: In the present research, four tea cultivars in Thailand were screening to search for the teaghrelin-like compounds and totally six components were identified. Among these, one new constituent isolated form Assam tea varieties was assigned as quercetin 3-*O*-[2-*O*-(*E*)-*p*-coumaroyl][*α*-L-rhamnopyranosyl(1→6)]-*β*-D-glucoside 4'-*α*-L-rhamnoside (**1**) through the comprehensive 1D- and 2D-NMR and mass spectrometric analysis. The isolated compounds were examined for their ghrelin receptor binding affinity *in silico* and antioxidant bioactivity by free radical scavenging model. However, no significant bioactivity was observed according to the experimental results.

Contents

Figure S1. MS/HRMS spectra of **1**.



Mass	Intensity	Calc. Mass	Mass Difference [mDa]	Mass Difference [ppm]	Possible Formula
925.23789	13534.23	925.23784	0.05	0.06	$^{12}C_{42}{}^{1}H_{46}{}^{23}Na_{1}{}^{16}O_{22}$

Figure S2. ^{1}H NMR spectrum of **1**.

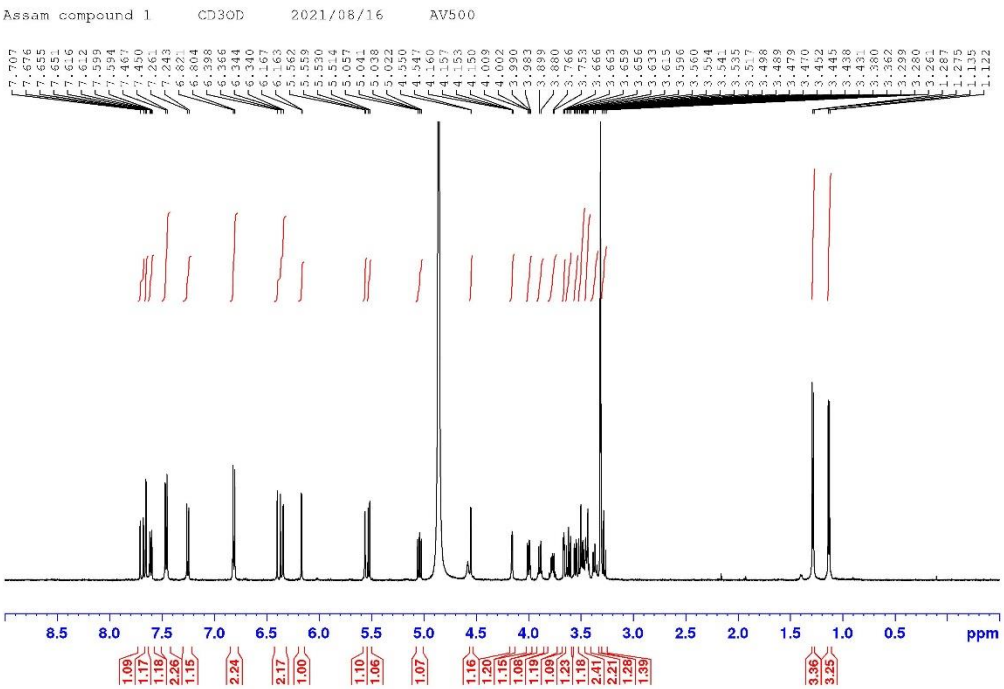


Figure S3. ^{13}C and DEPT NMR spectrum of **1**.

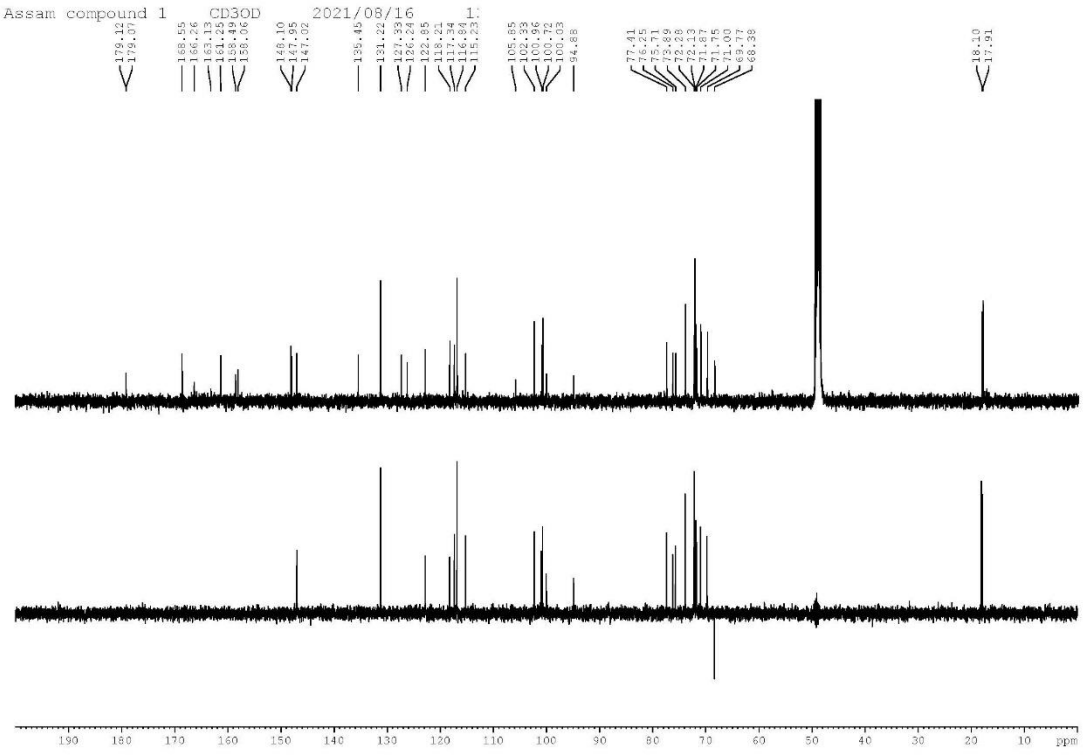


Figure S4. HMBC spectrum of **1**.

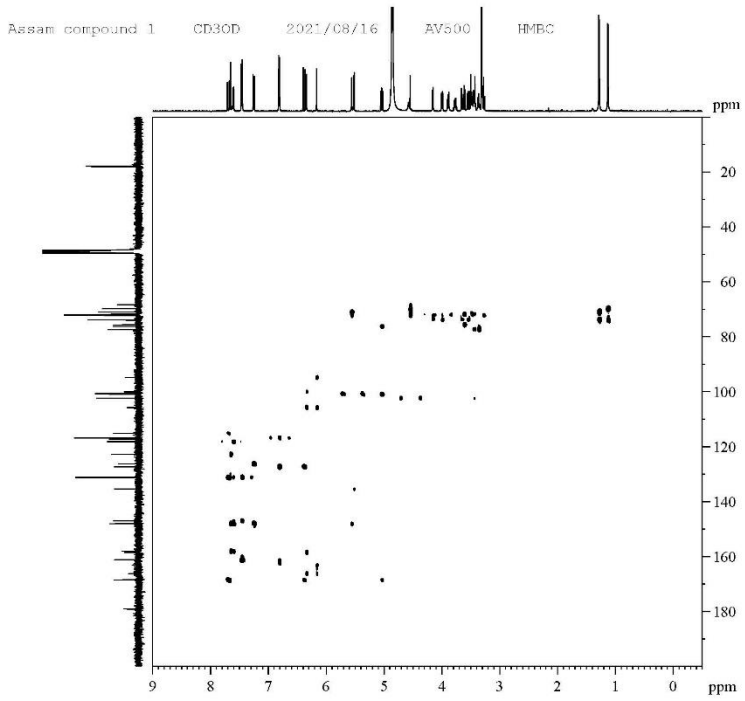


Figure S5. COSY spectrum of **1**.

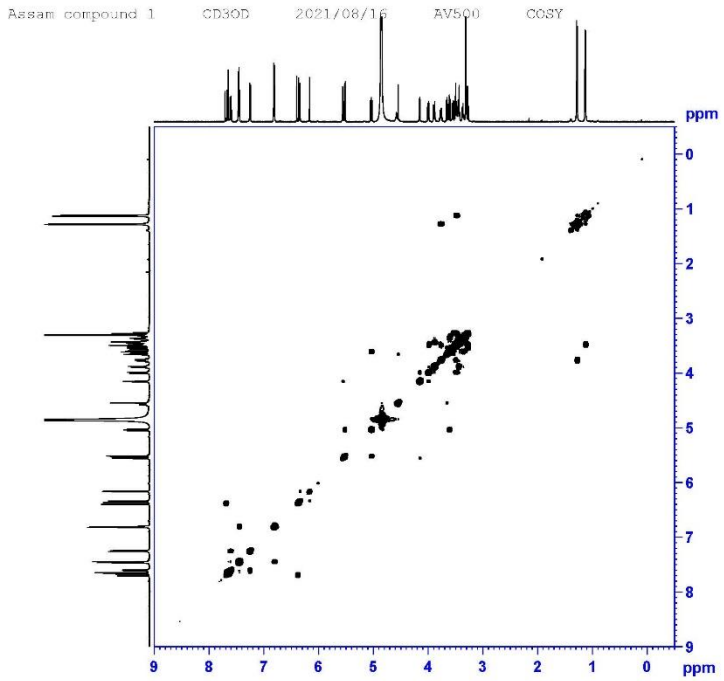


Figure S6. HSQC spectrum of **1**.

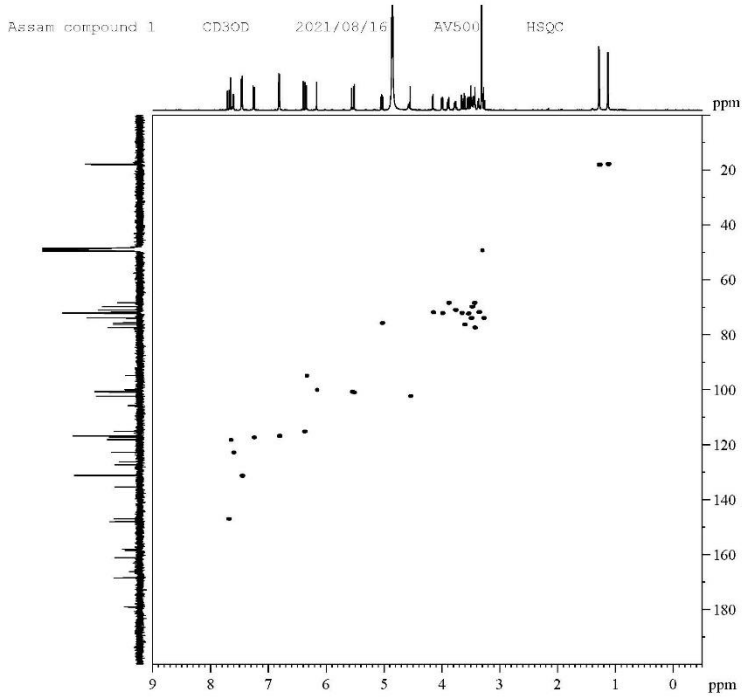


Figure S7. NOESY spectrum of **1**.

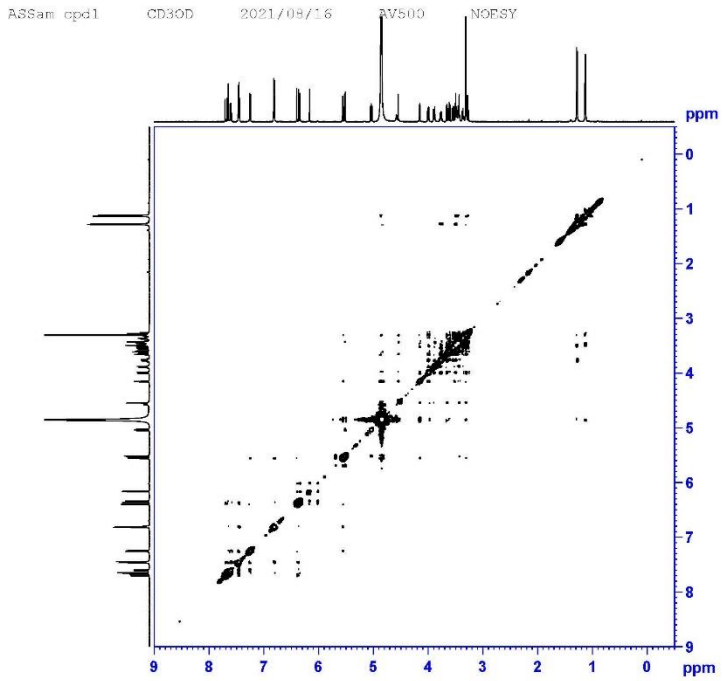
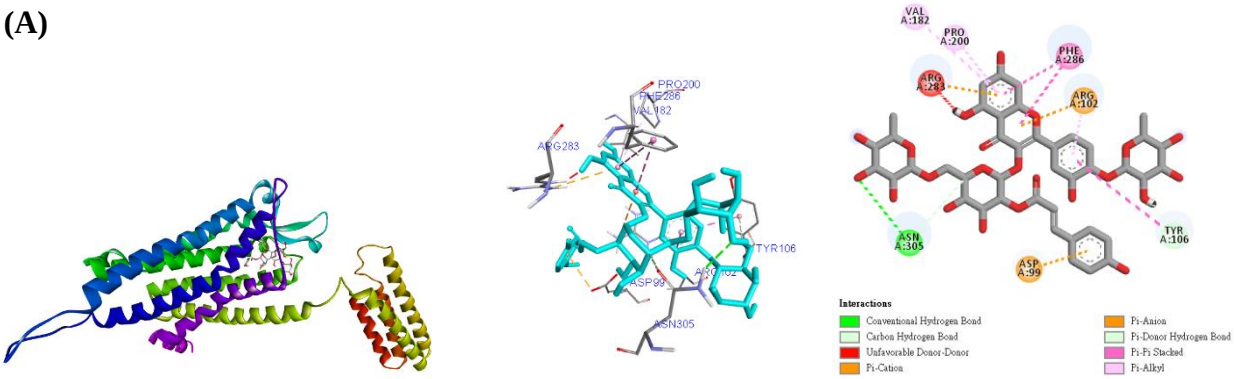
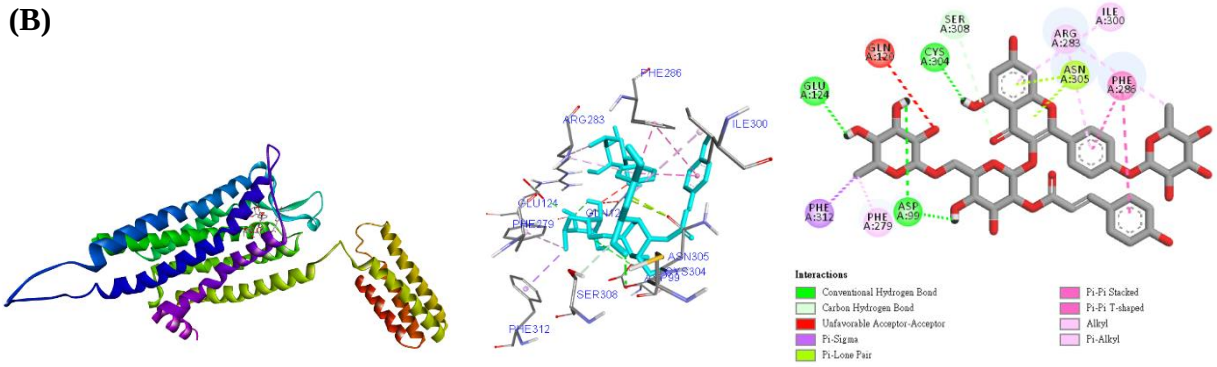


Figure S8. *In silico* modeling of (A) **1**, (B) **2**, and (C) **6** docking into the ghrelin receptor.

(A)



(B)



(C)