

# Proposed Mechanism for Emodin as Agent for Methicillin Resistant Staphylococcus Aureus: In Vitro Testing and In Silico Study

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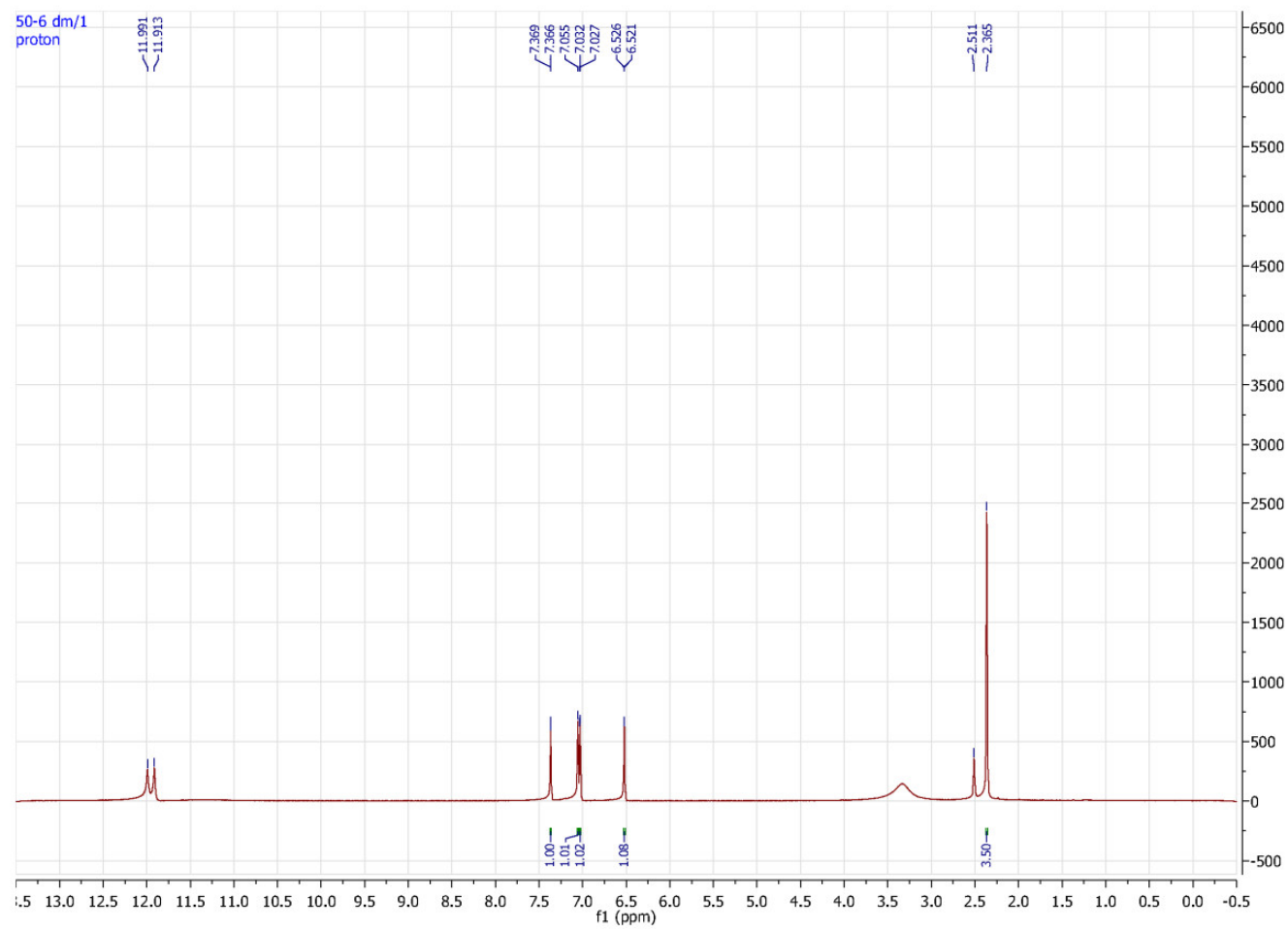
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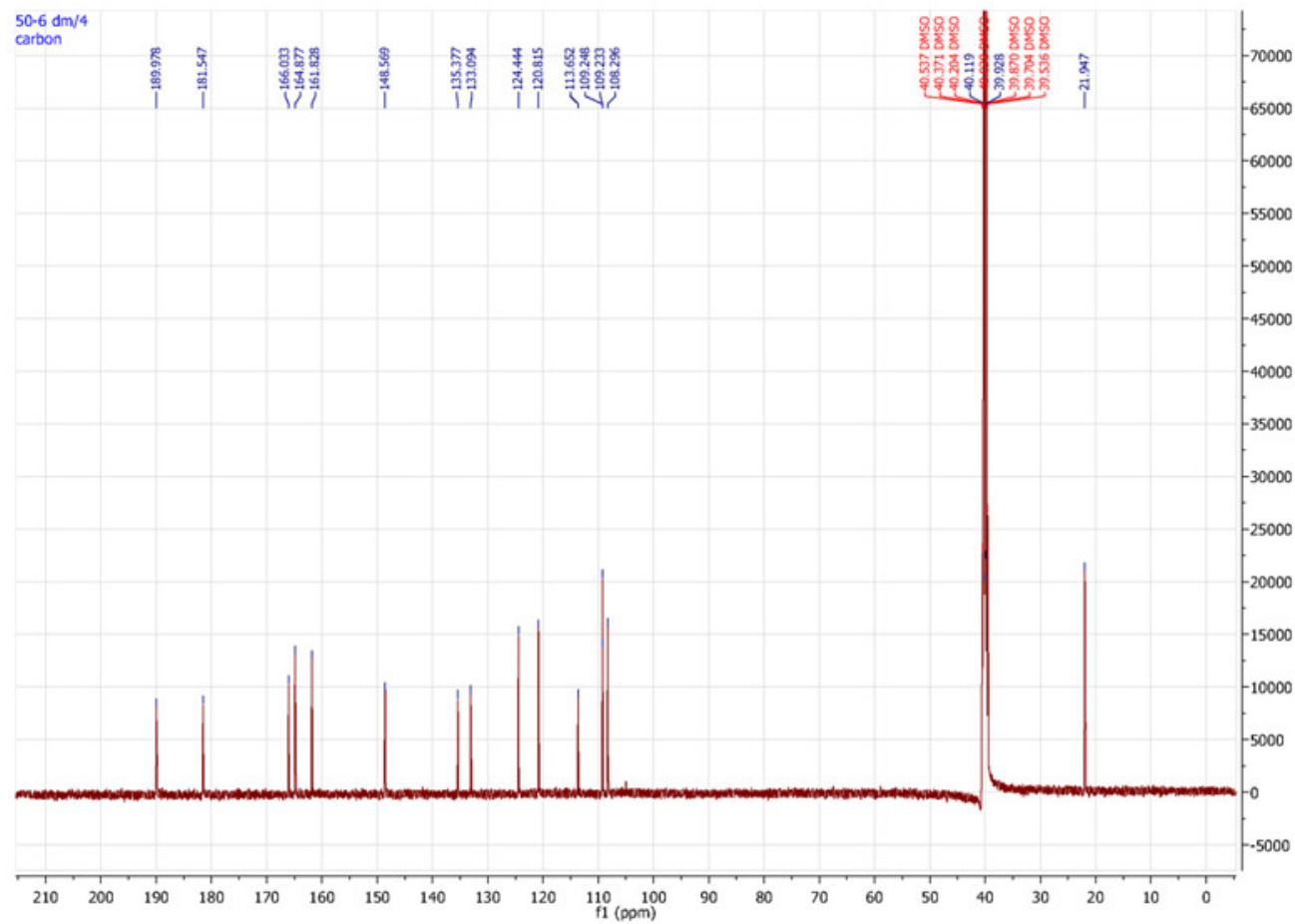
† These authors contributed equally to this work.

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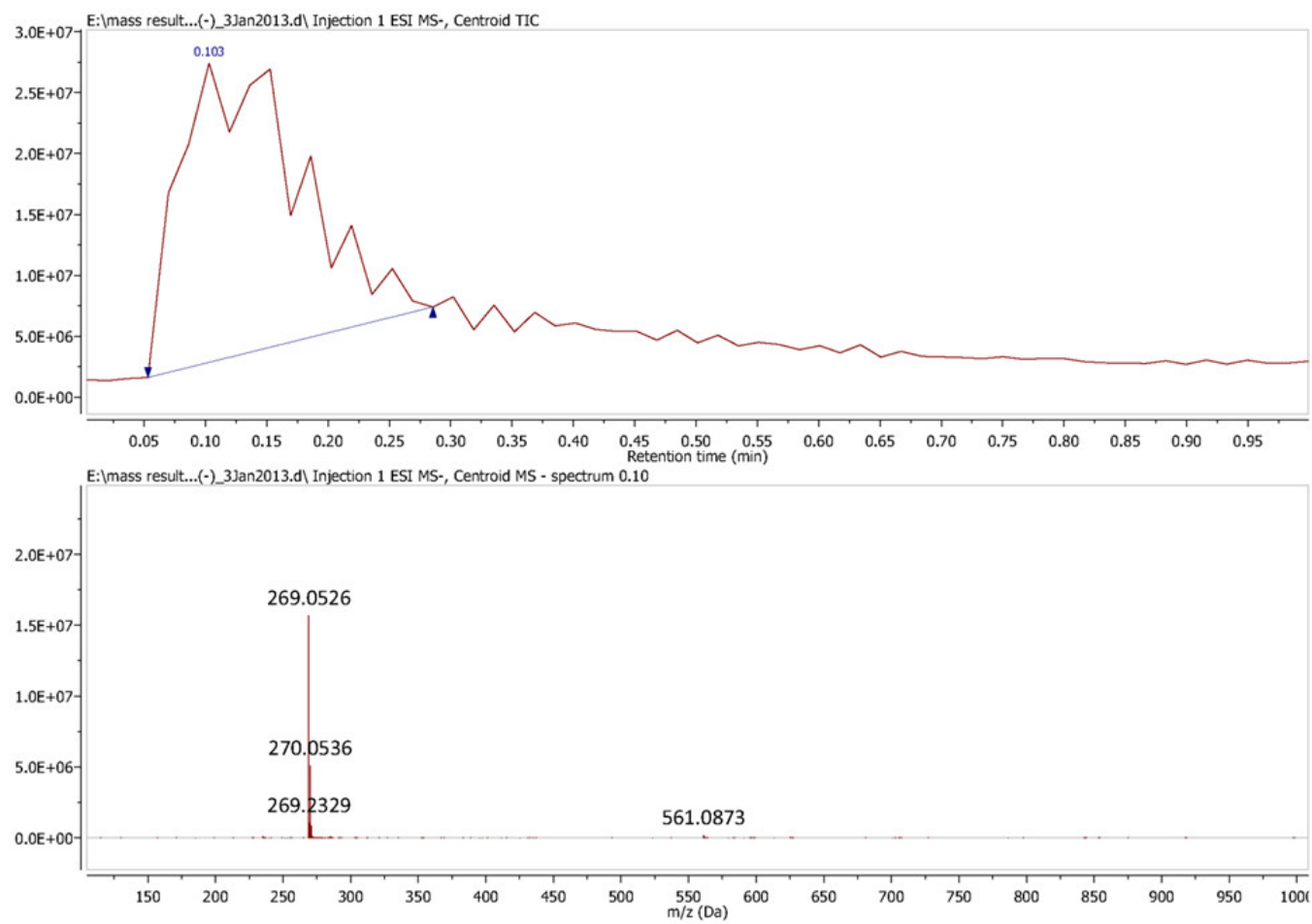
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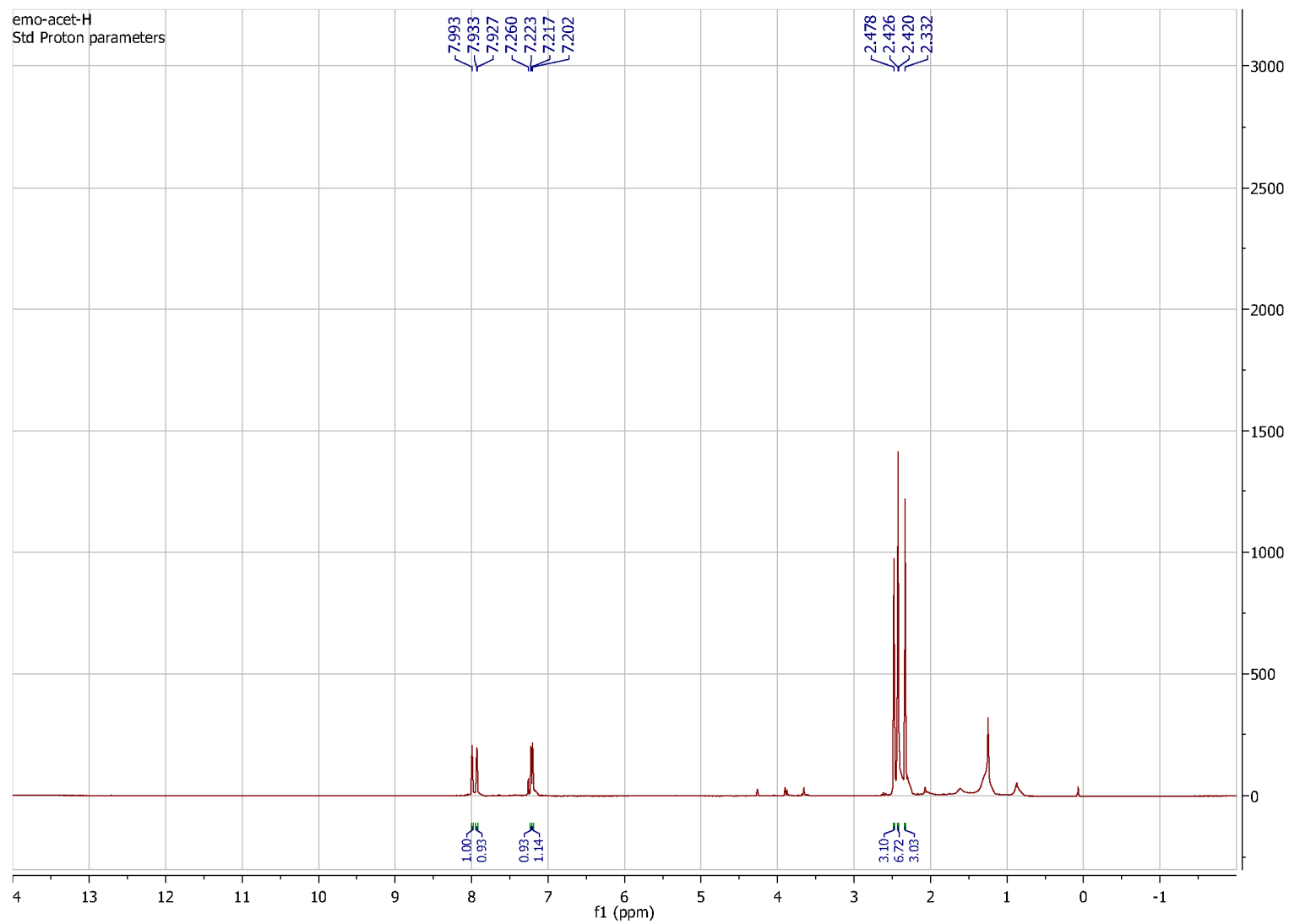
**Figure S1.**  $^1\text{H}$  NMR spectrum (400 MHz) for compound **1** in  $\text{DMSO-}d_6$ .



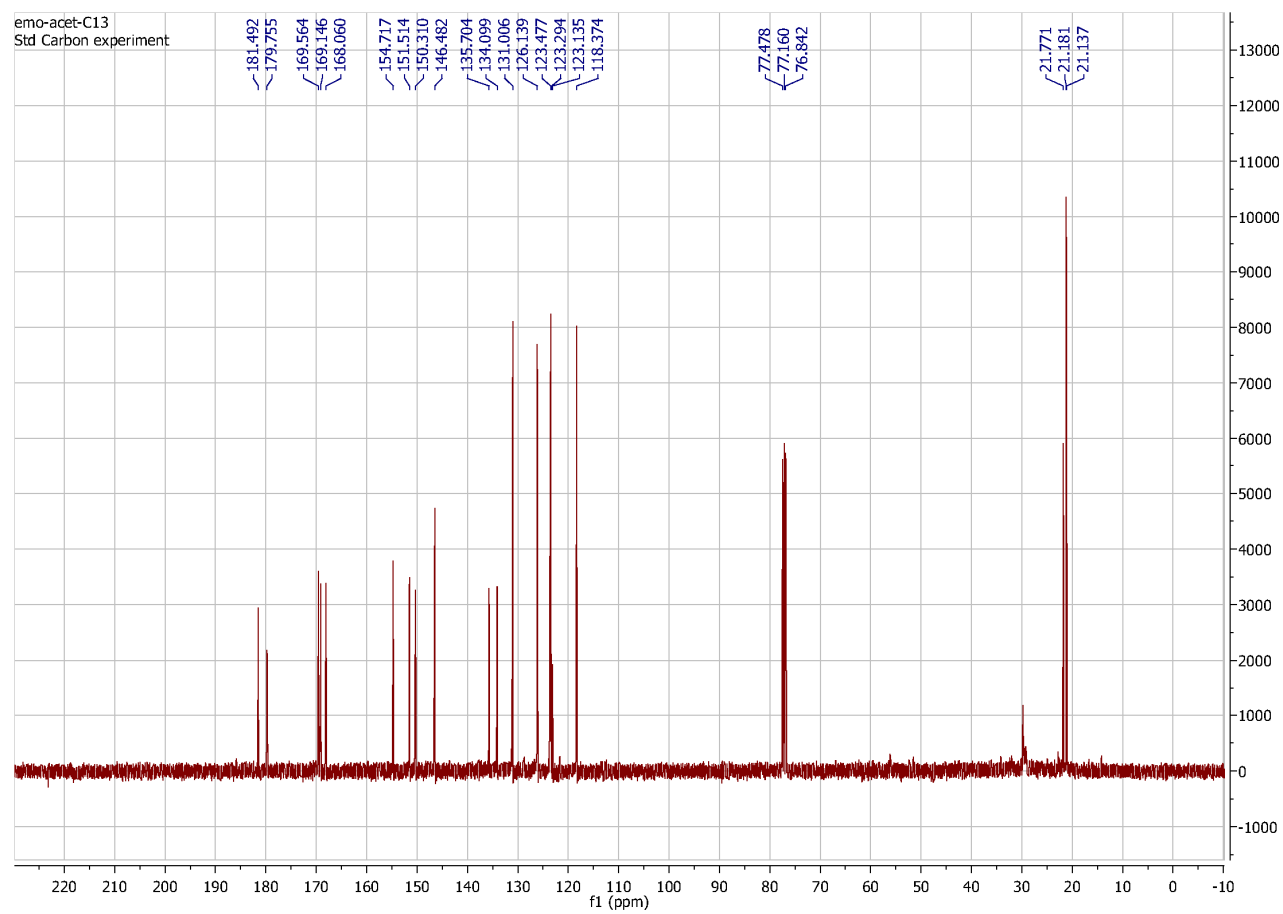
**Figure S2.**  $^{13}\text{C}$  NMR spectrum (400 MHz) for compound **1** in  $\text{DMSO-}d_6$



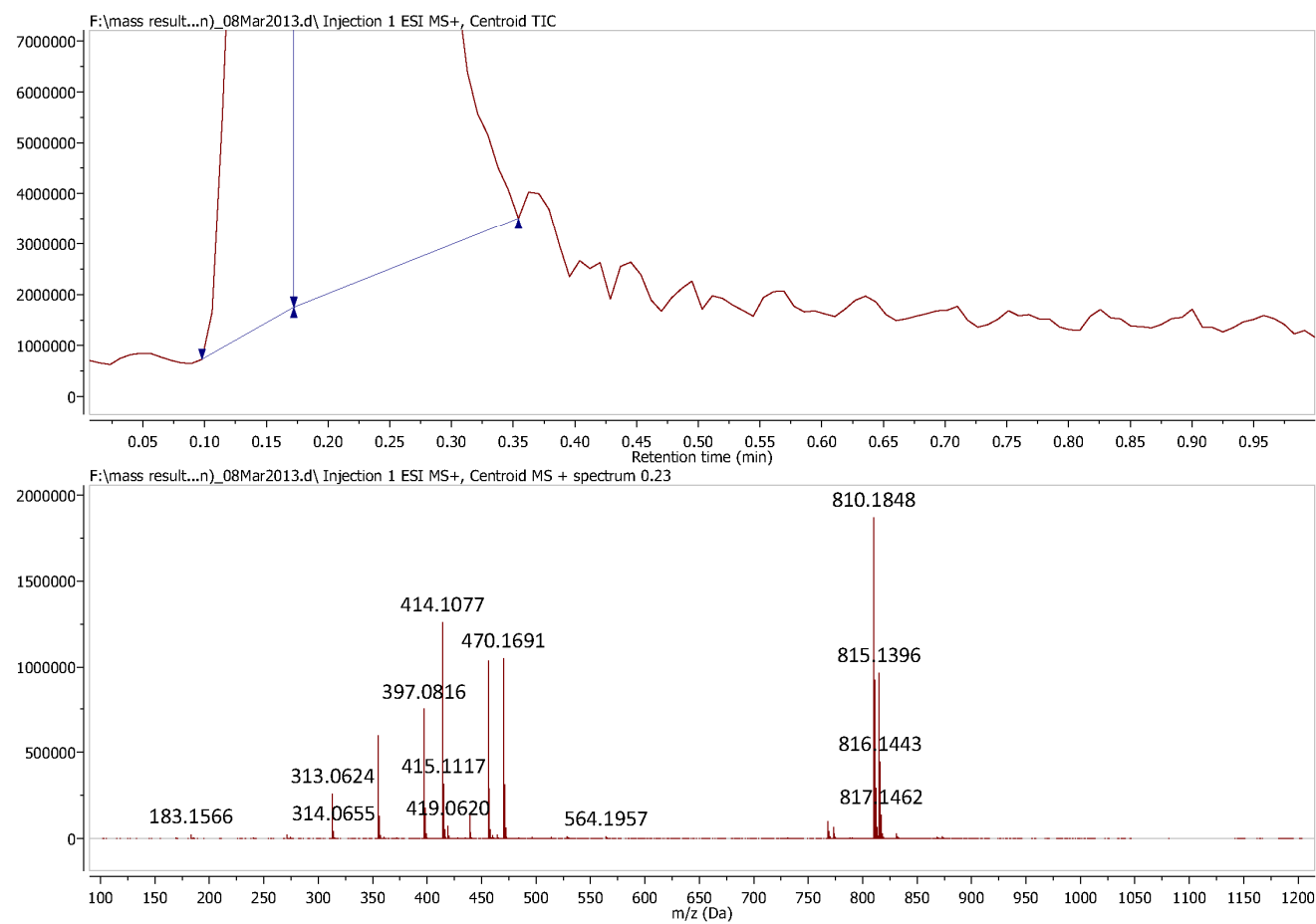
**Figure S3.** Negative ESI/MS spectrum for compound **1**



**Figure S4.**  $^1\text{H}$  NMR spectrum (400 MHz) for compound **2** in  $\text{CDCl}_3-d$ .

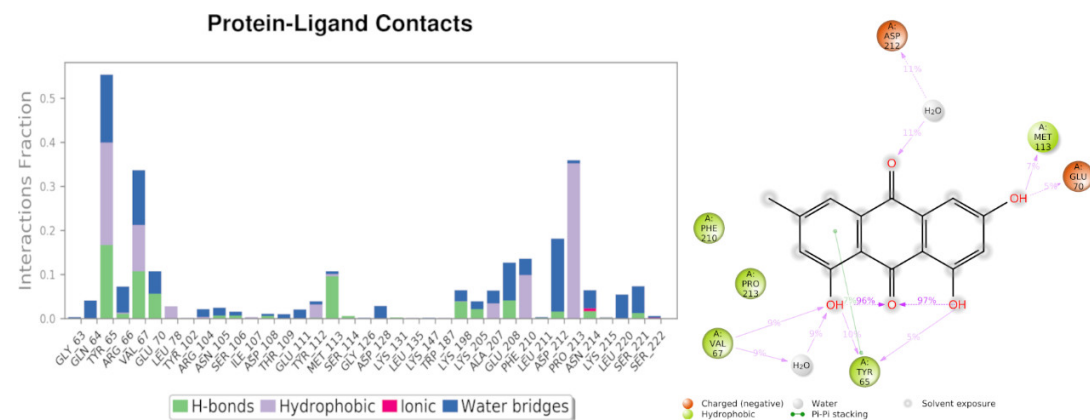


**Figure S5.**  $^{13}\text{C}$  NMR spectrum (400 MHz) for compound **2** in  $\text{CDCl}_3-d$

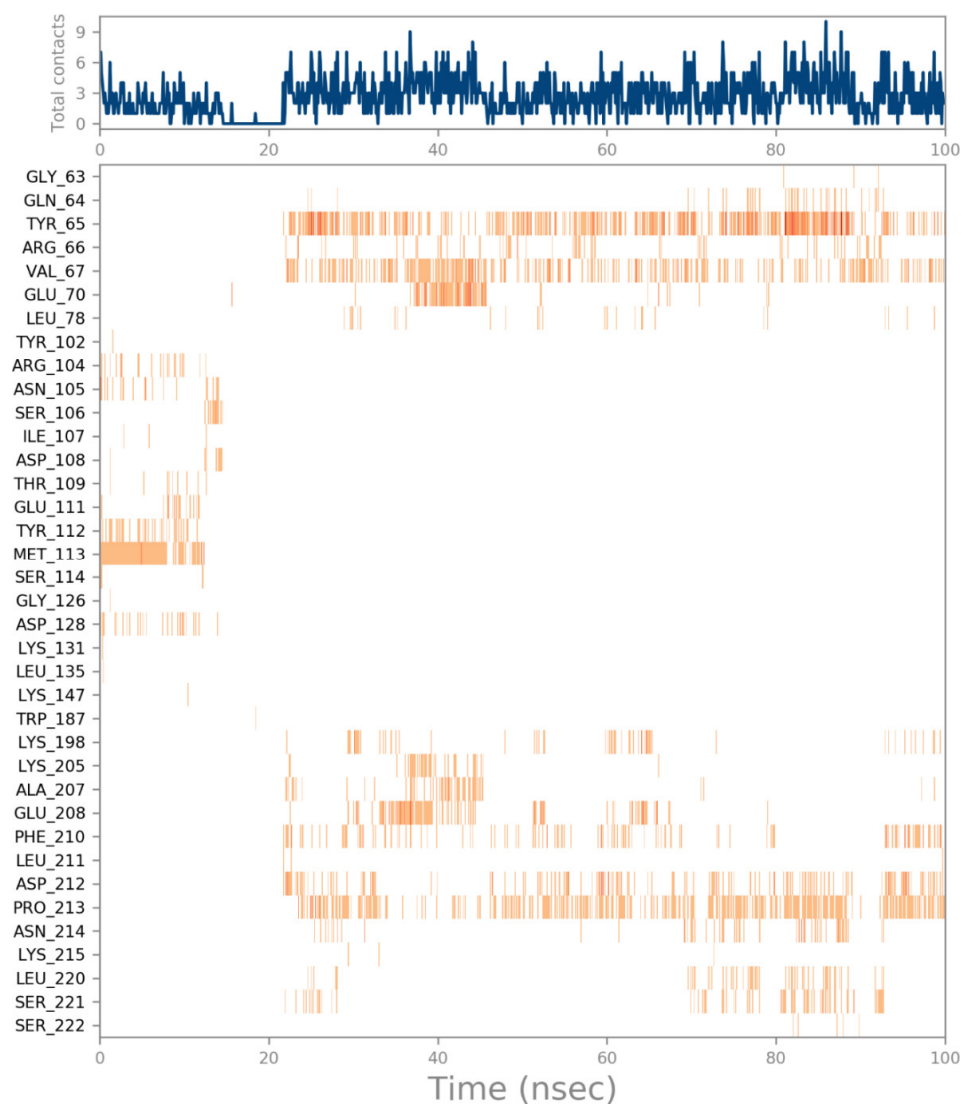


**Figure S6.** Positive ESI/MS spectrum for compound **2**

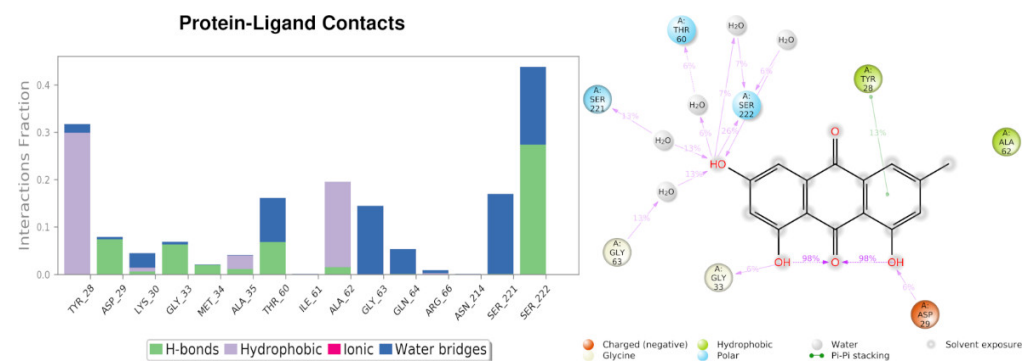




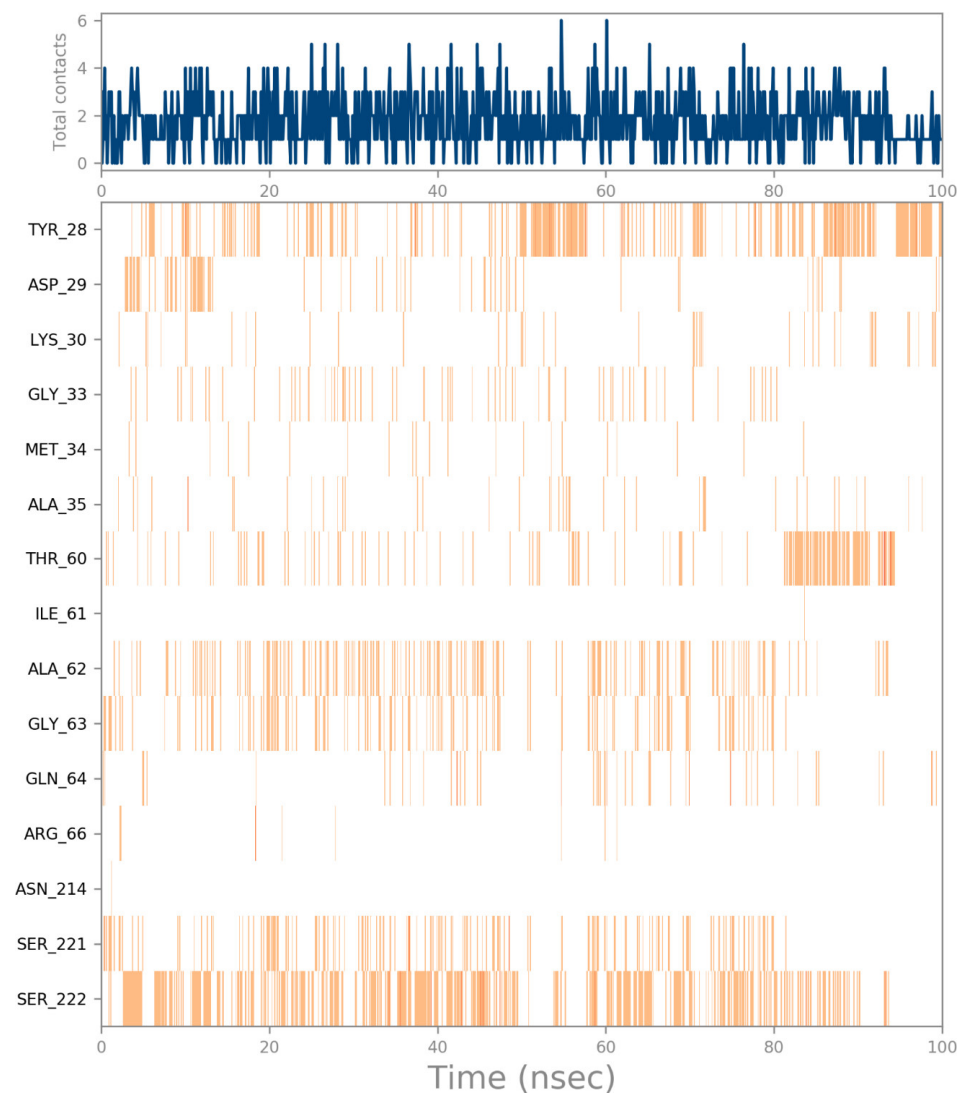
**Figure S7.** Emodin contacts with amino acids in site 2.



**Figure S8.** Average contacts of emodin in site 2.



**Figure S9.** Emodin contacts with amino acids in site 3.



**Figure S10.** Average contacts of emodin in site 3.