

Molecular Insights into the Potential Insecticidal Interaction of
β-Dihydroagarofuran Derivatives with the Subunit H of V-ATPase

Jielu Wei^{1,†}, Ding Li^{1,†}, Xin Xi¹, Lulu Liu¹, Ximei Zhao¹, Wenjun Wu², Jiwen
Zhang^{1,2,*}

1 College of Chemistry & Pharmacy, Northwest A&F University, Yangling, Shaanxi,
712100,
P. R. China

2 Key Laboratory of Botanical Pesticide R&D in Shaanxi Province, Yangling,
Shaanxi, 712100, P. R. China

*Corresponding author (Tel: +86-029-87092191; Fax: +86-029-87093987; E-mail:
nwzjw@nwsuaf.edu.cn)

† These authors contributed equally to this work.

Table of contents

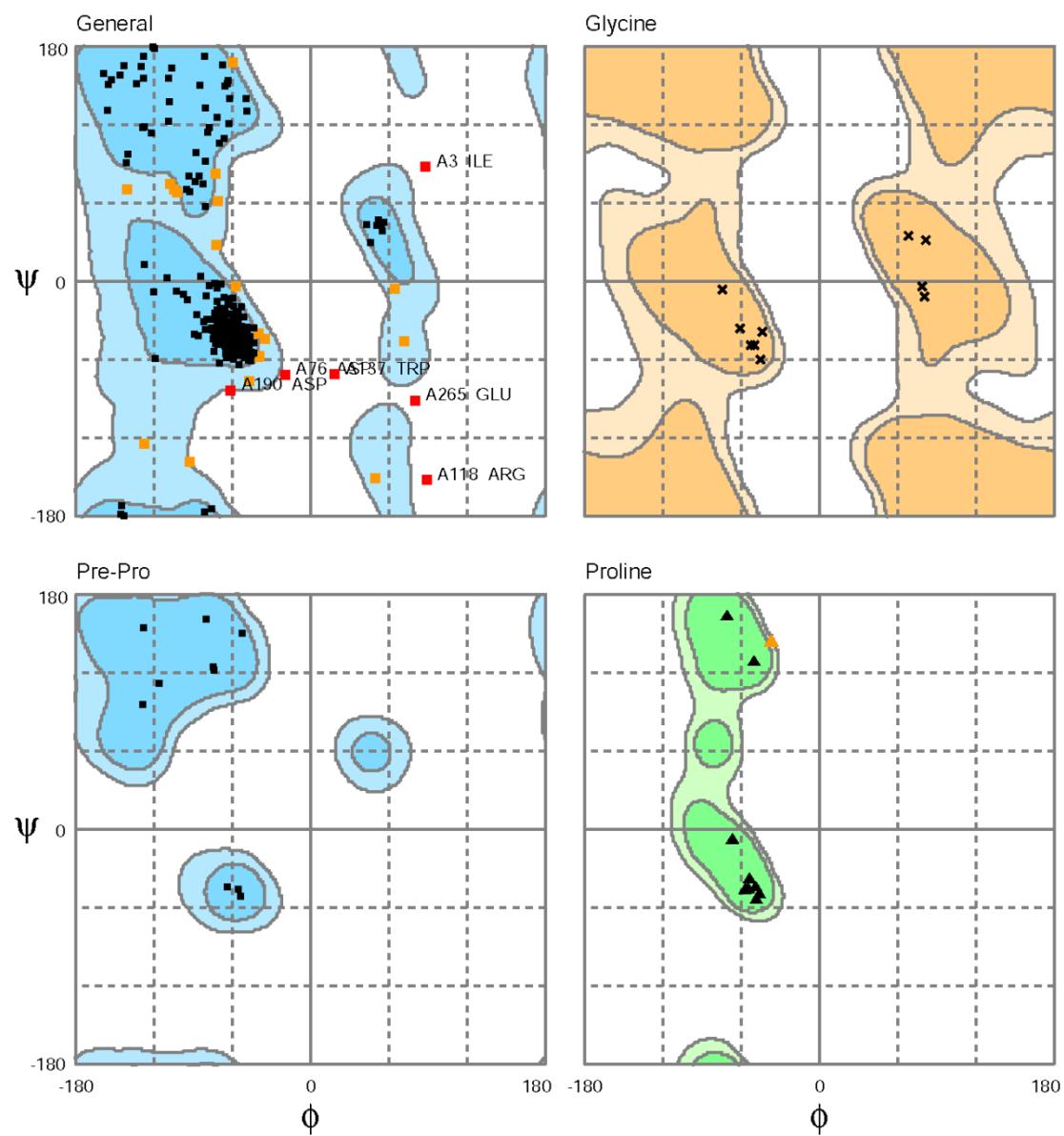
Figure S1	S1
Figure S2	S2

CLUSTAL 0(1.2.4) multiple sequence alignment

query	MANIGDGNVSQLMPPLGDEKIDMIAATSALQIRASEIRQENITWSSYLQSQMITQRDHDF
1ho8	<pre>-----GSMGATKILM--DSTHFNEIRSIIRSRSVAWDALARSEELSEIDAST :* ** * :: :: * * *...::*.: *: :: * .</pre>
query	IVNL-----DRGQHKDLPDKNP-----ELCAEVFLN---MLTHISKDNTIQYLLVMID
1ho8	<pre>AKALESILVKKNIGDG--LSSSNAHSGFKVNGKTLIPLIHLSTSDNEDCKSVQNLIA * : *: * ..* :: . .::: *: . ::: : : :*</pre>
query	DILSEDK---NRVKIFREGR-----TGNAWQPFLNLLNRQDEFVQHMT--ARI
1ho8	<pre>ELLSSDKYGDDTVKFFQEDPKQLEQLFDVSLKGDFQTVLISGFNVVSLLVQNGLHNVKLV ::**. ** : **: *: *. .*: ::. :* . **: . :::</pre>
query	AKLACWHTTVMERSDLLFYLSWLKDQLKLNNNEYVQSVARCLQM---MLRVDEYRFA---
1ho8	<pre>EK-----LLKNNNLINI-----LQNIEQMDTCYVCIRLLQELAVIPEYRDVIWL * :: . .: *: *: * * : : *::: : : *** .</pre>
query	-----FLT-----DGISTLLAILASRVNFQVQYQLTFCLWVLTFNPLLAEMNK
1ho8	<pre>HEKKFMPTLFKILQRATDSQLATRIVATNSNHLDIQLQYHSLLIWLLTFNPVFANELVQ :* : : : * . .: . *: **: : : *:*****: *: : :</pre>
query	FNAIPI--LADILSDSVKEKVTRIVLAVFRNLIEKPENQQVSKEHCIAMVQCKVLKQLSI
1ho8	<pre>KYLSDFLDLLKLVKITIKEKVSRLCISIILQCCSTRVKQHKKVI-KQLLLLGNALPTVQS : * . .: . :****: *: ::: : .. :*:. :: . * .</pre>
query	LEQKRSDDDEDIMNDVDFLNERLQTSVQDLSSFDQYATEVKSGRLEWSPVHKSAKFWRENA

1ho8	LSERKYSDEELRQDISNLKEILENEYQELTSFDEYVAELDSKLLCWSPPHVDNGFWSDNI *. ::: .**:: :*:. *;* *:.. *;*:****;*. ;*:. * * *** * . ** ;*
query	IRLNERGQELLRTLVLHLLEK-----SKDPVVLAVACYDVGEYVRHYPRGKHIIEQL
1ho8	DEFKKDNYKIFRQLIELLQAKVRNGDVNAKQEKKIIQVALNDITHVVELLPESIDVLDKT . ::: . ::::* *:.**: .::: ::: ** *: . *. *.. .:::
query	GGKQRVMHLLSHEDPNVRYEALLAVQKLMVHNWEYLGKQLEKEQIDKQAGTVVGAKA
1ho8	GGKADIMELLNHSDSRVKYEALKATQAIIGYTFK----- *** :*.**.*.*.:**** *.* :: .::

Figure S1. Multiple sequence alignment of the V-ATPase subunit H. from *M. separate* (query) and *yeast* (PDB:1ho8)



Number of residues in favoured region (~98.0% expected) : 403 (93.9%)
 Number of residues in allowed region (~2.0% expected) : 20 (4.7%)
 Number of residues in outlier region : 6 (1.4%)

Figure S2. Assessment of the Ramachandran plot of the model structure of the *M. separata* V-ATPase subunit H.