

1 **Supplementary Information**

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3 **Functional analysis of *CYP6ER1*, a P450 gene associated with imidacloprid resistance in *Nilaparvata lugens***

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5 **Author information**

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22 **Table S1. PCR primers used in this study.**

Primers name	Purpose	Primer sequence
6ER1-RNAi-F	ds <i>CYP6ER1</i> synthesis	5'-CCCCCTCTCACACCATCTGTT-3'
6ER1-RNAi-R	ds <i>CYP6ER1</i> synthesis	5'-CGACTCTTTGCTTTTTTCAATCTCC-3'
GFP-RNAi-F	ds <i>GFP</i> synthesis	5'-AAGGGCGAGGAGCTGTTCCACCG-3'
GFP-RNAi-R	ds <i>GFP</i> synthesis	5'-CAGCAGGACCATGTGATCGCGC-3'
ACTIN-F	RT-PCR (Actin)	5'-TGC GTGACATCAAGGAGAAGC-3'
ACTIN-R	RT-PCR (Actin)	5'- CCATACCCAAGAAGGAAGGCT-3'
6ER1-dsRNA-RT-F	RT-PCR (<i>CYP6ER1</i> in RNAi research)	5'-ATTCCGGTCTATGCGCTTC-3'
6ER1-dsRNA-RT-R	RT-PCR (<i>CYP6ER1</i> in RNAi research)	5'-TGGATTGGCGCTCTTACT-3'
6ER1-RT-F	RT-PCR (<i>CYP6ER1</i> , which was cloned in this research)	5'-TTCCGTTAGTGC GTTGGTTAC-3'
6ER1-RT-R	RT-PCR (<i>CYP6ER1</i> , which was cloned in this research)	5'-AATGGTTCTCCCACTGGATTT-3'

24 **Table S2. BLAST search and sequence alignment.**

Protocol		PSI-BLAST Search
Parameters	Target sequence	Cytochrome P450 <i>CYP6ER1</i>
	Database	PDB_nr95
	E-value Cutoff	10
	Maximum Hits	100
	Scoring Matrix	BLOSUM62
Result	PDB code	3NXU
	Identity	31%
	Sequence length	457
	Alignment length	480
	E-value	1.63273e-91
	Positive	52
	Resolution	2
	SCOP	a.104.1.1
	Ligand	HEM and RIT
	Description	Cytochrome P450 3A4

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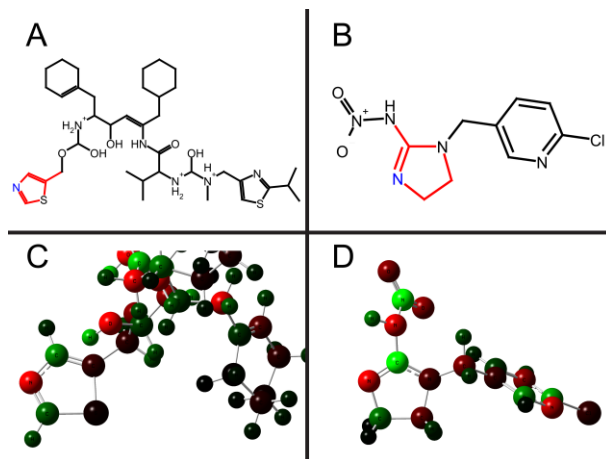
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30 **Table S3. Model scores from the homology modeling of *CYP6ER1*.**

Name	PDF Total Energy	PDF Physical Energy	DOPE Score
6ER1.M0011	4880.4561	1866.3110218	-52366.699219
6ER1.M0016	4991.5415	1956.281103	-52570.093750
6ER1.M0003	5013.8979	1924.61454914	-51440.234375
6ER1.M0009	5061.2505	2031.34542017241	-51891.925781
6ER1.M0014	5069.5327	1947.6158598	-52380.808594
6ER1.M0008	5095.7954	1914.9310658	-51684.746094
6ER1.M0005	5098.7485	1948.59656096	-51379.964844
6ER1.M0017	5154.1743	2079.17296940001	-51415.792969
6ER1.M0015	5168.4302	2012.83729205	-51804.324219
6ER1.M0001	5178.3896	1975.23588675	-51668.664063
6ER1.M0018	5230.6372	1987.3336503	-51077.031250
6ER1.M0007	5249.3813	2101.75486200001	-52651.351563
6ER1.M0019	5286.7007	2144.36547100024	-50818.742188
6ER1.M0006	5374.6938	2185.4297581	-51437.210938
6ER1.M0012	5381.5293	2126.134128	-51458.792969
6ER1.M0020	5406.6074	2088.49494070001	-51285.609375
6ER1.M0010	5543.0605	2130.575033245	-50681.925781
6ER1.M0002	5580.2217	2235.2910817	-51170.558594
6ER1.M0004	5736.0063	2166.807654	-50950.031250
6ER1.M0013	5754.1113	2080.516687	-51081.066406

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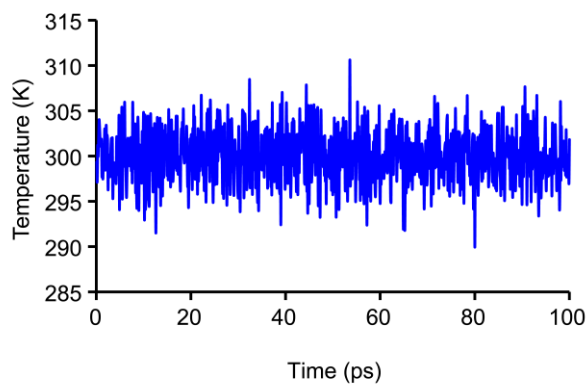
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35 **Figure S1. Molecular structure and approximate comparison of the ESP charge distribution**
 36 **of RIT (A, C) and IM4 (B, D).**

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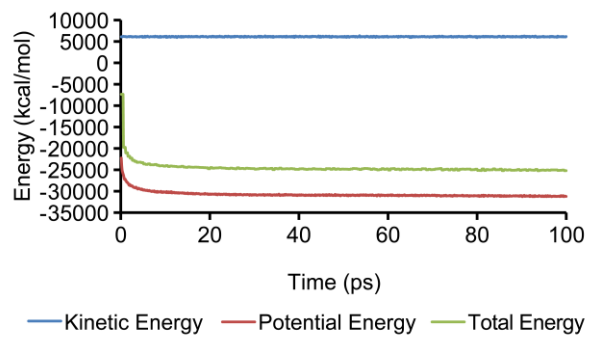
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40 **Figure S2. Temperature (K) fluctuation versus time (ps) during the 100 ps of MD simulation**
 41 **production**

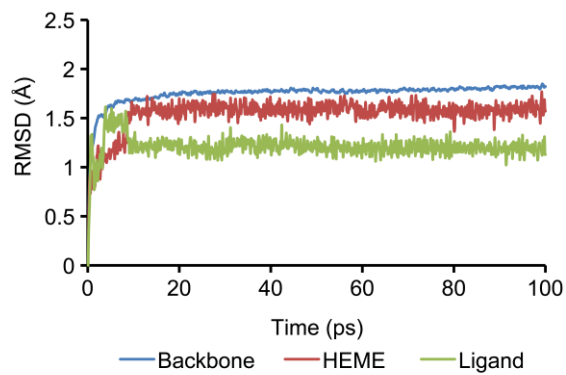
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44 **Figure S3. The total energy, kinetic energy and Molential energy (kcal/mol) fluctuations**
 45 **versus time (ps).**

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48 **Figure S4. RMSD of atomic coordination of protein backbone, HEME and ligand.**

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