

1 **Supplementary Materials:**2 **3D-QSAR and molecular docking studies on the *TcPMCA1*-mediated**  
3 **detoxification of scopoletin and coumarin derivatives**4 **Qiu-li Hou#, Jin-xiang Luo#, Bing-chuan Zhang, Gao-fei Jiang, Wei Ding, and Yong-qiang**  
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12 **Table S1. Primer sequences used in cloning and quantitative real-time PCR**

Experiments	Primer names and sequences (5' to 3')	Product length (bp)
Specific PCR	TcPMCA1-F: CGGGATCCCCTGCCCTTTGACATTTA	2000
	TcPMCA1-R: CCGCTCGAGCACGGACTTCATACCTCG	
5' RACE	TcPMCA1-F1: GTTTTAGGTGGTTTAGGAGGA	667
	TcPMCA1-F2: TCCTCTAAATCTTTGGGTGA	
3' RACE	TcPMCA1-R1: TCGAAACAGAGCCAAATTGGGAAGA	1355
	TcPMCA1-R2: AACTTGGCATCGAAGATCCCGTCC	
Full-length confirmation	TcPMCA1-1: CGGGATCCCCTGCCCTTTGACATTTA	2027
	TcPMCA1-2: CGCTCGAGCACGGACTTCATACCTCG	
	TcPMCA1-3: CGGGATCCCACGGACTTCATACCTCG	3056
	TcPMCA1-4: CCGCTCGAGCACCAAAGCCATTGTTCT	
	TcPMCA1-5: CGGGATCCCACGGACTTCATACCTCG	683
	TcPMCA1-6: CCGCTCGAGGCACCCAATAAAGCAAAT	
RT-qPCR	TcPMCA1-Q-F: GTTTGGCCTCGTTTACGTGT	201
	TcPMCA1-Q-R: TTCCTTGGCTACATCGGTTC	
<i>RPS18</i>	RPS18-F: ACGTGCTGGTGAACCTTACCGAAGA	99
	RPS18-R: TGCCTATTCAAGAACCAAAGTGGG	

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**Table S2.** Sequences and relevant information used in the phylogenetic analysis of plasma membrane Ca<sup>2+</sup>-ATPase (PMCA).

Organism	Accession number
<b>Ixodes</b>	
<i>Tetranychus urticae</i> PMCA1	tetur02g05600
<i>Tetranychus urticae</i> PMCA2	tetur09g02350
<i>Tetranychus urticae</i> SERCA1	tetur18g02100
<i>Ixodes scapularis</i> PMCA2	EEC15444.1
<i>Ixodes scapularis</i> E1-E2 ATPase	EEC11414.1
<b>Cnidaria (Outgroup)</b>	
<i>Stylophora pistillata</i>	AY360080
<b>Insect</b>	
<i>Aedes aegypti</i>	XP_001651107.1
<i>Anopheles gambiae</i>	XP_311357.4
<i>Apis mellifera</i> PMCA3	XP_003250350.1
<i>Acythosiphon pisum</i> PMCA1	XP_001945158.1
<i>Acythosiphon pisum</i> PMCA2	XP_001950494.1
<i>Camponotus floridanus</i>	EFN65040.1
<i>Culex quinquefasciatus</i>	XP_001847165.1
<i>Drosophila melanogaster</i>	NP_001033803.3
<i>Drosophila mojavensis</i>	XP_002011413.1
<i>Danaus plexippus</i>	EHJ74187.1
<i>Pediculus humanus corporis</i>	XP_002427234.1
<i>Tribolium castaneum</i>	XP_966434.1
<b>Chordate</b>	
<i>Branchiostoma floridae</i>	XP_002586028.1
<i>Ciona intestinalis</i>	XP_002126083.2
<i>Danio rerio</i> PMCA1	NP_001038222.1
<i>Danio rerio</i> PMCA2	NP_001116710.1
<i>Danio rerio</i> PMCA3	NP_001002472.1
<i>Danio rerio</i> PMCA4	EU559285.1
<i>Gallus gallus</i> PMCA1	NP_001161474.1
<i>Gallus gallus</i> PMCA2	XP_001231642.1
<i>Gallus gallus</i> PMCA4	XP_418055.2
<i>Homo sapiens</i> PMCA1	NP_001001323.1
<i>Homo sapiens</i> PMCA2	NP_001001331.1
<i>Homo sapiens</i> PMCA3	NP_068768.2
<i>Homo sapiens</i> PMCA4	NP_001001396.1
<i>Mus musculus</i> PMCA1	NP_080758.1
<i>Mus musculus</i> PMCA2	NP_033853.1
<i>Mus musculus</i> PMCA3	NP_796210.2
<i>Mus musculus</i> PMCA4	NP_998781.1
<i>Ornithorhynchus anatinus</i> PMCA1	XP_001512183.1
<i>Ornithorhynchus anatinus</i> PMCA3	XP_001510240.1
<i>Ornithorhynchus anatinus</i> PMCA4	XP_001518636.1
<i>Xenopus laevis</i> PMCA1	EU752492.1
<i>Xenopus laevis</i> PMCA2	NP_001087020.1
<i>Xenopus (Silurana) tropicalis</i> PMCA3	NP_001124515.1
<b>Nematoda</b>	
<i>Caenorhabditis briggsae</i> PMCA1	XP_002633689.1
<i>Caenorhabditis briggsae</i> PMCA2	XP_002634908.1
<i>Caenorhabditis briggsae</i> PMCA3	XP_002633968.1
<i>Caenorhabditis elegans</i> PMCA1	NP_741352.1
<i>Caenorhabditis elegans</i> PMCA2	NP_500161.1
<i>Caenorhabditis elegans</i> PMCA3	NP_501709.2

**Table S3.** Acaricidal activities of test compounds

Compo und	LC <sub>50</sub>				R	Compo und.	LC <sub>50</sub>				R
	(mg/L)		(mmol/L)				(mg/L)		(mmol/L)		
	LC <sub>50</sub>	SE(95% CL)	LC <sub>50</sub>	SE(95% CL)			LC <sub>50</sub>	SE(95% CL)	LC <sub>50</sub>	SE(95% CL)	
<b>1a</b>	0.4059	0.0493	1.2175	0.1479	0.9929	<b>16a</b>	1.3039	0.2671	6.0313	1.2355	0.9947
<b>2a</b>	0.3027	0.0234	0.8638	0.0668	0.9933	<b>17a</b>	1.2774	0.2075	5.188	0.8427	0.9612
<b>3a</b>	0.4788	0.0338	2.971	0.2097	0.9979	<b>18a</b>	1.4538	0.2574	5.3789	0.9523	0.9857
<b>4a</b>	0.6624	0.0696	3.52	0.3699	0.967	<b>19a</b>	1.2914	0.2317	6.2036	1.113	0.9958
<b>5b</b>	0.3975	0.0524	2.2563	0.2974	0.976	<b>20a</b>	2.2619	0.7932	12.6973	4.4527	0.8523
<b>6b</b>	9.9386	1.0688	61.2926	6.5914	0.9283	<b>21b</b>	0.6818	0.0878	3.8273	0.4929	0.9838
<b>7a</b>	5.7926	2.5973	22.784	10.2159	0.993	<b>22a</b>	3.2451	1.1658	20.0142	7.1901	0.955
<b>8a</b>	0.6344	0.1312	3.319	0.6864	0.8435	<b>23a</b>	2.0671	0.3547	14.1447	2.4271	0.9243
<b>9b</b>	1.398	0.3235	5.4987	1.2724	0.9775	<b>24a</b>	1.3959	0.313	4.876	1.0933	0.9932
<b>10b</b>	2.4756	0.5829	14.1318	3.3274	0.9903	<b>25a</b>	1.2512	0.155	5.0816	0.6295	0.9972
<b>11a</b>	5.9646	0.9378	33.8571	5.3233	0.9206	<b>26a</b>	2.473	0.7258	15.4398	4.5314	0.9922
<b>12b</b>	4.281	0.905	22.269	4.7077	0.9906	<b>27a</b>	0.4687	0.0504	1.9186	0.2063	0.9697
<b>13a</b>	0.2848	0.0302	1.3813	0.1465	0.9824	<b>28a</b>	3.2722	1.4539	15.1358	6.7251	0.9782
<b>14a</b>	4.7762	0.6985	25.6564	3.7521	0.9951	<b>29a</b>	0.7682	0.1033	3.8	0.511	0.9532
<b>15a</b>	1.2433	0.1278	6.4698	0.665	0.9618	<b>30a</b>	0.5732	0.0526	2.5798	0.2367	0.9139

**R:** Relative coefficient.

**a:** training compounds; **b:** test set compounds; the others same to **Table 2**.

1 ATGGAGGCCGCGCACTCCAAGAGCACAGGAATGTCTGGCCTATTTGGGGTGAGCGAGACCACAGGCCTACCCCGGACCAAGTGAAG  
1 M E A A H S K S T E E C L A Y F G V S E T T G L T P D Q V K

91 CGACATCTAGAGAAATACGGCCACAATGAGCTTCTGCTGAGGAAGGAAATCCCTGTGGGAGCTGGTGATAGAGCAGTTTGAAGACCTC  
31 R H L E K Y G H N E L P A E E G K S L W E L V I E Q F E D L

181 CTGGTGGGATTCTTCTGCTGGCCGCTGCATCTCCTTGTGCTGGCCTGGTTGAAGAAGGGGAAGAGACCATCACTGCCTTCGTTGAG  
61 L V R I L L L A A C I S F V L A W F E E G E E T I T A F V E

271 CCCTTTGTCATCCTCCTGATCCTCATTGCCAATGCCATCGTGGGAGTTTGGCAGGAGCGAACGCTGAGAACCCTATAGAGGCGCTGAAG  
91 P F V I L L I L I A N A I V G V W Q E R N A E N A I E A L K

361 GAATATGAGCCCGAGATGGGGAAGGTGTACCGGGCTGACCGCAAGTCAGTGCAAAGGATCAAGGCTCGGGACATCGTCCCGGGGACATC  
121 E Y E P E M G K V Y R A D R K S V Q R I K A R D I V P G D I

451 GTGGAGGTGGCGTTGGGGACAAAGTCCCTGCAGACATCCGCATCCTGTCTATCAAGTCCACCACCCTCCGCGTGGACCAGTCCATCCTG  
151 V E V A V G D K V P A D I R I L S I K S T T L R V D Q S I L

541 ACAGGCGAGTCTGTGCCGTCATCAAGCACACGGAGCCAGTCCCTGACCCGCGGGCTGTCAACCAGGACAAGAAGCATGCTTTTCTCG  
181 T G E S V S V I K H T E P V P D P R A V N Q D K K N M L F S

631 GGTACCAACATCGCGGCCGCAAGGCCCTGGGCATCGTGGCCACCACCGCGTGAGCACCGAGATCGGAAGATCCGTGACCAGATGGCC  
211 G T N I A A G K A L G I V A T T G V S T E I G K I R D Q M A

721 GCCACGGAGCAGGACAAGACGCGCTGCAGCAGAAGTGGATGAGTTCGGGGAGCAGCTGTCCAAGGTCATCCTCCTCATCGCGTGGCC  
241 A T E Q D K T P L Q Q K L D E F G E Q L S K V I S L I C V A

811 GTGTGGCTTATCAACATCGGCCACTTCAACGACCCCGTCCACGGGGCTCCTGGATCCGCGGTGCCATCTACTACTTCAAGATCGCCGTG  
271 V W L I N I G H F N D P V H G G S W I R G A I Y Y F K I A V

901 GCCTTGGCTGTGGCTGCGATCCAGAAGTCTTCCCGCTGTCATCACTACCTGCCTGGCCCTGGGACCCCGCGGATGGCAAGAAGAAC  
301 A L A V A A I P E G L P A V I T T C L A L G T R R M A K K N

991 GCCATCGTGAGGACCTGCCCTCTGTGGAGACCCTGGGCTGCACCTCTGTCATCTGCTCTGACAAGACTGGCACCCCTACCACCAACCAG  
331 A I V R S L P S V E T L G C T S V I C S D K T G T L T T N Q

1081 ATGTCTGTGTGCAAGATGTTTCATCATCGACAAGGTGGACGGAGACTTCTGTTGCTGAACGAGTTCTCCATACCGGCTCCACCTACGCT  
361 M S V C K M F I I D K V D G D F C S L N E F S I T G S T Y A

1171 CCAGAGGGGGAGTCTGAAGAATGATAAACCCATCCGGTCAGGGCAGTTTGATGGGCTGGTGGAGCTGGCCACCATTTGTGCCCTGTGC  
391 P E G E V L K N D K P I R S G Q F D G L V E L A T I C A L C

1261 AATGATTCTCCTTGGACTTCAATGAGACCAAAGCGTCTATGAGAAGGTGGGTGAGGCCACGGAGACGGCGCTCACCACCCTGGTGGAG  
421 N D S S L D F N E T K G V Y E K V G E A T E T A L T T L V E

1351 AAGATGAATGTGTTCAACACGGAAGTTCGGAACCTCTCGAAGGTGGAGAGACCAACGCCTGCAACTCGGTGATCCGCCAGCTCATGAAG  
451 K M N V F N T E V R N L S K V E R A N A C N S V I R Q L M K

1441 AAAGAGTTCACCCCTGGAGTCTCCCGAGACAGGAAGTCCATGTCTGTGTACTGTTCTCCAGCAAATCTCCCGCGCTGCTGTGGCAAC  
481 K E F T L E F S R D R K S M S V Y C S P A K S S R A A V G N

1531 AAGATGTTTGTCAAGGGCGCCCGAGGGGTTCATGACCCTGTAACACGTGCGAGTCGGCACCACCCGGTGCCCATGACTGGGCCG  
511 K M F V K G A P E G V I D R C N Y V R V G T T R V P M T G P

1621 GTGAAGGAGAAGATCCTCTCCGTGATCAAGGAGTGGGGACCCGGCCGGACACGCTGCGCTGCCTGGCCCTGGCCACCCGCGACACGCCG  
541 V K E K I L S V I K E W G T G R D T L R C L A L A T R D T P

1711 CCCAAGCGAGAGAAAATGGTGCTGGACGACTCCTCCCGTTCATGGAGTACGAGACGGACCTGACGTTTCGTGGGCGTCTGGGCATGCTG  
571 P K R E E M V L D D S S R F M E Y E T D L T F V G V V G M L

1801 GACCCGCCCCGCAAGGAGTTCATGGGCTCCATCCAGCTGTGCCGGGACCCGGGATCCGTGTCATCATGATCACCGGCACAACAAGGGC  
601 D P P R K E V M G S I Q L C R D A G I R V I M I T G D N K G

1891 ACGGCCATCGCCATCTGCCGCCATCGGCATCTTTGGGAGAACGAGGAGGTGGCAGACCCGCTACACCCGGCCGAGTTTGACGAC  
631 T A I A I C R R I G I F G E N E E V A D R A Y T G R E F D D

1981 CTGCCCTGGCCGAGCAGCGGGAAGCCTGCCGCCGCGCTGCTGCTCGCGCGGTGGAACCTCCACAAGTCCAAGATCGTGAATAC  
661 L P L A E Q R E A C R R A C C F A R V E P S H K S K I V E Y

2071 CTGCAGTCTACGATGAGATCAGGCCATGACAGGGGATGGCGTCAACGATGCCCTGCCCTGAAGAAGCCGAGATCGGCATAGCTATG  
691 L Q S Y D E I T A M T G D G V N D A P A L K K A E I G I A M

2161 GGATCTGGCACCCTGGCCAAGACAGCTGTGAGATGGTCTGGCGGACGACAACTTCTCCACCATCGTGCCCGCGTGGAGAGGGC  
721 G S G T A V A K T A S E M V L A D D N F S T I V A A V E E G

2251 CGGGCCATCTACAACAACATGAAGCAGTTCATCCGCTACCTCATCTCTCCAACGTGGCGAGGTGGTCTGCATCTTCTGACGGCCGCC  
751 R A I Y N N M K Q F I R Y L I S S N V G E V V C I F L T A A

2341 TTGGGGCTGCCCGAGGCCCTGATCCCCGTGACGTGCTGTGGGTGAACCTGGTGACGGACGGGCTCCCGGCCACAGCCCTGGGCTTCAAC  
781 L G L P E A L I P V Q L L W V N L V T D G L P A T A L G F N

2431 CCACCAGACCTGGACATCATGGACCGCCCCCGGAGTCCCAAGGAGCCCTGATCAGTGGTGGCTCTTCTCCGCTACATGGCCATC  
811 P P D L D I M D R P P R S P K E P L I S G W L F F R Y M A I

2521 GGGGGCTATGTTGGTGCAGCCACCGTGGGAGCCGCTGCCTGGTGGTTCATGTATGCGGAGGATGGGCCGGGTGTACCTACCACCAGCTG  
841 G G Y V G A A T V G A A A W W F M Y A E D G P G V T Y H Q L

2611 ACCCACTTCATGCAGTGCACCGAGGACCACCTCACTTTGAGGGTCTGGACTGTGAGATCTTTGAGGCCACAGCCCATGACCATGGCC

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871 T H F M Q C T E D H P H F E G L D C E I F E A P E P M T M A

2701 TTGTCTGTGCTGGTGACCATCGAGATGTGCAATGCTCTCAACAGCCTGTCCGAGAACCAGTCCTTGATGCGGATGCCGCCCTGGGTGAAC

901 L S V L V T I E M C N A L N S L S E N Q S L M R M P P W V N

2791 ATCTGGCTGCTGGGCTCCATCTGCCTGTCCATGTCCCTCCACTTCCTCATCCTCTACGTCGACCCCTGCCGATGATCTTCAAGCTCAAG

931 I W L L G S I C L S M S L H F L I L Y V D P L P M I F K L K

2881 GCCCTAGACCTCACCCAGTGGCTCATGGTCCTCAAGATCTCACTTCCAGTCATCGGGCTGGATGAAATACTCAAGTTCATTGCTCGGAAC

961 A L D L T Q W L M V L K I S L P V I G L D E I L K F I A R N

2971 TACCTGGAGGATCCAGAAGATGAAAGGAGGAAGTAA

991 Y L E D P E D E R R K \*

**Figure S1.** Nucleotide and amino acid sequence of the crystallographic structure of SERCA Ca<sup>2+</sup>-ATPase used as template for homology modeling (PDB ID code: 3BA6).