Supplementary Material

Support Vector Machine (SVM) Classification Model Based Rational Design of Novel Tetronic Acid Derivatives as Potent Insecticidal and Acaricidal Agents

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Table of Contents

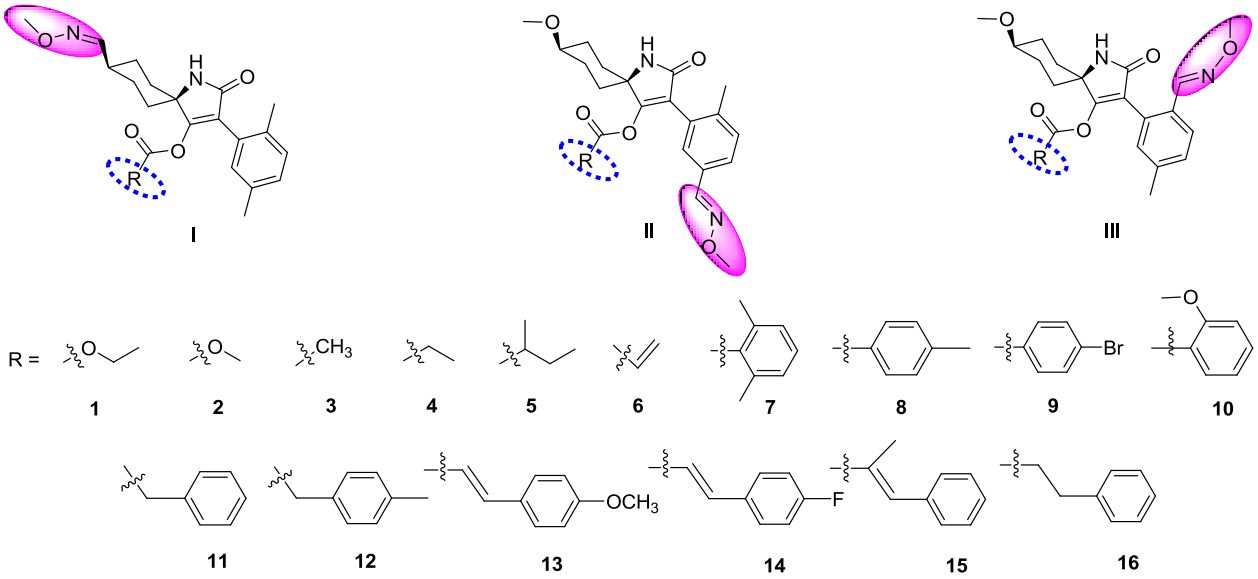

Fig. S1. The proposed tetronic acid derivatives by introduction of oxime ether moieties onto different site of spirotetramat for virtual evaluation.

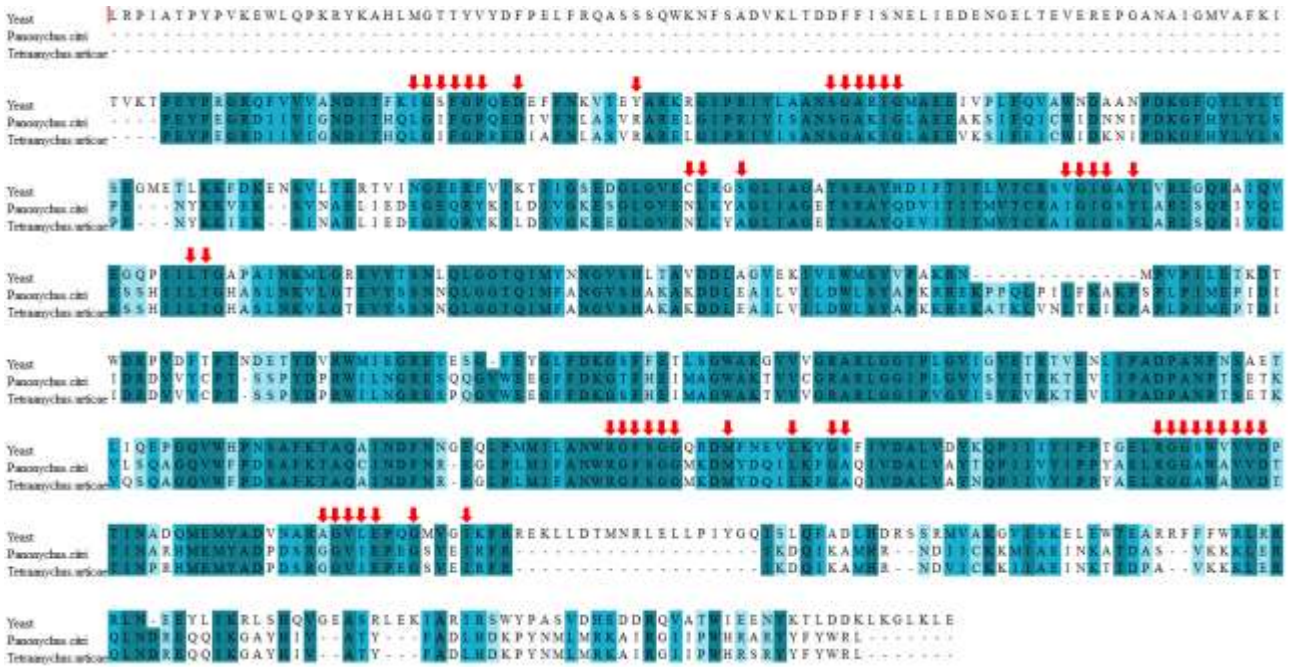

Fig. S2. Sequence alignment of the carboxyltransferase domain of ACCase (identity: 43.0% and 42.4%; similarity: 57.4% and 57.4%, respectively) between yeast and two insects (*Panonychus citri and Tetranychus urticae*). The amino acids in the binding site were highlighted by the red arrows (identity: 78.4% and 78.4%; similarity: 92.2% and 92.2%, respectively). Deep blue color shows conserved residue in all three sequences.

Table S1. The biological data of compounds **1-86** for SVM model development.

No.	Compd. (reference No.)	Concentrations (mg/L)	Mol. Weight	Inhibition percentage against *A. fabae* (%)
1	**Spirodiclofen** (13)	100	411.32	60
2	**Spiromesifen** (13)	100	370.49	62
3	**5a** (20)	100	286.37	22
4[b]	**5b** (20)	100	300.40	19
5[b]	**5l** (20)	100	402.49	72
6	**5c** (20)	100	404.55	26
7	**5d** (20)	100	463.40	46
8	**5e** (20)	100	496.95	35
9[b]	**5o** (20)	100	326.39	80
10	**5f** (20)	100	467.00	19
11	**5g** (20)	100	390.48	72
12	**5m** (20)	100	433.50	79
13[b]	**5s** (20)	100	356.46	100
14	**5q** (20)	100	328.41	85
15	**5r** (20)	100	342.44	94
16	**5t** (20)	100	370.49	87
17	**5u** (20)	100	384.52	93
18[b]	**8-I-b** (20)	100	417.51	73
19	**8-I-a** (20)	100	403.48	96
20	**8-I-c** (20)	100	431.53	76
21	**8-I-d** (20)	100	445.56	69
22	**8-I-f** (20)	100	421.47	94
23[b]	**8-I-e** (20)	100	433.50	92
24	**8-I-g** (20)	100	437.92	97
25	**8-I-i** (20)	100	437.92	90
26	**8-I-j** (20)	100	472.36	86
27	**8-I-k** (20)	100	472.36	97
28	**8-I-m** (20)	100	471.48	99
29	**8-I-n** (20)	100	448.48	92
30[b]	**8-II-b** (20)	100	445.56	99
31	**8-II-a** (20)	100	447.53	94
32	**8-II-c** (20)	100	473.61	62
33	**8-II-d** (20)	100	443.54	86
34	**8-II-f** (20)	100	493.60	25
35	**8-II-g** (20)	100	514.02	68
36[b]	**5n** (3)	100	453.96	35
37	**5b** (3)	100	419.52	79
38	**5e** (3)	300	496.04	26
39	**5f** (3)	100	419.52	96
40[b]	**5r** (3)	300	451.61	69
41	**5p** (3)	100	431.53	95
42	**5q** (3)	100	465.97	85

43	**5s** (3)	300	492.44	46
44	**5u** (3)	100	493.36	100
45[b]	**7d** (3)	100	564.46	27
46	**7a** (3)	100	523.63	40
47	**7c** (3)	300	579.74	36
48	**7e** (3)	300	531.56	39
49	**7f** (3)	300	483.65	51
50[b]	**7h** (3)	300	427.54	44
51	**7g** (3)	100	371.43	85
52	**7i** (3)	300	423.51	33
53	**7j** (3)	300	455.60	28
54	**7k** (3)	300	676.68	29
55[b]	**8** (3)	100	359.42	98
56	**Spirotetramat** (13)	100	373.45	100
57	**9b** (3)	300	457.57	62
58	**9c** (3)	300	519.64	10
59[b]	**4Ia** (26)	200	690.87	77
60	**4Ib** (26)	2	684.91	93
61	**4Ic** (26)	200	684.91	77
62[b]	**4Ig** (26)	200	654.84	74
63	**4Ie** (26)	200	866.73	73
64	**4Ii** (26)	200	708.86	57
65	**4Ij** (26)	200	720.90	75
66	**4Ik** (26)	200	720.90	69
67[b]	**4Il** (26)	200	704.90	56
68	**4Im** (26)	200	704.90	63
69	**6Ic** (26)	200	740.33	68
70[b]	**4IIm** (26)	1	849.07	100
71	**4IIa** (26)	10	835.04	100
72	**4IIb** (26)	2.5	829.08	100
73	**4IIn** (26)	1	892.10	100
74	**6IIb** (26)	10	864.09	100
75[b]	**4IIc** (26)	10	829.09	80
76	**5Ia** (26)	200	752.34	0
77[b]	**5Ib** (26)	200	747.93	6
78	**5Ic** (26)	200	717.90	7
79	**5Id** (26)	200	735.89	0
80[b]	**5Ie** (26)	200	774.95	7
81	**5IIa** (26)	200	880.06	9
82	**5IIb** (26)	200	892.10	9
83[b]	**5IIc** (26)	200	862.07	6
84	**5IId** (26)	200	880.06	11
85	**5IIe** (26)	200	919.12	16
86	**Ivemectin** (26)	2	875.11	100

Table S2. The most relevant molecular descriptors in the established SVM classification model and their corresponding definition.

Symbol	Class	Definition
ALOGP2	Molecular properties	Squared Ghose-Crippen octanol-water partition coeff. (logP^2)
PW3	Toplogical descriptors	Path/walk 3-Randic shape index
Lop	Toplogical descriptors	Lopping centric index
R6m	GETAWAY descriptors	R autocorrelation of lag6 /weighted by atomic masses
EEig02r	Edge adjacency indices	Eigenvalue 02 from edge adj.matrix weighted by resonance integrals
BELm6	Burden eigenvalues	Lowest eigenvalue n.6 of Burden matrix / weighted by atomic masses

Table S3. Correlation matrix of the selected molecular descriptors.

	ALOGP2	PW3	Lop	R6m	EEig02r	BELm6
ALOGP2	1.000000					
PW3	0.407019	1.000000				
Lop	-0.061773	-0.292785	1.000000			
R6m	0.123322	0.071002	-0.171371	1.000000		
EEig02r	0.470450	0.571521	0.100949	0.082104	1.000000	
BELm6	0.605989	0.583439	0.006698	-0.032633	0.773382	1.000000