QSAR study for antifungal activity of coumarin derivatives

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COMPUTER-AIDED MOLECULAR DESIGN

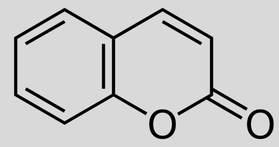
screening

optimization

design

new potent agents in plant protection

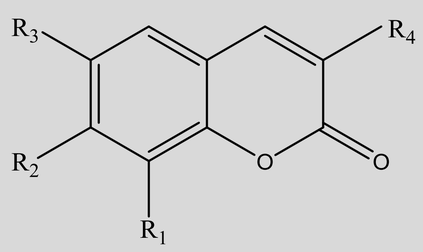
COUMARINS



biological activities

antifungal
antibacterial
nematocidal
antiviral
antioxidant

Synthesized of Coumarin Derivatives



antifungal evaluation
(*Macropomina phaseolina*, *Sclerotinia sclerotiorum*)

Quantitative **S**tructure **A**ctivity **R**elationship) QSAR

The artificial neural networks (ANN) analysis

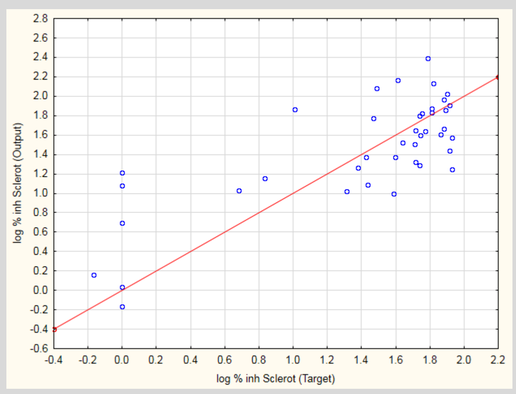
Mol. no.	log % inh Macrop.	log % inh Sclerot
1	1.729	1.864
2	1.761	1.598
3	1.729	1.812
4	1.752	1.891
5	1.806	1.884
6	1.822	1.917
7	1.818	1.924
8	1.822	1.928
9	1.872	1.928
10	1.858	1.812
11	1.725	1.715
12	1.844	1.774
13	1.394	1.83
14	1.748	1.914
15	1.778	1.884
16	1.79	1.641
17	1.79	1.59
18	1.778	1.436
19	1.844	1.738
20	1.818	0.68
21	1.847	1.641
22	1.904	1.743
23	1.922	0
24	1.872	1.738
25	1.878	1.789
26	1.881	1.903
27	1.888	1.821
28	1.829	1.426
29	1.829	1.468
30	1.854	0.98
31	1.847	1.743
32	1.833	1.488
33	1.829	1.71
34	1.84	1.59
35	1.814	1.312
36	1.822	1.754
37	1.875	1.613
38	1.861	1.379
39	1.851	0
40	1.84	-0.166
41	1.901	0
42	1.836	0.834
43	1.825	0
44	1.894	0
45	1.898	1.715
46	1.806	1.135
47	1.904	1.011

S. sclerotiorum
Used molecular descriptors:
3D-MoRSE (*Mor19v*); Moran autocorrelation (*MATS7v*); relative negative charge (*RNCG AM1*); and E-States, the sum of (- CH2 -) (*SssCH2*),

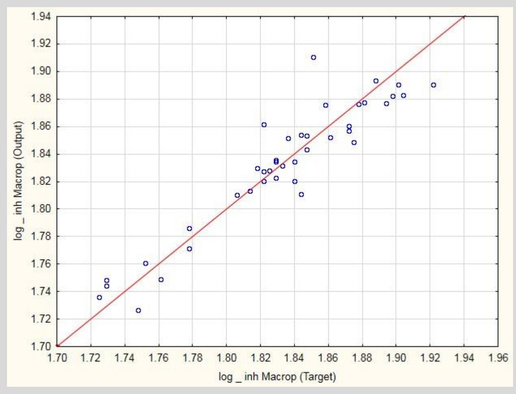
M. phaseolina
Used molecular descriptors:
geometrical symmetry (SYMM2); MATS4m; MATS5m; and sum of (= C<) (SdssC)

Results of ANN analysis

	Training perf.	Test perf.	Training error	Test error	Training algorithm	Error function	Hidden activation	Output activation
S. sclerotiorum	0.76	0.88	0.09	0.02	BFGS 37	SOS	Logistic	Exponential
M. phaseolina	0.94	0.92	0.00	0.00	BFGS 64	SOS	Tanh	Logistic



a)



b)

Graphs of observed against calculated values using ANN models for:
a) Sclerotinia sclerotiorum;
b) Macropomina phaseolina .

Conclusions:

- relationship between the structures of coumarine and antifungal activity is not linear
- ANN could be performed for further research of more effective coumarin agents against the pathogen fungi.

Literature:

Melita Lončarić, Martina Sušjenka, Maja Molnar, Current Organic Synthesis, 2020, 17, 98-108

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