

Electronic supplementary information (ESI)

## **Bioactivity-guided mixed synthesis and evaluation of $\alpha$ -alkenyl- $\gamma$ and $\delta$ -lactone derivatives as potential fungicidal agents**

### **Authorship:**

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Table 1 The difference between the experimental pIC<sub>50</sub> and predicted pIC<sub>50</sub>

No.	Compd.	Calc.pIC <sub>50</sub>	Exp.pIC <sub>50</sub>	Difference
1	2-1	-1.9479	-1.9775	0.0296
2	2-2	-1.7686	-1.8028	0.0342
3	2-3	-1.8142	-1.7002	-0.1140
4	2-4	-1.6175	-1.6664	0.0489
5	2-5	-1.7616	-1.7839	0.0223
6	2-6	-1.7348	-1.7674	0.0326
7	2-7	-1.6315	-1.7069	0.0754
8	2-8	-1.6456	-1.6929	0.0473
9	2-9	-1.5657	-1.5940	0.0283
10	2-10	-1.3724	-1.4522	0.0798
11	2-11	-2.0678	-2.1337	0.0659
12	2-12	-2.1999	-2.1053	-0.0946
13	2-13	-2.0557	-2.0323	-0.0234
14	2-14	-2.2269	-2.1622	-0.0647
15	2-15	-1.9646	-2.1412	0.1766
16	2-16	-2.0651	-2.1193	0.0543
17	2-17	-1.2719	-1.3354	0.0635
18	2-18	-1.7079	-1.7625	0.0546
19	2-19	-1.6878	-1.6003	-0.0875
20	2-20	-1.8744	-2.0286	0.1542
21	2-21	-1.5656	-1.6311	0.0655
22	2-22	-2.1516	-2.0557	-0.0959
23	2-23	-2.0414	-2.1632	0.1218
24	2-24	-2.0278	-2.1821	0.1543
25	2-25	-1.6990	-1.6205	-0.0785
26	2-26	-1.2919	-1.3246	0.0327
27	4-1	-2.0030	-2.0765	0.0735
28	4-2	-1.8180	-1.9144	0.0964
29	4-3	-1.9468	-1.8976	-0.0492
30	4-4	-1.7283	-1.8224	0.0941
31	4-5	-2.0024	-1.9221	-0.0803
32	4-6	-1.8319	-1.8947	0.0628
33	4-7	-1.7416	-1.8458	0.1042
34	4-8	-1.7251	-1.9022	0.1771
35	4-9	-1.9077	-1.8713	-0.0364
36	4-10	-1.7670	-1.8246	0.0576
37	4-11	-2.1249	-2.2186	0.0937
38	4-12	-2.0920	-2.1681	0.0761
39	4-13	-2.0899	-2.1148	0.0249
40	4-14	-2.2785	-2.2436	-0.0349
41	4-15	-2.3222	-2.2384	-0.0838

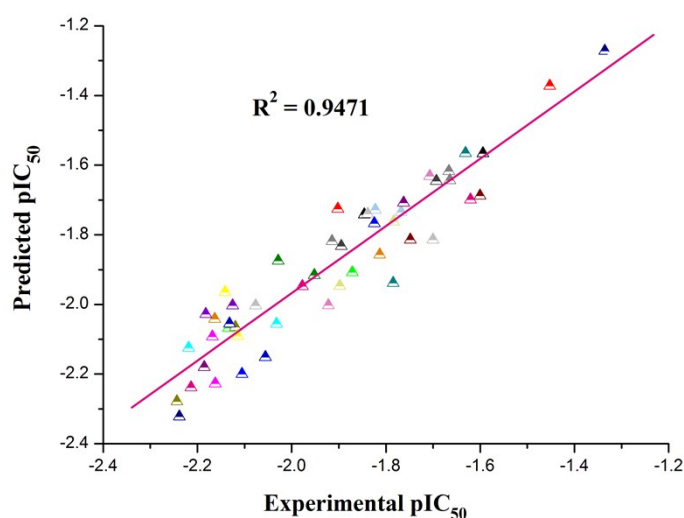
42	4-16	-2.1799	-2.1855	0.0056
43	4-17	-1.8136	-1.7482	-0.0654
44	4-18	-1.9157	-1.9521	0.0364
45	4-19	-1.9388	-1.7845	-0.1543
46	4-20	-2.0554	-2.1319	0.0765
47	4-21	-1.8564	-1.8132	-0.0432
48	4-22	-2.0028	-2.1253	0.1225
49	4-23	-2.2382	-2.2136	-0.0246
50	4-24	-2.1793	-2.2471	0.0678
51	4-25	-1.7391	-1.8385	0.0994
52	4-26	-1.6430	-1.6643	0.0213

Table 2 Fungicidal activity and structural descriptors of the title compounds

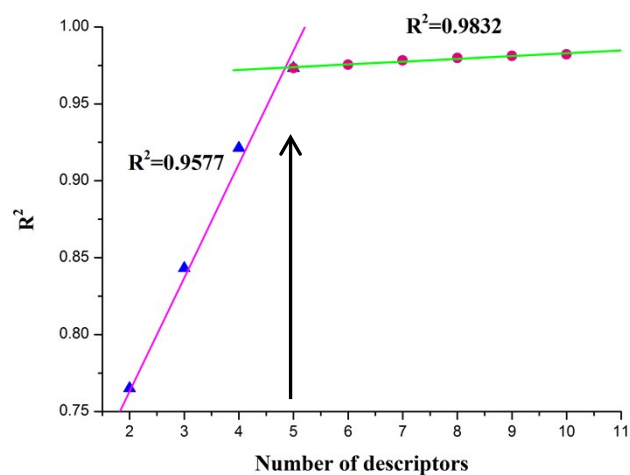
No.	Compd.	pIC <sub>50</sub>	Structural descriptors				
			$q_{\max}^O$ <sup>a</sup>	$n_o$ <sup>b</sup>	MAOEP <sup>c</sup>	$\mu_c$ <sup>d</sup>	$q_{\max}$ <sup>e</sup>
1	2-1	-1.9479	-0.2470	1.4348	1.9118	4.8340	0.3316
2	2-2	-1.7686	-0.2609	1.5652	1.9855	4.8610	0.2884
3	2-3	-1.8142	-0.2455	1.5652	1.9820	4.6130	0.3309
4	2-4	-1.6175	-0.2455	1.5652	1.9820	3.6000	0.3309
5	2-5	-1.7616	-0.2467	1.5652	1.9844	4.9890	0.3328
6	2-6	-1.7348	-0.2453	1.5652	1.9667	4.5830	0.3309
7	2-7	-1.6315	-0.2450	1.5652	1.9730	3.9350	0.3305
8	2-8	-1.6456	-0.2462	1.5652	1.9576	5.2870	0.3321
9	2-9	-1.5657	-0.2452	1.5652	1.9433	4.6340	0.3307
10	2-10	-1.3724	-0.2455	1.5652	1.9376	3.2410	0.3312
11	2-11	-2.0678	-0.2476	1.3846	1.9118	4.5690	0.3322
12	2-12	-2.1999	-0.2473	1.3846	1.9118	4.9560	0.3317
13	2-13	-2.0557	-0.2474	1.3846	1.9118	5.2420	0.3318
14	2-14	-2.2269	-0.2062	1.4444	1.9118	5.0240	0.3325
15	2-15	-1.9646	-0.2083	1.4444	1.9117	5.6670	0.3314
16	2-16	-2.0651	-0.2062	1.4444	1.9118	5.0240	0.3325
17	2-17	-1.2719	-0.2432	1.7308	1.9615	2.0340	0.4656
18	2-18	-1.7079	-0.2471	1.4483	1.9118	4.7400	0.3323
19	2-19	-1.6878	-0.2518	1.4444	1.9113	4.9390	0.3427
20	2-20	-1.8744	-0.2437	1.5417	1.9118	2.4280	0.3299
21	2-21	-1.5656	-0.2453	1.6957	1.9822	4.2240	0.3319
22	2-22	-2.1516	-0.1015	1.5500	1.9118	4.8100	0.3337
23	2-23	-2.0414	-0.2474	1.3448	1.9118	5.2710	0.3318
24	2-24	-2.0278	-0.2475	1.3125	1.9118	5.2800	0.3318
25	2-25	-1.6990	-0.2469	1.3448	1.9118	5.1390	0.3301
26	2-26	-1.2919	-0.2444	1.4483	1.9674	4.7630	0.3311
27	4-1	-2.0030	-0.2584	1.3846	1.9129	3.5750	0.3456
28	4-2	-1.8180	-0.2453	1.5000	1.9820	2.6530	0.3436

29	4-3	-1.9468	-0.2559	1.5000	1.9820	4.7240	0.3422
30	4-4	-1.7283	-0.2562	1.5000	1.9819	4.5660	0.3445
31	4-5	-2.0024	-0.2554	1.5000	1.9665	3.1570	0.3430
32	4-6	-1.8319	-0.2554	1.5000	1.9663	4.3290	0.3417
33	4-7	-1.7416	-0.2558	1.5000	1.9829	4.2620	0.3439
34	4-8	-1.7251	-0.2467	1.5000	1.9331	5.7840	0.3348
35	4-9	-1.9077	-0.2557	1.5000	1.9534	5.1480	0.3421
36	4-10	-1.7670	-0.2561	1.5000	1.9126	4.8890	0.3451
37	4-11	-2.1249	-0.2477	1.3448	1.9129	3.9210	0.3452
38	4-12	-2.0920	-0.2589	1.3448	1.9129	3.2820	0.3461
39	4-13	-2.0899	-0.2588	1.3448	1.9129	3.3720	0.3461
40	4-14	-2.2785	-0.2166	1.4000	1.9125	4.0690	0.3480
41	4-15	-2.3222	-0.2047	1.4000	1.9131	3.2420	0.3418
42	4-16	-2.1799	-0.2073	1.4000	1.9129	4.0620	0.3466
43	4-17	-1.8136	-0.2534	1.7308	1.9654	2.6543	0.3765
44	4-18	-1.9157	-0.2657	1.5203	1.9129	4.6754	0.3543
45	4-19	-1.9388	-0.2576	1.4062	1.9130	3.5030	0.3452
46	4-20	-2.0554	-0.2437	1.5417	1.9118	2.4280	0.3299
47	4-21	-1.8564	-0.2434	1.6154	1.9821	3.6590	0.3425
48	4-22	-2.0028	-0.1179	1.4783	1.9127	3.1270	0.3494
49	4-23	-2.2382	-0.2590	1.3125	1.9129	3.3040	0.3462
50	4-24	-2.1793	-0.2589	1.2857	1.9129	3.3660	0.3461
51	4-25	-1.7391	-0.2567	1.3333	1.9126	3.6630	0.3499
52	4-26	-1.6430	-0.2439	1.4242	1.9672	3.1860	0.3470

Note: <sup>a</sup> Max. net atomic charge for a O atom. <sup>b</sup> Number of occupied electronic levels of atoms. <sup>c</sup> Max. atomic orbital electronic population. <sup>d</sup> Total point-charge composition of the molecular dipole. <sup>e</sup> Max. net atomic charge.



**Fig. 1** Experimental pIC<sub>50</sub> vs. predicted pIC<sub>50</sub>.



**Fig. 2** The “breaking point” rule results  
**Table 3** Internal validation of the QSAR model <sup>a</sup>

Training set	<i>N</i>	<i>R</i> <sup>2</sup>	<i>F</i>	<i>S</i> <sup>2</sup>	Test set	<i>N</i>	<i>R</i> <sup>2</sup>	<i>F</i>	<i>S</i> <sup>2</sup>
A+B	34	0.954	65.79	0.0031	C	18	0.945	64.54	0.0026
B+C	35	0.932	64.34	0.0029	A	17	0.932	65.22	0.0031
A+C	35	0.945	65.54	0.0027	B	17	0.944	64.99	0.0032
Average		0.943	65.22	0.0029	Average		0.941	64.92	0.0030

Note: <sup>a</sup>Compds. A: 1, 4, 7, 10, 13, 16, 19, 22, 25, 28, 31, 34, 37, 40, 43, 46, 49, 52. Compds. B: 2, 5, 8, 11, 14, 17, 20, 23, 26, 29, 32, 35, 38, 41, 44, 47, 50. Compds. C: 3, 6, 9, 12, 15, 18, 21, 24, 27, 30, 33, 36, 39, 42, 45, 48, 51.