Supporting Information

Natural osthole-based ester derivatives as potential fungicidal agents: design, synthesis and quantitative structure-activity relationship (QSAR)

Authorship:

Authors: Yong-Ling Wu [1, 2, *], Yong Yan [1], Tin-Tin Pan [1, 2], Dou-dou Wang [1]

[1] College of Biology Pharmacy and Food Engineering, Shangluo University, Shangluo 726000, Shaanxi, China.

[2] Shaanxi Qinling Industrial Technology Research Institute of Special Biological Resources, Shangluo 726000, Shaanxi, China.

*Corresponding Author: Telephone +86-0914-2986016; fax +86-0914-2986016; E-Mail: wuyongling39@126.com

Supplementary content:

General Information:

1. The difference between the experimental pIC_{50} and predicted pIC_{50}

Table 1 The difference between the experimental pIC_{50} and predicted pIC_{50}

No.	Compd.	Calc.pIC_{50}	Exp.pIC_{50}	Difference
1	**Os1**	-2.1619	-2.0554	-0.1065
2	**Os2**	-1.9762	-1.9987	0.0225
3	**Os3**	-1.7493	-1.7177	-0.0316
4	**Os4**	-1.4263	-1.5250	0.0987
5	**Os5**	-1.1221	-1.1335	0.0114
6	**Os6**	-1.2717	-1.4099	0.1382
7	**Os7**	-0.9691	-1.0334	0.0643
8	**Os8**	-1.2774	-1.2989	0.0215
9	**Os9**	-1.3973	-1.4440	0.0467
10	**Os10**	-1.1532	-1.2355	0.0823
11	**Os11**	-1.1617	-1.1004	-0.0613
12	**Os12**	-1.3752	-1.2878	-0.0874
13	**Os13**	-1.1431	-1.0899	-0.0532
14	**Os14**	-0.9049	-0.9395	0.0346
15	**Os15**	-1.0461	-1.2227	0.1766
16	**Os16**	-1.2865	-1.3096	0.0231
17	**Os17**	-1.1746	-1.2380	0.0634
18	**Os18**	-1.4132	-1.3997	-0.0135
19	**Os19**	-1.5232	-1.4548	-0.0684
20	**Os20**	-1.2141	-1.3284	0.1143
21	**Os21**	-1.4372	-1.4639	0.0267
22	**Os22**	-1.6530	-1.5658	-0.0872
23	**Os23**	-1.3829	-1.4843	0.1014
24	**Os24**	-1.5617	-1.6599	0.0982
25	**Os25**	-1.6535	-1.7267	0.0732
26	**Os26**	-1.7498	-1.7033	-0.0465
27	**Os27**	-1.8575	-1.7752	-0.0823
28	**Os28**	-1.6617	-1.7882	0.1265
29	**Os29**	-1.7637	-1.7505	-0.0132
30	**Os30**	-1.7276	-1.8041	0.0765
31	**Os31**	-1.1116	-1.0492	-0.0624
32	**Os32**	-1.0984	-1.1987	0.1003

2. Fungicidal activity and structural descriptors of the title compounds

Table 2 Fungicidal activity and structural descriptors of the title compounds

No.	Compd.	pIC_{50}	Structural descriptors				
			Total charge [a]	q^{O}_{max} [b]	n_o [c]	q^{C}_{min} [d]	μ_h [e]
1	Os1	-2.1619	-0.1802	-0.1667	1.2054	0.6465	3.7439
2	Os2	-1.9762	-0.1819	-0.1709	1.2236	0.6309	3.9028
3	Os3	-1.7493	-0.1824	-0.1723	1.2287	0.6362	4.0650
4	Os4	-1.4263	-0.1855	-0.1742	1.2364	0.6385	4.3036
5	Os5	-1.1221	-0.2067	-0.1789	1.2478	0.5643	4.5799
6	Os6	-1.2717	-0.1953	-0.1735	1.2403	0.5951	4.4232
7	Os7	-0.9691	-0.2080	-0.1796	1.2553	0.5322	4.6781
8	Os8	-1.2774	-0.1962	-0.1757	1.2512	0.5587	4.4266
9	Os9	-1.3973	-0.2052	-0.1909	1.4846	0.4409	4.7386
10	Os10	-1.1532	-0.2155	-0.2109	1.5652	0.3309	5.0676
11	Os11	-1.1617	-0.2166	-0.2109	1.5652	0.3323	5.0679
12	Os12	-1.3752	-0.2158	-0.2109	1.5652	0.3328	4.9290
13	Os13	-1.1431	-0.2182	-0.2129	1.5637	0.3359	5.0931
14	Os14	-0.9049	-0.2188	-0.2131	1.5637	0.3365	5.2482
15	Os15	-1.0461	-0.2182	-0.2131	1.5637	0.3367	5.1559
16	Os16	-1.2865	-0.2141	-0.2109	1.5665	0.3389	4.9835
17	Os17	-1.1746	-0.2143	-0.2122	1.5665	0.3378	5.0592
18	Os18	-1.4132	-0.2141	-0.2122	1.5665	0.3371	4.9063
19	Os19	-1.5232	-0.2018	-0.2054	1.4682	0.4015	4.6430
20	Os20	-1.2141	-0.2022	-0.2062	1.4685	0.4033	4.8454
21	Os21	-1.4372	-0.2018	-0.2059	1.4682	0.4082	4.7032
22	Os22	-1.6530	-0.1865	-0.1629	1.3846	0.4365	4.2410
23	Os23	-1.3829	-0.1864	-0.1635	1.3842	0.4332	4.4117
24	Os24	-1.5617	-0.1864	-0.1626	1.3842	0.4301	4.2932
25	Os25	-1.6535	-0.1832	-0.1685	1.4412	0.4582	4.3467
26	Os26	-1.7498	-0.1835	-0.1687	1.4456	0.4563	4.2933
27	Os27	-1.8575	-0.1832	-0.1687	1.4467	0.4521	4.2228
28	Os28	-1.6617	-0.1753	-0.1534	1.3426	0.5602	4.1614
29	Os29	-1.7637	-0.1753	-0.1534	1.3467	0.5671	4.1070
30	Os30	-1.7276	-0.1753	-0.1534	1.3485	0.5684	4.1335
31	Os31	-1.1116	-0.2187	-0.2367	1.6252	0.3347	5.2906
32	Os32	-1.0984	-0.2101	-0.2319	1.6648	0.3392	5.3104

Note: [a] Total charge of the substituent groups on the osthole-based backbone structure. [b] Max. net atomic charge for an O atom. [c] Number of occupied electronic levels of atoms. [d] Minimum net atomic charge for a C atom. [e] Tot hybridization composite of the molecular dipole.