

Supplementary Information

Peel Diffusion and Antifungal Efficacy of Different Fungicides in Pear Fruit: Structure-Diffusion-Activity Relationships

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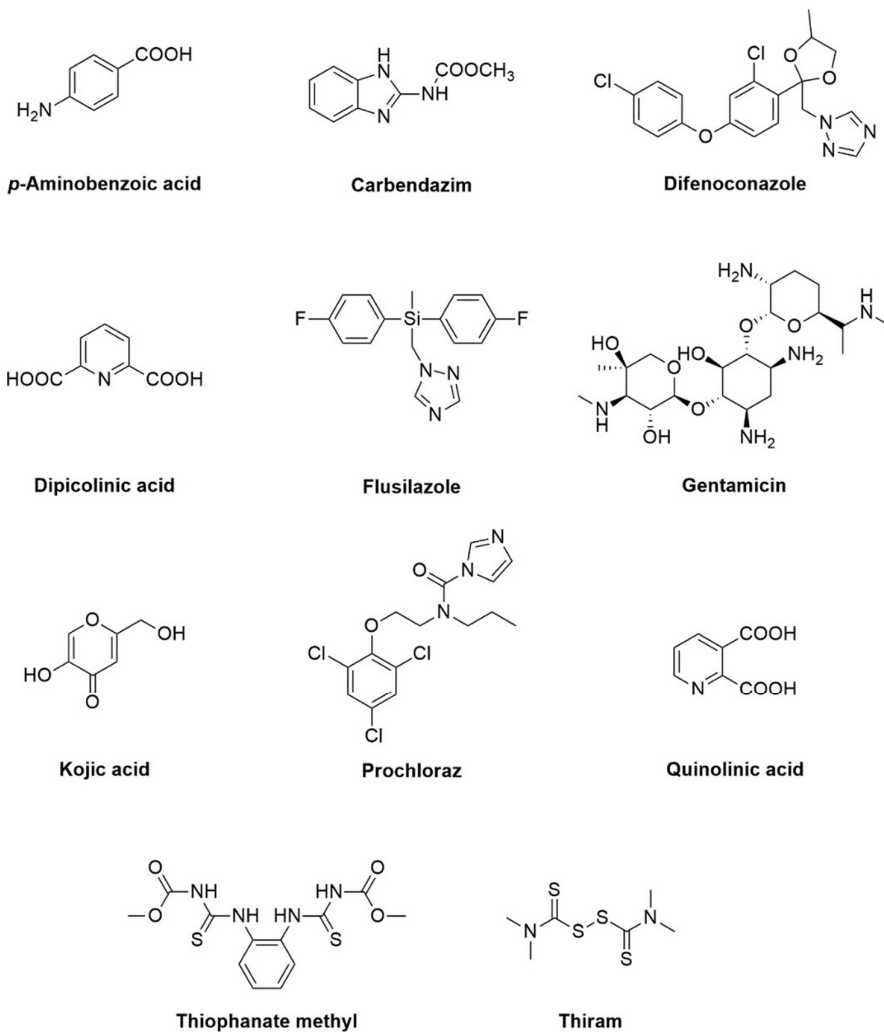


Figure S1. Structures of the studied fungicides.

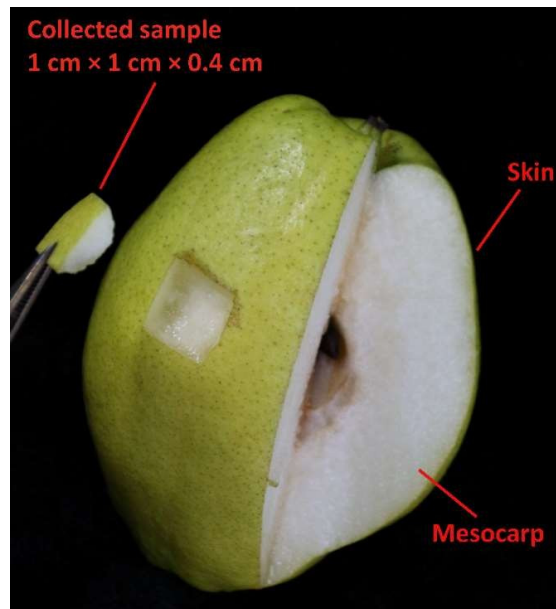


Figure S2. Extraction of samples from pears.

Table S1. DFT absolute energies (in a.u.) for the optimized structures calculated at the M062X(SMD)/6-311G(d,p) level.

Compound	Energy
<i>p</i> -Aminobenzoic acid	-476.12605
Carbendazim	-663.05413
Difenoconazole	-2044.41503
Dipicolinic acid	-625.38770
Flusilazole	-1272.05188
Gentamicin	-1586.97382
Kojic acid	-533.06635
Prochloraz	-2276.40178
Quinolinic acid	-625.38128
Thiophanate methyl	-1781.92663
Thiram	-1938.03024

Table S2. Cartesian coordinates (in a.u.) for all optimized structures (**A:** *p*-aminobenzoic acid; **B:** carbendazim; **C:** difenoconazole; **D:** dipicolinic acid; **E:** flusilazole; **F:** gentamicin; **G:** kojic acid; **H:** prochloraz; **I:** quinolinic acid; **J:** thiophanate methyl; and **K:** thiram).

A:

6	-2.107167	-0.036632	0.000043
6	-1.375504	-1.221596	0.000095
6	0.012703	-1.193388	0.000057
6	0.678874	0.030227	0.000005
6	-0.045564	1.221597	-0.000018
6	-1.430637	1.186021	-0.000015
1	-1.920784	-2.156943	0.000188
1	0.583467	-2.113041	0.000100
1	0.496173	2.159671	-0.000065
1	-2.001829	2.108264	-0.000065
6	2.162608	0.120445	-0.000025
8	2.787256	1.146535	0.000037
8	2.761423	-1.086064	-0.000072
1	3.712623	-0.919538	-0.000073
7	-3.541940	-0.128234	0.000066
1	-3.918743	0.348747	0.812838
1	-3.918643	0.346662	-0.813973

B:

6	4.187364	-0.312401	0.000047
6	3.170160	-1.253918	-0.000059
6	1.853097	-0.795586	-0.000058
6	1.596199	0.589404	0.000042
6	2.609246	1.540862	0.000144

6	3.912047	1.063763	0.000143
1	5.219015	-0.642724	0.000059
1	3.374311	-2.317109	-0.000123
1	2.394977	2.602364	0.000191
1	4.734255	1.768638	0.000228
1	-0.375625	1.511950	-0.000122
6	-0.253324	-0.586748	-0.000101
7	0.662418	-1.508560	-0.000099
7	0.215129	0.693180	0.000004
7	-1.608476	-0.880026	-0.000132
1	-1.845742	-1.861181	0.000903
6	-2.610316	0.049108	-0.000127
8	-2.451023	1.246480	-0.000443
8	-3.800183	-0.559540	0.000205
6	-4.924136	0.325121	0.000233
1	-4.908827	0.955649	-0.888510
1	-5.799191	-0.318220	0.000051
1	-4.909051	0.955324	0.889223

C:

6	6.194014	-0.623604	0.163517
6	6.177070	0.560583	-0.559212
6	5.059236	1.383040	-0.494916
6	3.981056	1.016080	0.297833
6	4.005182	-0.166076	1.030675
6	5.117117	-0.993201	0.959288
1	7.027946	0.832116	-1.170238
1	5.013113	2.312478	-1.047810
1	3.159524	-0.435172	1.652036

1	5.153496	-1.916719	1.522103
17	7.590613	-1.663353	0.073321
8	2.922927	1.894153	0.381523
6	1.644827	1.410878	0.285406
6	1.317706	0.329294	-0.524806
6	0.657506	2.084429	0.991925
6	-0.006741	-0.078541	-0.609223
1	2.080358	-0.192883	-1.087886
6	-0.658823	1.664462	0.882717
1	0.936563	2.927270	1.610803
6	-1.026033	0.577949	0.086979
1	-1.438020	2.180572	1.427616
17	-0.333665	-1.446238	-1.642244
6	-2.491088	0.140559	0.027900
6	-4.142805	1.726718	-0.369560
6	-3.480998	1.253471	-1.659382
1	-5.141863	1.285582	-0.276388
1	-4.176519	1.100259	-2.481894
1	-2.678836	1.938409	-1.965037
6	-2.713299	-1.176498	0.780505
1	-2.146850	-1.983537	0.320851
1	-2.394889	-1.040323	1.815412
6	-5.142957	-1.020571	1.426360
7	-4.564129	-2.465336	-0.131228
1	-5.010262	-0.255562	2.175465
6	-5.862150	-2.439779	0.080294
1	-6.537186	-3.078077	-0.467513
7	-6.274431	-1.562214	1.034554
7	-4.107727	-1.551035	0.745323

6	-4.187140	3.226329	-0.180751
1	-4.817740	3.684948	-0.945739
1	-4.599443	3.476818	0.797206
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8	-2.949706	-0.004575	-1.286911

D:

6	1.194091	1.544409	-0.000020
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6	-1.194071	1.544429	0.000044
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6	1.134777	0.150483	-0.000049
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1	0.000025	3.333581	0.000031
1	-2.152604	2.044415	0.000069
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8	2.432259	-1.870734	0.000086
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1	4.254310	-0.498005	0.000046

E:

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1	0.127942	-1.655499	-1.715153
6	-2.077801	-0.367195	0.192083
6	-2.769369	0.608700	0.924610
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6	-4.128205	-0.806542	-1.048176
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6	1.050027	3.087383	-0.528909
1	-0.791204	2.006739	-0.604867
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7	3.959057	-1.859694	-0.939234

F:

6	-3.851123	0.643976	-0.222525
6	-2.782228	-0.325537	0.287057
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6	1.626115	0.367349	-0.836528
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1	0.757763	-0.214410	1.076892
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1	1.256131	0.435963	-1.867851
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6	5.964452	-1.580427	-0.536043
6	5.445765	-0.174494	-0.249795
1	5.187035	-3.515904	-1.161064
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1	6.754167	-1.518074	-1.290286
1	5.089393	0.306515	-1.167792
1	4.449687	-2.131787	-1.978817
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1	2.860818	2.302463	-2.200201
1	3.505832	3.112510	-0.942072
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1	-1.290537	4.002047	0.516642
7	-6.117664	0.925287	-0.964475
1	-5.701530	1.551378	-1.648723
6	6.497609	0.713893	0.415151
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6	6.008459	2.157951	0.535727
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1	5.081771	2.184953	1.114882
1	6.758734	2.770790	1.042010
7	6.878249	0.108657	1.693627
1	7.555418	0.697975	2.165206
1	6.051521	0.072469	2.283510
6	-7.392467	0.447234	-1.501672
1	-7.269739	-0.267667	-2.325302
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1	-7.962491	1.308707	-1.852593

G:

6	1.653815	-0.414409	0.000030
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6	-1.072618	-0.277399	0.000001

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1	1.279949	-2.534587	-0.000047
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1	3.255398	0.500707	-0.000005
6	-2.561715	-0.446105	0.000054
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8	-0.460600	-1.470227	-0.000063

H:

6	-4.474391	0.398774	-0.459639
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6	-2.927834	-1.163410	0.466813
6	-1.977042	-0.156307	0.635752
6	-2.312921	1.134767	0.222371
6	-3.554192	1.427832	-0.320285
1	-4.904418	-1.692150	-0.185971
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1	0.216609	-1.733483	-0.037554
1	0.201991	-0.044710	-0.590746

6	1.574666	-0.423647	1.043750
1	1.559325	-1.000633	1.973994
1	1.628384	0.629473	1.313775
7	2.735949	-0.818310	0.254390
6	3.805811	-0.009418	-0.004809
6	4.498402	2.339200	0.222630
6	2.432290	2.082351	-0.516047
6	2.778417	3.397254	-0.460147
1	1.545160	1.586079	-0.865593
1	2.180275	4.249310	-0.741906
1	5.474835	2.049211	0.577436
7	4.065856	3.546267	0.011521
7	3.543337	1.390545	-0.058589
8	4.925223	-0.413087	-0.201520
6	3.015822	-2.259085	0.170522
1	3.959456	-2.467556	0.682305
1	2.218340	-2.776933	0.708834
6	3.085201	-2.758954	-1.268266
1	2.132987	-2.548619	-1.765834
1	3.860899	-2.197883	-1.794427
6	3.393457	-4.252638	-1.318234
1	3.436842	-4.611014	-2.347339
1	4.357176	-4.465207	-0.849501
1	2.628840	-4.832069	-0.793846

I:

6	2.391538	1.233050	0.007660
6	2.763158	-0.106741	-0.024100
6	1.761946	-1.062211	-0.017745

6	0.432856	-0.650313	0.016963
6	0.169696	0.722900	0.022498
7	1.126094	1.645790	0.024572
1	1.976980	-2.124093	-0.032507
1	3.143465	2.015731	0.016475
1	3.808348	-0.386326	-0.046164
6	-1.224058	1.307853	-0.002114
6	-0.608907	-1.715968	0.075373
8	-1.705355	1.944998	0.883210
8	-0.399407	-2.869380	-0.176735
8	-1.821833	1.073203	-1.179619
1	-2.698575	1.478959	-1.136415
8	-1.800458	-1.257786	0.482491
1	-2.413829	-2.004508	0.480620

J:

6	-0.630824	3.291132	0.291409
6	0.631401	3.290800	-0.291353
6	1.262268	2.090013	-0.585607
6	0.639996	0.877080	-0.289739
6	-0.639960	0.877447	0.290994
6	-1.261965	2.090631	0.586247
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1	1.123789	4.224897	-0.529531
1	2.232101	2.080378	-1.067473
1	-2.231820	2.081399	1.068084
7	1.226940	-0.370131	-0.595372
1	0.641449	-1.053274	-1.058675
7	-1.227319	-0.369473	0.597276

1	-0.642351	-1.052270	1.061736
6	2.540054	-0.762468	-0.501587
6	-2.540455	-0.761563	0.502907
16	3.048421	-2.140588	-1.251100
16	-3.049548	-2.139264	1.252819
7	3.281939	0.075422	0.306166
1	2.772926	0.731921	0.885756
7	-3.281712	0.076198	-0.305524
1	-2.772210	0.732174	-0.885289
6	4.648754	0.132627	0.595380
6	-4.648210	0.132664	-0.596535
8	-5.048546	0.840408	-1.480573
8	5.050043	0.841472	1.478110
8	-5.390888	-0.611256	0.197772
8	5.390642	-0.611979	-0.199041
6	-6.791580	-0.587848	-0.094943
1	-6.967401	-0.927218	-1.115371
1	-7.242588	-1.267749	0.621498
1	-7.184957	0.421582	0.023257
6	6.791746	-0.587443	0.091568
1	7.242079	-1.268022	-0.624660
1	7.184441	0.422024	-0.028504
1	6.969241	-0.925395	1.112184

K:

7	-3.304807	0.481779	0.000400
6	-2.184844	-0.263122	-0.000276
6	-4.597015	-0.198936	0.000955
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1	-4.688187	-0.835684	0.882678
1	-5.383475	0.551944	0.002465
6	-3.263778	1.941940	0.001125
1	-4.281463	2.321817	0.000157
1	-2.751481	2.317558	0.891197
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16	-0.716474	0.765787	-0.000365
16	0.716478	-0.765682	-0.000396
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6	2.184833	0.263124	-0.000118
6	3.263604	-1.941992	0.001396
1	2.749574	-2.317385	0.890558
1	2.751187	-2.318485	-0.888240
1	4.281240	-2.322001	0.002560
6	4.597064	0.198746	0.000469
1	4.689370	0.834106	-0.882148
1	4.688992	0.835178	0.882349
1	5.383448	-0.552217	0.001090
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16	2.171997	1.923803	-0.000813

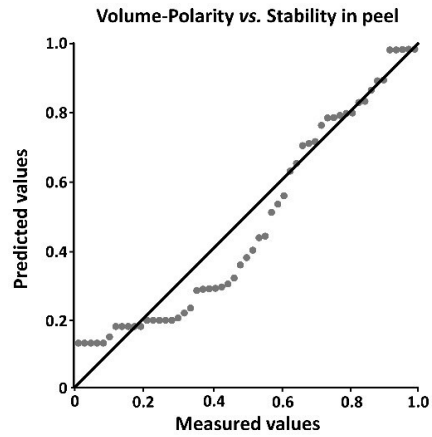
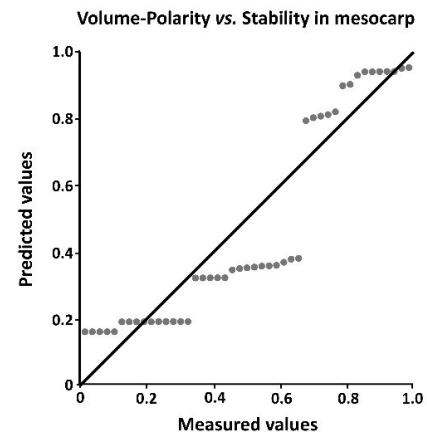
A**B**

Figure S3. Correlations between (A) volume, polarity and stability in pear peel, and (B) volume, polarity and stability in pear mesocarp. Linear regression analyses were performed using SPSS software version 16.0.