Supplementary Information

Urease Inhibitors of Agricultural Interest Inspired by Structures of Plant Phenolic Aldehydes

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Thermogravimetric analysis

Thermogravimetric measurements were carried out in a Shimadzu TGA-50 Thermogravimetric Analyzer using a nitrogen flow of 100 mL min^{-1}. Mass losses of phenolic aldehydes derivatives and *N*-(butyl)thiophosphorictriamide (NBPT) (standard soil inhibitor) were monitored at temperatures in the range from 35 to 500 ºC.

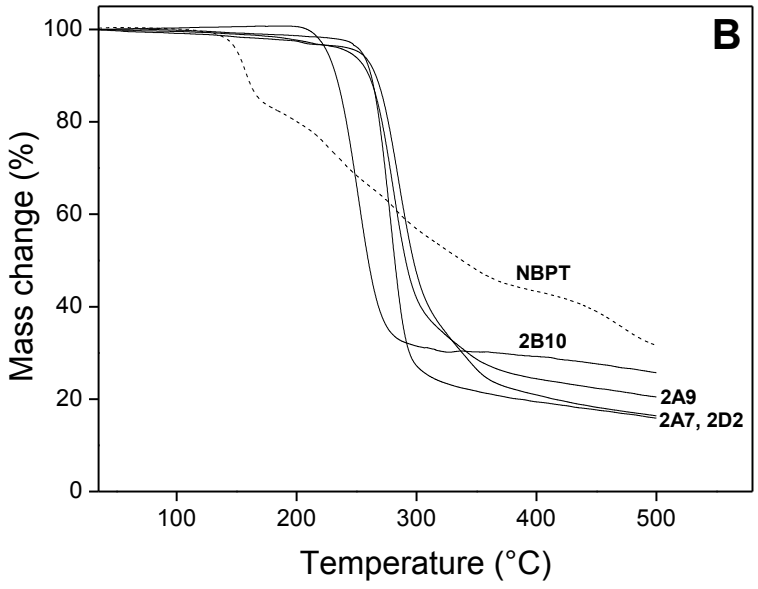

Figure S1. Thermal stability of phenolic aldehyde derivatives **2A7** and **2B10** (PA derivatives), **2A9** (SA derivative), **2D2** (VN derivative) and the reference urease inhibitor *N*-(butyl)thiophosphorictriamide (NBPT) assessed by monitoring compounds mass changes as a function of increments in temperature.

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Characterization data for compounds **2A7**, **2A9**, **2B10** and **2D2**

Compound **2A7**

Solid (red crystal); m.p. 233.0-235.1 ºC (lit.[1] 243.0-244.0); ^{1}H NMR (200 MHz, DMSO-d_6) δ 1.11 (t, 3H, *J* 6.9 Hz), 2.23 (s, 3H), 3.99 (q, 2H, *J* 6.9 Hz), 4.99 (bs, 1H), 6.78-6.41 (m, 3H), 7.60 (s, 1H), 8.78 (s, 1H), 8.88 (s, 1H), 9.10 (s, 1H); ^{13}C NMR (50 MHz, DMSO-d_6) 14.2, 17.8, 53.6, 59.2, 99.9, 113.8, 115.2, 117.2, 136.1, 144.6, 145.0, 147.5, 152.3, 165.6; IR (ATR) ν / cm^{-1} 3303, 2989, 2900, 1678, 1652, 1522, 1474, 1443, 1369, 1337, 1264, 1234, 1094, 1003, 943, 868, 771, 754.

Compound **2A9**

Solid (yellow crystal); m.p. 206.0-208.0 ºC (lit.[2] 205.0-206.0 ºC); ^{1}H NMR (200 MHz, DMSO-d_6) δ 1.11 (t, 3H, *J* 7.2 Hz), 2.27 (s, 3H), 3.72 (s, 3H), 4.01 (q, 2H, *J* 7.2 Hz), 5.08 (d, 1H, *J* 2.9 Hz), 6.89-6.50 (m, 3H), 9.00 (s, 1H), 9.56 (s, 1H), 10.25 (s, 1H); ^{13}C NMR (50 MHz, DMSO-d_6) 14.0, 17.1, 53.7, 55.6, 59.6, 101.0, 110.9, 115.4, 118.6, 134.6, 144.6, 146.2, 147.4, 165.3, 174.1; IR (ATR) ν / cm^{-1} 3474, 3315, 3165, 3101, 2973, 1667, 1603, 1572, 1518, 1451, 1373, 1329, 1270, 1236, 1179, 1116, 1026, 850, 833, 771, 739.

Compound **2B10**

Solid (gray crystal); m.p. 183.0-185.1 ºC; ^{1}H NMR (200 MHz, DMSO-d_6) δ 1.11 (t, 3H, *J* 7.1 Hz), 2.27 (s, 3H), 4.00 (q, 2H, *J* 7.1 Hz), 5.00 (d, 1H, *J* 3.4 Hz), 6.80-6.36 (m, 3H), 8.94 (s, 2H), 9.53 (s, 1H), 10.22 (s, 1H); ^{13}C NMR (50 MHz, DMSO-d_6) 14.1, 17.2, 53.7, 59.5, 101.2, 113.9, 115.3, 117.4, 134.6, 144.3, 144.9, 145.1, 165.3, 173.8; IR (ATR) ν / cm^{-1} 3309, 3245, 3012, 1661, 1608, 1567, 1510, 1463, 1449, 1375, 1340, 1284, 1270, 1192, 1113, 988, 943, 862, 763.

Compound **2D2**

Solid (yellow crystal); m.p. 189.3-191.6 ºC; ^{1}H NMR (200 MHz, DMSO-d_6) δ 1.14 (t, 3H, *J* 7.0 Hz), 2.28 (s, 3H), 3.71 (s, 6H), 4.04 (q, 2H, *J* 7.0 Hz), 5.11 (d, 1H, *J* 3.2 Hz), 6.46 (s, 2H), 8.42 (s, 1H), 9.58 (s, 1H), 10.29 (s, 1H); ^{13}C NMR (50 MHz, DMSO-d_6) 14.1, 17.1, 53.9, 56.0, 59.6, 100.9, 103.9, 133.7, 135.3, 144.7, 147.9, 165.3, 174.3; IR (ATR) ν / cm^{-1} 3473, 3326, 3193, 2945, 2840, 1663, 1619, 1516, 1454, 1432, 1371, 1330, 1278, 1217, 1184, 1148, 1119, 859, 821, 789, 753, 672.

References

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