***Plants, People, Planet* Supporting Information**

Article title: The role of strigolactone structural diversity in the host specificity and control of *Striga*, a major constraint to Sub-Saharan agriculture

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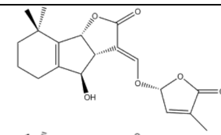
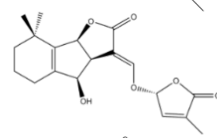
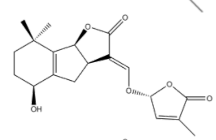
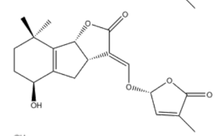
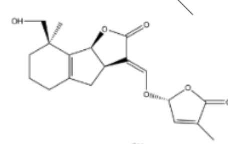
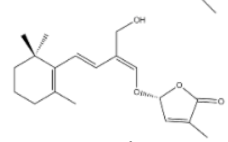
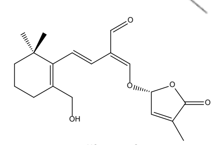
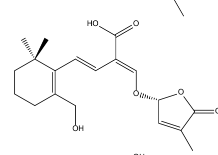
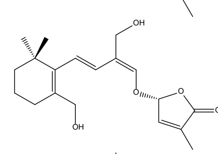
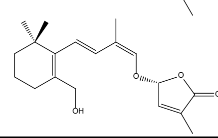
The following Supporting Information is available for this article:

**Table S1-** A series of potential sorghum strigolactone biosynthesis intermediates were used for docking to evaluate which strigolactone-like molecule would best fit as substrate into the active site of Sorghum bicolor sulfotransferase (SbSOT4A).

**Table S1. To evaluate which strigolactone-like molecule would best fit as substrate into the active site of *Sorghum bicolor* sulfotransferase (SbSOT4A), a series of potential sorghum strigolactone biosynthesis intermediates were used for docking. A homology model of SbSOT4A was constructed using MODELLER (Šali and Blundell, 1993) (version 9.18), using the X-ray structure of *Arabidopsis thaliana* sulfotransferase 18 (AtSOT18), Protein Data Bank (PDB) ID 5MEX, Uniprot ID Q9C9C9, co-crystallized with the substrate sinigrin (which was sulfated) and the (desulfated) cofactor PAPS as template. GOLD (using Gold Score fitness score, flexible amino acid sidechains) was used for docking the putative substrates into the active site of the modelled SbSOT4A (Shimels, 2019)**.

| Name of the compound | Chemical Formula | Molecular weight | Structure | Docking score |
|---|---|---|---|---|
| **Orobanchol** | $C_{19}H_{22}O_6$ | 346.38 |  | 41.759 |
| ***ent-2`-epi*-orobanchol** | $C_{19}H_{22}O_6$ | 346.38 |  | 43.717 |
| **Strigol** | $C_{19}H_{22}O_6$ | 346.38 |  | 55.117 |
| ***ent-2`-epi*-strigol** | $C_{19}H_{22}O_6$ | 346.38 |  | 51.041 |
| **Sorgomol** | $C_{19}H_{22}O_6$ | 346.38 |  | 50.196 |
| **C19-hydroxycarlactone** | $C_{19}H_{26}O_4$ | 318.41 |  | 58.163 |
| **Carlactonoic aldehyde_C18OH** | $C_{19}H_{24}O_5$ | 332.40 |  | 63.287 |
| **C18-hydroxycarlactonoic acid** | $C_{19}H_{24}O_6$ | 348.40 |  | 59.607 |
| **C19-hydroxycarlactone _C18OH** | $C_{19}H_{26}O_5$ | 334.41 |  | 66.547 |
| **C18-hydroxycarlactone** | $C_{19}H_{26}O_4$ | 318.41 |  | 66.704 |

## *References*

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Shimels, M.Z., 2019. The mechanism underlying strigolactone diversification in sorghum and its role in resistance against the parasitic weed *Striga hermonthica*. PhD thesis Wageningen University. https://doi.org/10.18174/498779