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Structural insights into the ligand-LsrK kinase binding mode. A step forward in the discovery of novel antimicrobial agents.

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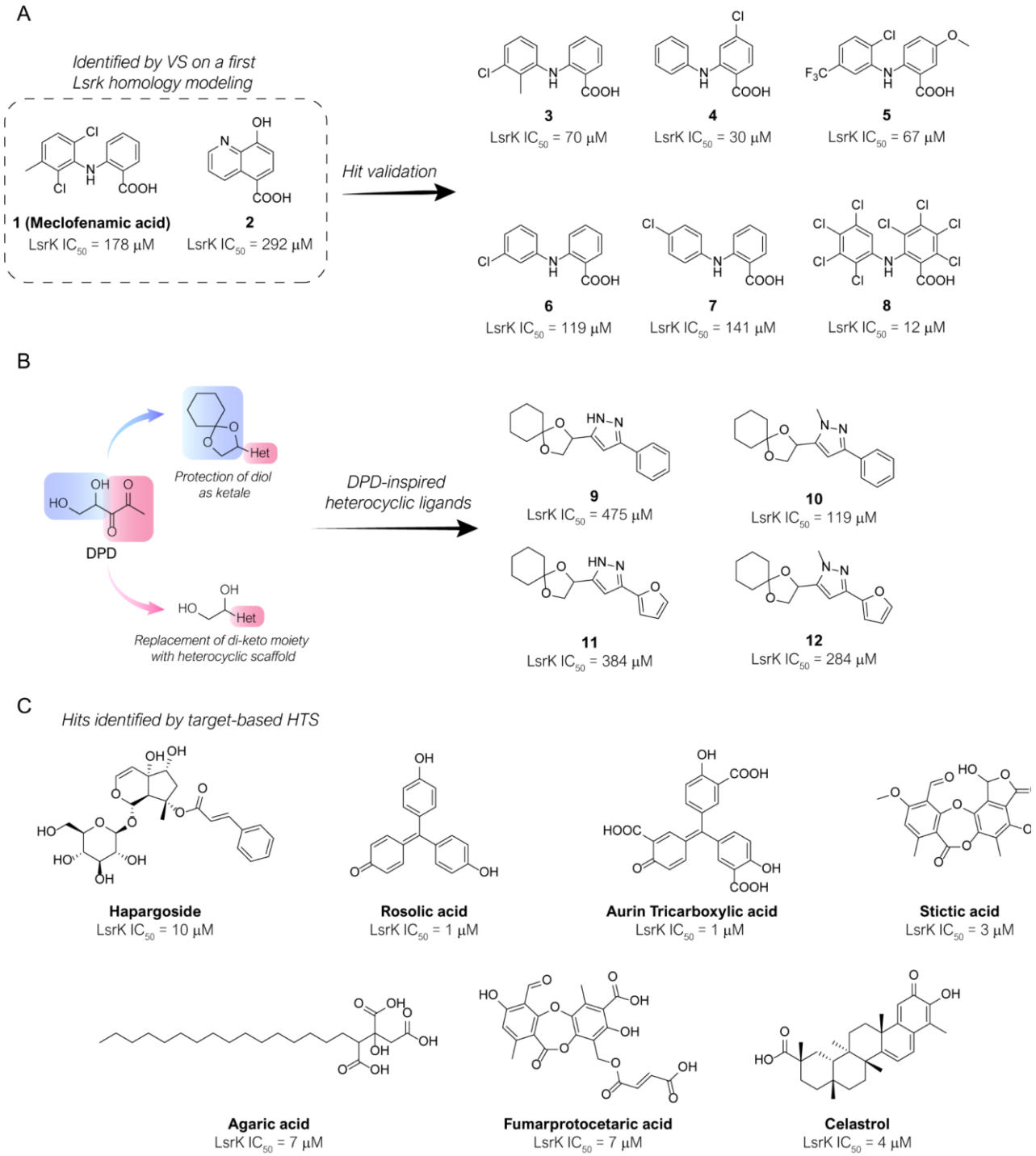

Figure SI-1. Chemical structure, LsrK inhibitory activity and approach exploited for the identification of the LsrK inhibitors reported in literature.

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Table SI-1. Percentage of secondary structural components in LsrK.

	α-Helix	**β-Strand**	**Turns**	**Other**
from UV-CD spectra[a]	44.4 ± 1.5 %	16.9 ± 2.4 %	3.2 ± 0.3 %	35.7 ± 0.3 %
from apo-LsrK X-ray structure[b]	39.6 %	20.4 %	37.9 %	

a. The values are an average of results obtained using the BestSel deconvolution programs.; b. calculated with the EMBL-EBI PDBsum utility