TimTec Natural Products Library, NPL, was used for in silico virtual ligand screening to identify new ligands of the AhR.

Bisson, W. H., et. al. Modeling of the Aryl Hydrocarbon Receptor (AhR) Ligand Binding Domain and Its Utility in Virtual Screening to Predict New AhR Ligands. J. Med. Chem. 2009, Vol. 52, No 18., p 5635-5641

Abstract:

The aryl hydrocarbon receptor (AhR) is a ligand-activated transcription factor; the AhR Per-AhR/Arnt-Sim (PAS) domain binds ligands. We developed homology models of the AhR PAS domain to characterize previously observed intra- and interspecies differences in ligand binding using molecular docking. In silico structure-based virtual ligand screening using our model resulted in the identification of pinocembrin and 5-hydroxy-7-methoxyflavone, which promoted nuclear translocation and transcriptional activation of AhR and AhR-dependent induction of endogenous target genes.

Six compounds-activators of AhR transcription are available from TimTec stock for re-supply

Download known activators of AhR transcription

To compliment published results with relevantly diverse chemical material, TimTec assembled small collection of 167 analogs to identified in virtual screen AhR ligands. Download PDF

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ST055658

MFCD00143506
C16H12O3
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ST056012

MFCD00143511
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270.24

ST057541

MFCD00016945
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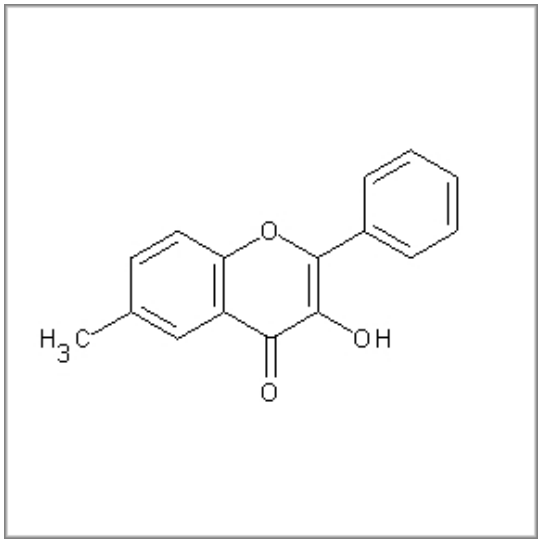

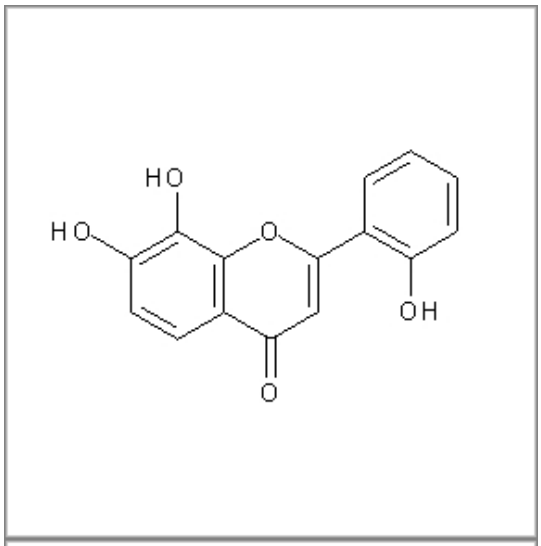
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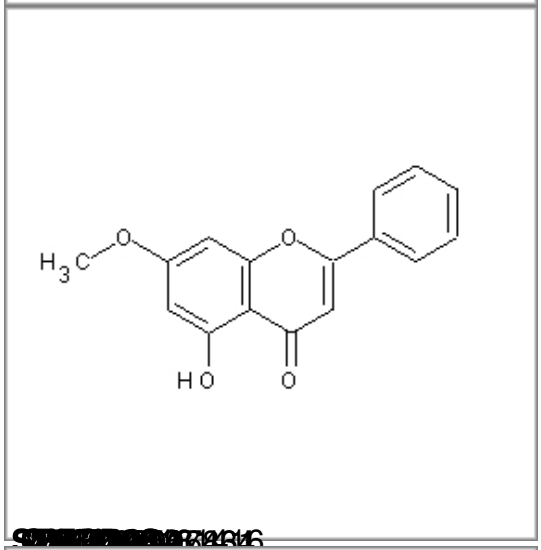
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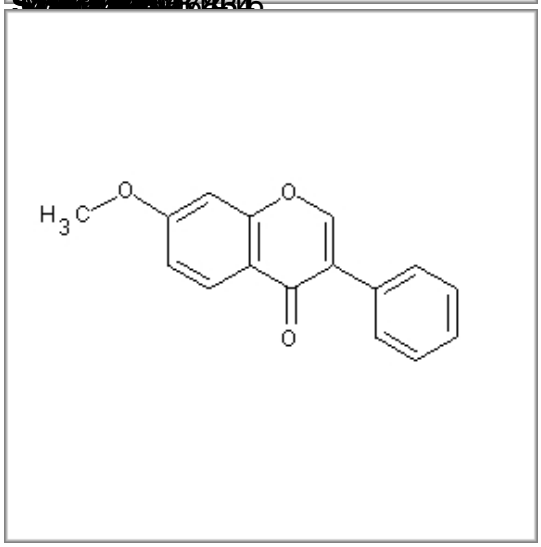
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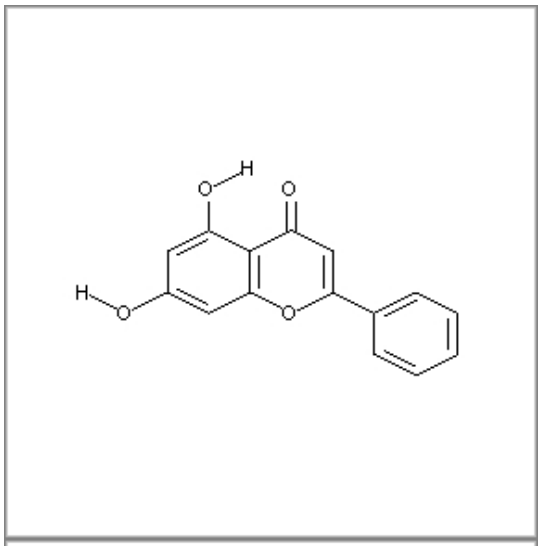

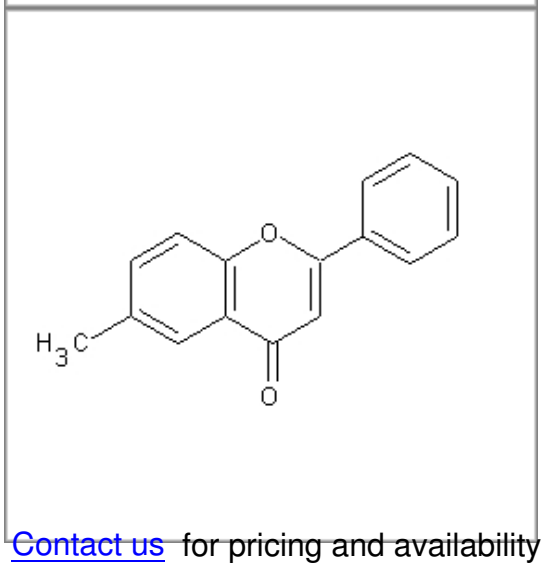

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