

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

C<sub>16</sub>H<sub>12</sub>O<sub>3</sub>

252.27

**ST056012**

MFCD00143511

C<sub>15</sub>H<sub>10</sub>O<sub>5</sub>

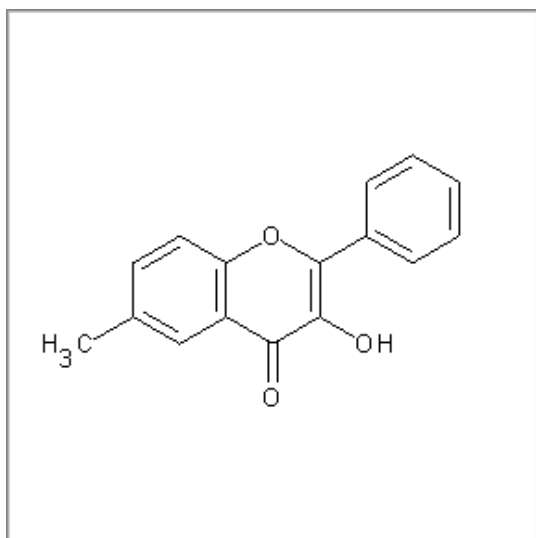
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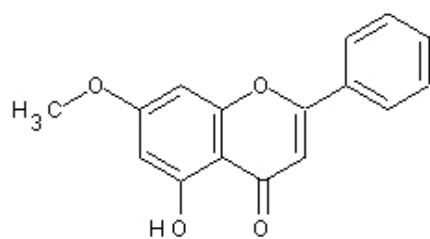
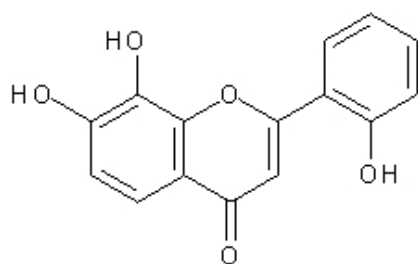
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MFCD00016945

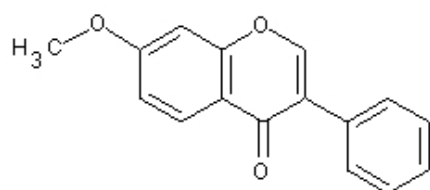
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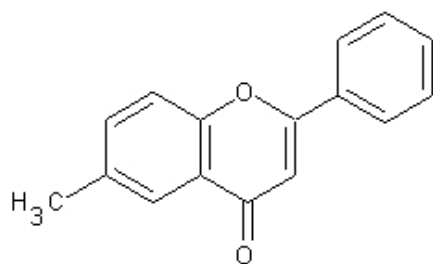
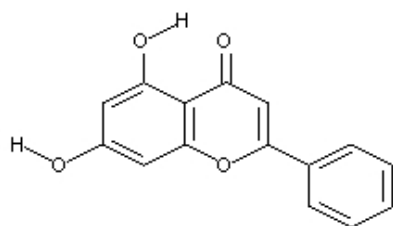
268.27





~~Chemical structure of 6-methoxy-2-phenylchromone (6-MeO-Pic)~~





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