



**TimTec LLC**

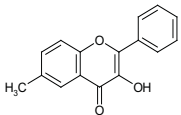
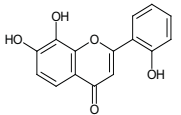
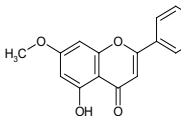
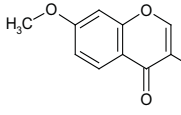
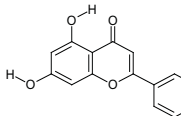
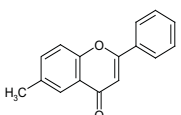
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**Aryl Hydrocarbon Receptor (AhR) Ligands**

ID	structure	fmla structure	MW	IUPACNAME	Binding Energy	Induction of AhR Transcriptional Activity
ST055658		C16H12O3	252.27	3-hydroxy-6-methyl-2-phenylchromen-4-one	-4.3	11.3 fold
ST056012		C15H10O5	270.24	7,8-dihydroxy-2-(2-hydroxyphenyl)chromen-4-one	-3.75	2.7 fold
ST057541		C16H12O4	268.27	5-hydroxy-7-methoxy-2-phenylchromen-4-one	-3.52	4.8 fold
ST066905		C16H12O3	252.27	7-methoxy-3-phenylchromen-4-one	-3.37	2.5 fold
ST069324		C15H10O4	254.24	5,7-dihydroxy-2-phenylchromen-4-one	-2.97	8.0 fold
ST069348		C16H12O2	236.27	6-methyl-2-phenylchromen-4-one	-2.74	2.8 fold

**Table 2. Activation of AhR Transcription by Compounds Identified by Virtual Docking into AhR LBD**

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