

Table S1. Average hydrogen bond Results for Three Small Molecules with PPARG

System	Average hydrogen bond
<i>Hederagenin</i>	2.06
<i>Triptotriterpenic Acid B</i>	0.411
<i>Triptotriterpenic Acid C</i>	1.419

Table S2. Average hydrogen bond Results for Three Small Molecules with PTGS2

System	Average hydrogen bond
<i>Hederagenin</i>	0.671
<i>Triptotriterpenic Acid B</i>	0.949
<i>Ursolic Acid</i>	0.384

Table S3. Average hydrogen bond Results for Three Small Molecules with PPARG

System	No.	donor	acceptor	occupancy
<i>Hederagenin</i>	1	ARG81-Side	6Q5271-Side	92.50%
	2	GLU136-Main	6Q5271-Side	71.30%
	3	SER135-Main	6Q5271-Side	15.70%
<i>Triptotriterpenic Acid B</i>	1	GLY137-Main	UNK271-Main	11.60%
	2	GLU136-Main	UNK271-Side	5.20%
	3	UNK271-Side	LEU133-Main	4.70%
<i>Triptotriterpenic Acid C</i>	1	UNK271-Side	GLU136-Side	67.20%
	2	GLU136-Main	UNK271-Main	35.40%
	3	GLU136-Main	UNK271-Side	16.10%

Table S4. Average hydrogen bond Results for Three Small Molecules with PTGS2

System	No.	donor	acceptor	occupancy
<i>Hederagenin</i>	1	HIE176-Side	6Q5552-Side	32.80%
	2	TYR378-Side	6Q5552-Side	23.60%
	3	6Q5552-Side	TYR378-Side	6.20%
<i>Triptotriterpenic Acid B</i>	1	UNK552-Side	ALA168-Main	59.30%
	2	UNK552-Side	ASN351-Side	9.00%
	3	UNK552-Side	GLN172-Side	7.30%
<i>Ursolic Acid</i>	1	UNK552-Side	TYR354-Main	17.90%
	2	UNK552-Side	THR175-Side	4.80%
	3	ASN351-Side	UNK552-Side	3.40%