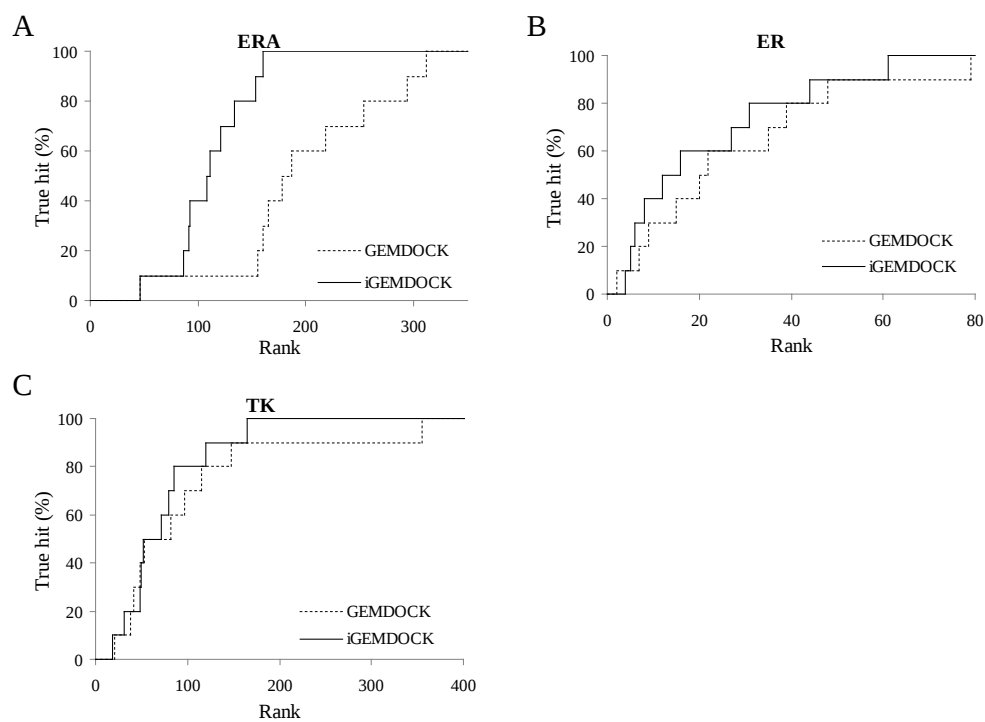




Supplementary Figure S1 - Comparison of iGEMDOCK (pharmacological scoring function) with GEMDOCK (energy-based scoring function) for (A) ERA, (B) ER, and (C) TK.

Supplementary Table S1 - Comparing iGEMDOCK with GOLD on the CCDC/Astex set by using the success rate

RMSD	iGEMDOCK				GOLD ^a			
	All entries ^b	Clean set ^c	Clean set with R<2.5Å ^c	Clean set with R<2.0 Å ^c	All entries ^b	Clean set ^c	Clean set with R<2.5Å ^c	Clean set with R<2.0 Å ^c
<0.5 Å	14 %	16 %	17 %	22 %	14 %	17 %	19 %	19 %
<1.0 Å	51 %	55 %	55 %	57 %	44 %	50 %	51 %	56 %
<1.5 Å	71 %	73 %	73 %	75 %	59 %	65 %	66 %	72 %
<2.0 Å	78 %	82 %	83 %	83 %	68 %	72 %	73 %	78 %
<2.5 Å	84 %	86 %	86 %	87 %	75 %	78 %	80 %	85 %
<3.0 Å	86 %	89 %	89 %	89 %	80 %	82 %	83 %	88 %

^a Summarized from Nissink *et al* (Nissink, *et al.*, 2002).

^b 305 complexes.

^c The clean set contains three subsets: all clean complexes (224 complexes), the complexes (180 complexes) with resolution (R) < 2.5 Å, and the complexes (92 complexes) with resolution < 2.0 Å.

Supplementary Table S2 - Comparing the pharmacological scoring function with other methods on ER and TK by the false-positive rates (%)

Protein	TP (%) ^a	iGEMDOCK ^b	GEMDOCK	DOCK ^c	FlexX ^c	GOLD ^c
ER	80	2.3 ^d	3.1	13.3	57.8	5.3
	90	3.5	3.9	17.4	70.9	8.3
	100	5.2	7.0	18.9	NA	23.4
TK	80	7.8	10.8	23.4	8.8	8.3
	90	11.2	14.0	25.5	13.3	9.1
	100	15.7	34.9	27.0	19.4	9.3

^a The true-positive rate (percentage).

^b The pharmacological scoring function.

^c Summarized from Bissantz *et al.*

^d The false-positive rate from 990 random compounds (percentage).