

CASF 2016 pose rank benchmark

Table S9. Success rates when the native ligand binding pose is not included in each decoy set

Scoring function	Rank ^a	Top 1 ^b	Top 2 ^c	Top 3 ^d	90% confidence interval ^e
RTCNN@ICM		86.7%	93.0%	95.8%	
$\Delta_{\text{vinaRF}_{20}}$	1	84.9%	91.6%	93.3%	[80.7% ~ 87.7%]
GlideScore-SP	2	84.6%	90.5%	92.6%	[80.0% ~ 87.0%]
Autodock Vina	2	84.6%	90.2%	92.6%	[80.4% ~ 87.4%]
ChemPLP@GOLD	3	83.2%	90.5%	93.3%	[78.6% ~ 86.3%]
GBVI/WSA-dG@MOE	4	82.1%	88.4%	91.6%	[77.5% ~ 85.3%]
GlideScore-XP	5	81.8%	89.5%	93.0%	[76.8% ~ 84.6%]
PLP1@DS	6	81.1%	88.4%	91.6%	[76.5% ~ 84.2%]
LigScore2@DS	7	80.4%	91.2%	94.4%	[75.8% ~ 83.9%]
DrugScore ^{CSD}	8	80.4%	89.5%	91.9%	[76.1% ~ 83.9%]
DrugScore2018	9	79.3%	86.3%	92.3%	[74.7% ~ 82.8%]
ChemScore@GOLD	9	79.3%	85.6%	90.2%	[74.4% ~ 82.5%]
ASP@GOLD	10	78.9%	85.6%	90.5%	[74.4% ~ 82.5%]
PLP2@DS	11	77.2%	87.4%	91.6%	[72.5% ~ 80.7%]
GoldScore@GOLD	12	74.7%	86.3%	90.5%	[69.8% ~ 78.6%]
LigScore1@DS	13	74.0%	82.7%	87.7%	[69.1% ~ 77.0%]

Table data: Su M, Yang Q, Du Y, et al. Comparative Assessment of Scoring Functions: The CASF-2016 Update. *J Chem Inf Model.* 2019;59(2):895-913.

CASF 2016 screening benchmark $EF_{1\%}$

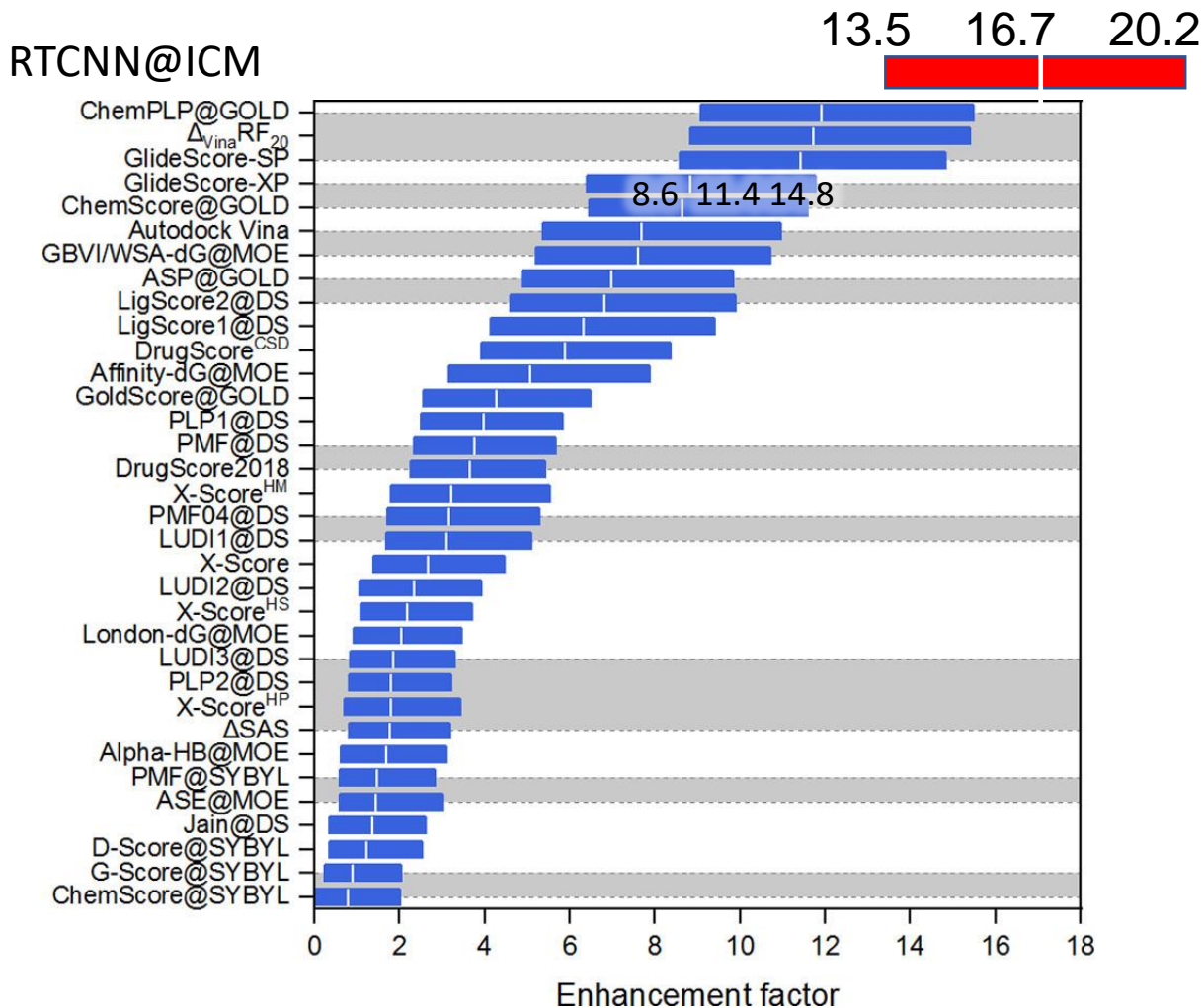


Figure: Su M, Yang Q, Du Y, et al. Comparative Assessment of Scoring Functions: The CASF-2016 Update. *J Chem Inf Model*. 2019;59(2):895-913.