1.0 - 1.0 - 0.5 -	KDE of B in target 11betaHSD1 and its decoys	Density	KDE of B in target 17betaHSD1 and its decoys  Actives Decoys	Density	KDE of B in target A2A and its decoys  — Actives — Decoys
0.0	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target ACE and its decoys	-	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target ACE2 and its decoys	<u> </u>	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target ACHE and its decoys
0.0 - 5.0	-1.0 -0.5 0.0 0.5 1.0	Density	-1.0 -0.5 0.0 0.5 1.0	Density	-1.0 -0.5 0.0 0.5 1.0
Density 1.0 -	Values  KDE of B in target ADAM17 and its decoys  Actives Decoys	Density	Values  KDE of B in target ADRB2 and its decoys  — Actives — Decoys	Density	Values  KDE of B in target AKT1 and its decoys  — Actives — Decoys
0.0	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target ALR2 and its decoys	Der	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target AR and its decoys	Der	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target AURKA and its decoys
1.0 - 1.0 - 0.5 -	Actives Decoys	Density	Actives Decoys	Density	Actives Decoys
0.0 \( \frac{1e7}{} \)	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target AURKB and its decoys	- - - -	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target BCL2 and its decoys  — Actives	<u>*</u>	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target BRAF and its decoys  — Actives
0.0 0.0 - c.0	-1.0 -0.5 0.0 0.5 1.0 Values	Density	-1.0 -0.5 0.0 0.5 1.0 Values	Density	-1.0 -0.5 0.0 0.5 1.0 Values
1.0 - 1.0 - 0.5 -	KDE of B in target CATL and its decoys  Actives Decoys	Density	KDE of B in target CDK2 and its decoys  Actives Decoys	Density	KDE of B in target COX1 and its decoys  Actives Decoys
0.0   1.0	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target COX2 and its decoys  — Actives		-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target CTSK and its decoys  —— Actives		-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target CYP2A6 and its decoys  Actives
0.0 0.0	-1.0 -0.5 0.0 0.5 1.0	Density	-1.0 -0.5 0.0 0.5 1.0	Density	-1.0 -0.5 0.0 0.5 1.0
1.0 - 1.0 - 0.5 -	Values  KDE of B in target DHFR and its decoys  Actives Decoys	Density	Values  KDE of B in target EGFR and its decoys  — Actives — Decoys	Density	Values  KDE of B in target EPHB4 and its decoys  — Actives — Decoys
0.0 le7	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target ER-beta and its decoys		-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target ERBB2 and its decoys		-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target FGFR1 and its decoys
0.0 Density	-1.0 -0.5 0.0 0.5 1.0	Density	-1.0 -0.5 0.0 0.5 1.0	Density	— Actives — Decoys
1.0 - 1.0 - 0.5 -	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target FKBP1A and its decoys	Density	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target FXA and its decoys	Density	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target GBA and its decoys
0.0	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target GR and its decoys	Der	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target GSK3B and its decoys	Der	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target HDAC2 and its decoys
1.0 - Density 0.5 - 0.0	Actives Decoys	Density	Actives Decoys	Density	Actives Decoys
1e7 1.0 <del>-</del>	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target HDAC8 and its decoys	, T	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target HIV1PR and its decoys  — Actives — Decoys		-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target HIV1RT and its decoys
0.0 0.0	-1.0 -0.5 0.0 0.5 1.0 Values	Density	-1.0 -0.5 0.0 0.5 1.0 Values	Density	-1.0 -0.5 0.0 0.5 1.0 Values
1.0 - 1.0 - 1.0 -	KDE of B in target HMGR and its decoys  —— Actives —— Decoys	Density	KDE of B in target HSP90 and its decoys  — Actives — Decoys	Density	KDE of B in target IGF1R and its decoys  — Actives — Decoys
0.0 Le7	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target INHA and its decoys  — Actives		-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target ITK and its decoys  —— Actives		-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target JAK3 and its decoys  — Actives
0.0 0.0	-1.0 -0.5 0.0 0.5 1.0	Density	-1.0 -0.5 0.0 0.5 1.0	Density	-1.0 -0.5 0.0 0.5 1.0
1e7 1.0 - 0.5 -	Values  KDE of B in target JNK1 and its decoys  Actives Decoys	Density	Values  KDE of B in target JNK2 and its decoys  ———————————————————————————————————	Density	Values  KDE of B in target JNK3 and its decoys  — Actives — Decoys
0.0 le7	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target KIF11 and its decoys		-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target LCK and its decoys		-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target MDM2 and its decoys
1.0 - Density	-1.0 -0.5 0.0 0.5 1.0	Density	-1.0 -0.5 0.0 0.5 1.0	Density	-1.0 -0.5 0.0 0.5 1.0
1e7 1.0 - 0.5 -	Values  KDE of B in target MK2 and its decoys  Actives Decoys	Density	Values  KDE of B in target MMP2 and its decoys  Actives Decoys	Density	Values  KDE of B in target NA and its decoys  — Actives — Decoys
0.0	-1.0 $-0.5$ $0.0$ $0.5$ $1.0$ Values  KDE of B in target P38-alpha and its decoys	Den	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target PARP-1 and its decoys	Den	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target PDE4B and its decoys
1.0 - Density 0.5 - 0.0	Actives Decoys	Density	Actives Decoys	Density	Actives Decoys
1e7 1.0 <del>-</del>	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target PDE5 and its decoys	- - - - -	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target PDK1 and its decoys	- - - -	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target PI3Kg and its decoys
0.0 0.0 0.0	-1.0 -0.5 0.0 0.5 1.0 Values	Density	-1.0 -0.5 0.0 0.5 1.0 Values	Density	-1.0 -0.5 0.0 0.5 1.0 Values
1.0 - 1.0 - 1.0 -	KDE of B in target PIM-1 and its decoys  Actives Decoys	Density	KDE of B in target PIM-2 and its decoys  Actives Decoys	Density	KDE of B in target PNP and its decoys  Actives Decoys
0.0 Le7	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target PPARA and its decoys		-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target PPARG and its decoys  — Actives		-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target PR and its decoys  Actives
0.0 0.0	-1.0 -0.5 0.0 0.5 1.0 Values	Density	-1.0 -0.5 0.0 0.5 1.0 Values	Density	-1.0 -0.5 0.0 0.5 1.0 Values
Density 1.0 -	KDE of B in target PRKCQ and its decoys  Actives Decoys	Density	KDE of B in target PYGL-in and its decoys  Actives Decoys	Density	KDE of B in target PYGL-out and its decoys  Actives Decoys
0.0 le7	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target QPCT and its decoys		-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target ROCK-1 and its decoys		-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target RXR and its decoys
0.0 0.0	-1.0 -0.5 0.0 0.5 1.0	Density	-1.0 -0.5 0.0 0.5 1.0	Density	-1.0 -0.5 0.0 0.5 1.0
Density 1.0 -	Values  KDE of B in target SARS-HCoV and its decoys	Density	Values  KDE of B in target SIRT2 and its decoys  ———————————————————————————————————	Density	Values  KDE of B in target SRC and its decoys  — Actives — Decoys
0.0 le7	-1.0 $-0.5$ $0.0$ $0.5$ $1.0$ Values  KDE of B in target Thrombin and its decoys	D¢	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target TIE2 and its decoys	ğ <u> </u>	-1.0
1.0 Density	Actives Decoys	Density	Actives Decoys	Density	— Actives — Decoys
1e7 1.0 <del> </del>	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target TP and its decoys  Actives Decoys	ity	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target TPA and its decoys  — Actives — Decoys	ity	-1.0 -0.5 0.0 0.5 1.0  Values  KDE of B in target TS and its decoys  Actives Decoys
Density 0.0 - 5.0	-1.0 -0.5 0.0 0.5 1.0 Values	Density	-1.0 -0.5 0.0 0.5 1.0 Values	Density	-1.0 -0.5 0.0 0.5 1.0 Values
1.0 - 1.0 - 1.0 -	KDE of B in target uPA and its decoys  Actives Decoys	Density	KDE of B in target VEGFR1 and its decoys  Actives Decoys	Density	KDE of B in target VEGFR2 and its decoys  — Actives — Decoys
0.0	-1.0 -0.5 0.0 0.5 1.0 Values 1e13		-1.0 -0.5 0.0 0.5 1.0 Values 1e13		-1.0 -0.5 0.0 0.5 1.0 Values 1e13