

SUPPLEMENTARY INFORMATION

Comparing AutoDock and Vina in Ligand/Decoy Discrimination for Virtual Screening

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Table S1. Docking parameters used for Vina and AutoDock

Targets	Vina			AutoDock			
	Box size ¹	Box center ¹	Exhaustiveness	Box size ¹	Box center ¹	Spacing ¹	N ^o GA runs
AA2AR	x=12; y=14; z=16	x=-9.26; y=-7.14; z=55.58	8	x=32; y=37; z=42	x=-9.26; y=-7.14; z=55.58	0.375	10
ABL1	x=18; y=14; z=14	x=16.02; y=15.82; z=4.02	8	x=48; y=37; z=37	x=16.02; y=15.82; z=4.02	0.375	10
ACE	x=16; y=16; z=18	x=45.05; y=44.92; z=44.77	8	x=42; y=42; z=48	x=45.05; y=44.92; z=44.77	0.375	10
ACES	x=12; y=14; z=12	x=4.60; y=68.95; z=66.25	8	x=32; y=37; z=32	x=4.60; y=68.95; z=66.25	0.375	10
ADA	x=16; y=16; z=16	x=50.74; y=54.87; z=19.94	8	x=42; y=42; z=42	x=50.74; y=54.87; z=19.94	0.375	10
ADA17	x=16; y=16; z=16	x=44.44; y=27.97; z=2.31	8	x=16; y=16; z=16	x=44.44; y=27.97; z=2.31	0.375	10
ADRB1	x=16; y=14; z=16	x=26.64; y=4.49; z=1.25	8	x=42; y=37; z=42	x=26.64; y=4.49; z=1.25	0.375	10
ADRB2	x=14; y=14; z=14	x=2.10; y=4.63; z=51.12	8	x=37; y=37; z=37	x=2.10; y=4.63; z=51.12	0.375	10
AKT1	x=14; y=14; z=16	x=5.43; y=3.15; z=19.91	8	x=37; y=37; z=42	x=5.43; y=3.15; z=19.91	0.375	10
AKT2	x=16; y=16; z=16	x=22.21; y=-19.16; z=7.41	8	x=42; y=42; z=42	x=22.21; y=-19.16; z=7.41	0.375	10
ALDR	x=16; y=16; z=16	x=17.03; y=-6.72; z=13.58	8	x=42; y=42; z=42	x=17.03; y=-6.72; z=13.58	0.375	10
AMPC	x=16; y=16; z=16	x=80.89; y=5.40; z=31.58	8	x=42; y=42; z=42	x=80.89; y=5.40; z=31.58	0.375	10
ANDR	x=14; y=14; z=12	x=27.11; y=2.70; z=5.20	8	x=37; y=37; z=32	x=27.11; y=2.70; z=5.20	0.375	10

AOFB	x=16; y=16; z=16	x=52.37; y=153.95; z=25.56	8	x=42; y=42; z=42	x=52.37; y=153.95; z=25.56	0.375	10
BACE1	x=18; y=18; z=18	x=24.59; y=12.19; z=22.99	8	x=48; y=48; z=48	x=24.59; y=12.19; z=22.99	0.375	10
BRAF	x=18; y=16; z=18	x=84.64; y=6.64; z=-6.76	8	x=48; y=42; z=48	x=84.64; y=6.64; z=-6.76	0.375	10
CAH2	x=14; y=14; z=14	x=-5.85; y=1.07; z=16.80	8	x=37; y=37; z=37	x=-5.85; y=1.07; z=16.80	0.375	10
CASP3	x=16; y=16; z=16	x=34.73; y=35.35; z=33.42	8	x=42; y=42; z=42	x=34.73; y=35.35; z=33.42	0.375	10
CDK2	x=18; y=16; z=16	x=1.38; y=26.15; z=9.40	8	x=48; y=42; z=42	x=1.38; y=26.15; z=9.40	0.375	10
COMT	x=16; y=16; z=16	x=-4.11; y=-12.23; z=-17.39	8	x=42; y=42; z=42	x=-4.11; y=-12.23; z=-17.39	0.375	10
CP2C9	x=16; y=16; z=16	x=8.49; y=33.27; z=-1.31	8	x=42; y=42; z=42	x=8.49; y=33.27; z=-1.31	0.375	10
CP3A4	x=18; y=18; z=18	x=37.26; y=-14.81; z=30.68	8	x=48; y=48; z=48	x=37.26; y=-14.81; z=30.68	0.375	10
CSF1R	x=16; y=16; z=18	x=7.07; y=30.32; z=9.66	8	x=42; y=42; z=48	x=7.07; y=30.32; z=9.66	0.375	10
CXCR4	x=16; y=16; z=18	x=19.95; y=-8.67; z=71.18	8	x=42; y=42; z=48	x=19.95; y=-8.67; z=71.18	0.375	10
DEF	x=18; y=18; z=18	x=-36.54; y=25.66; z=67.29	8	x=48; y=48; z=48	x=-36.54; y=25.66; z=67.29	0.375	10
DHI1	x=16; y=18; z=16	x=55.25; y=24.56; z=39.10	8	x=42; y=48; z=42	x=55.25; y=24.56; z=39.10	0.375	10
DPP4	x=18; y=16; z=16	x=-18.30; y=-5.12; z=59.36	8	x=48; y=42; z=42	x=-18.30; y=-5.12; z=59.36	0.375	10

DRD3	x=16; y=16; z=16	x=9.14; y=21.19; z=24.26	8	x=42; y=42; z=42	x=9.14; y=21.19; z=24.26	0.375	10
DYR	x=16; y=18; z=16	x=15.06; y=5.31; z=0.57	8	x=42; y=48; z=42	x=15.06; y=5.31; z=0.57	0.375	10
EGFR	x=18; y=18; z=16	x=16.76; y=35.71; z=91.27	8	x=48; y=48; z=42	x=16.76; y=35.71; z=91.27	0.375	10
ESR1	x=18; y=16; z=16	x=30.89; y=-2.02; z=24.19	8	x=48; y=42; z=42	x=30.89; y=-2.02; z=24.19	0.375	10
ESR2	x=18; y=16; z=16	x=96.09; y=20.70; z=-4.36	8	x=48; y=42; z=42	x=96.09; y=20.70; z=-4.36	0.375	10
FA10	x=16; y=16; z=18	x=2.63; y=-7.91; z=-12.59	8	x=16; y=16; z=18	x=2.63; y=-7.91; z=-12.59	0.375	10
FA7	x=16; y=16; z=16	x=10.39; y=41.72; z=31.89	8	x=42; y=42; z=42	x=10.39; y=41.72; z=31.89	0.375	10
FABP4	x=16; y=16; z=16	x=4.53; y=7.61; z=18.57	8	x=42; y=42; z=42	x=4.53; y=7.61; z=18.57	0.375	10
FAK1	x=16; y=16; z=16	x=10.12; y=2.76; z=5.11	8	x=42; y=42; z=42	x=10.12; y=2.76; z=5.11	0.375	10
FKB1A	x=16; y=16; z=16	x=-35.29; y=39.17; z=32.11	8	x=42; y=42; z=42	x=-35.29; y=39.17; z=32.11	0.375	10
FNTA	x=16; y=16; z=16	x=18.39; y=-23.91; z=3.24	8	x=42; y=42; z=42	x=18.39; y=-23.91; z=3.24	0.375	10
FPPS	x=16; y=16; z=16	x=15.39; y=33.27; z=-8.30	8	x=42; y=42; z=42	x=15.39; y=33.27; z=-8.30	0.375	10
GCR	x=16; y=18; z=16	x=40.84; y=30.89; z=9.61	8	x=42; y=48; z=42	x=40.84; y=30.89; z=9.61	0.375	10
GLCM	x=16; y=16; z=16	x=36.56; y=31.75; z=0.88	8	x=42; y=42; z=42	x=36.56; y=31.75; z=0.88	0.375	10
GRIA2	x=16; y=16; z=16	x=7.92; y=32.59; z=-0.89	8	x=42; y=42; z=42	x=7.92; y=32.59; z=-0.89	0.375	10

GRIK1	x=16; y=16; z=16	x=38.83; y=5.07; z=5.97	8	x=42; y=42; z=42	x=38.83; y=5.07; z=5.97	0.375	10
HDAC2	x=16; y=16; z=16	x=66.96; y=30.52; z=2.14	8	x=42; y=42; z=42	x=66.96; y=30.52; z=2.14	0.375	10
HDAC8	x=16; y=16; z=16	x=-26.33; y=28.31; z=-41.83	8	x=42; y=42; z=42	x=-26.33; y=28.31; z=-41.83	0.375	10
HIVINT	x=16; y=16; z=16	x=10.16; y=-26.76; z=-10.91	8	x=42; y=42; z=42	x=10.16; y=-26.76; z=-10.91	0.375	10
HIVPR	x=16; y=16; z=16	x=20.51; y=-2.79; z=18.77	8	x=42; y=42; z=42	x=20.51; y=-2.79; z=18.77	0.375	10
HIVRT	x=16; y=16; z=16	x=9.34; y=12.19; z=18.23	8	x=42; y=42; z=42	x=9.34; y=12.19; z=18.23	0.375	10
HMDH	x=16; y=16; z=16	x=-15.94; y=8.30; z=44.72	8	x=42; y=42; z=42	x=-15.94; y=8.30; z=44.72	0.375	10
HS90A	x=16; y=16; z=16	x=2.40; y=12.75; z=22.66	8	x=42; y=42; z=42	x=2.40; y=12.75; z=22.66	0.375	10
HXK4	x=16; y=16; z=16	x=-9.99; y=2.37; z=20.17	8	x=42; y=42; z=42	x=-9.99; y=2.37; z=20.17	0.375	10
IGF1R	x=16; y=16; z=16	x=5.76; y=-7.75; z=20.68	8	x=42; y=42; z=42	x=5.76; y=-7.75; z=20.68	0.375	10
INHA	x=16; y=16; z=16	x=9.34; y=32.33; z=60.66	8	x=42; y=42; z=42	x=9.34; y=32.33; z=60.66	0.375	10
ITAL	x=16; y=16; z=16	x=-10.33; y=2.41; z=27.49	8	x=42; y=42; z=42	x=-10.33; y=2.41; z=27.49	0.375	10
JAK2	x=16; y=16; z=16	x=114.75; y=65.50; z=11.11	8	x=42; y=42; z=42	x=114.75; y=65.50; z=11.11	0.375	10
KIF11	x=16; y=16; z=16	x=17.62; y=17.08; z=109.31	8	x=42; y=42; z=42	x=17.62; y=17.08; z=109.31	0.375	10

KIT	x=16; y=16; z=16	x=34.58; y=-2.8; z=-27.96	8	x=42; y=42; z=42	x=34.58; y=-2.8; z=-27.96	0.375	10
KITH	x=16; y=14; z=16	x=-9.93; y=5.08; z=35.14	8	x=42; y=37; z=42	x=-9.93; y=5.08; z=35.14	0.375	10
KPCB	x=16; y=16; z=16	x=38.87; y=55.35; z=34.84	8	x=42; y=42; z=42	x=38.87; y=55.35; z=34.84	0.375	10
LCK	x=16; y=16; z=16	x=27.07; y=39.82; z=84.43	8	x=42; y=42; z=42	x=27.07; y=39.82; z=84.43	0.375	10
LKHA4	x=16; y=16; z=16	x=11.42; y=40.20; z=68.38	8	x=42; y=42; z=42	x=11.42; y=40.20; z=68.38	0.375	10
MAPK2	x=16; y=16; z=16	x=37.62; y=6.04; z=16.97	8	x=42; y=42; z=42	x=37.62; y=6.04; z=16.97	0.375	10
MCR	x=16; y=16; z=16	x=18.82; y=72.28; z=20.37	8	x=42; y=42; z=42	x=18.82; y=72.28; z=20.37	0.375	10
MET	x=24; y=16; z=16	x=-1.39; y=3.96; z=27.01	8	x=64; y=42; z=42	x=-1.39; y=3.96; z=27.01	0.375	10
MK01	x=16; y=16; z=16	x=-13.77; y=13.53; z=41.29	8	x=42; y=42; z=42	x=-13.77; y=13.53; z=41.29	0.375	10
MK10	x=16; y=16; z=16	x=47.90; y=7.09; z=31.50	8	x=42; y=42; z=42	x=47.90; y=7.09; z=31.50	0.375	10
MK14	x=16; y=16; z=20	x=-1.86; y=-1.28; z=23.68	8	x=42; y=42; z=53	x=-1.86; y=-1.28; z=23.68	0.375	10
MMP13	x=16; y=16; z=16	x=-4.97; y=27.19; z=53.13	8	x=42; y=42; z=42	x=-4.97; y=27.19; z=53.13	0.375	10
MP2K1	x=16; y=16; z=16	x=-1.40; y=58.44; z=32.96	8	x=42; y=42; z=42	x=-1.40; y=58.44; z=32.96	0.375	10
NOS1	x=16; y=16; z=16	x=1.37; y=-0.37; z=59.29	8	x=42; y=42; z=42	x=1.37; y=-0.37; z=59.29	0.375	10
NRAM	x=16; y=16; z=16	x=31.88; y=-9.77; z=63.83	8	x=42; y=42; z=42	x=31.88; y=-9.77; z=63.83	0.375	10

PA2GA	x=16; y=16; z=16	x=-39.92; y=64.89; z=34.84	8	x=42; y=42; z=42	x=-39.92; y=64.89; z=34.84	0.375	10
PARP1	x=16; y=16; z=16	x=26.41; y=11.28; z=27.24	8	x=42; y=42; z=42	x=26.41; y=11.28; z=27.24	0.375	10
PDE5A	x=16; y=16; z=16	x=1.67; y=68.32; z=83.84	8	x=42; y=42; z=42	x=1.67; y=68.32; z=83.84	0.375	10
PGH1	x=16; y=16; z=16	x=20.52; y=50.05; z=11.24	8	x=42; y=42; z=42	x=20.52; y=50.05; z=11.24	0.375	10
PGH2	x=16; y=16; z=16	x=30.10; y=-22.56; z=-15.76	8	x=42; y=42; z=42	x=30.10; y=-22.56; z=-15.76	0.375	10
PLK1	x=16; y=16; z=16	x=0.28; y=23.32; z=66.86	8	x=42; y=42; z=42	x=0.28; y=23.32; z=66.86	0.375	10
PNPH	x=16; y=16; z=16	x=15.59; y=10.58; z=58.28	8	x=42; y=42; z=42	x=15.59; y=10.58; z=58.28	0.375	10
PPARA	x=16; y=16; z=16	x=15.32; y=39.88; z=27.77	8	x=42; y=42; z=42	x=15.32; y=39.88; z=27.77	0.375	10
PPARD	x=16; y=16; z=16	x=15.67; y=2.31; z=39.48	8	x=42; y=42; z=42	x=15.67; y=2.31; z=39.48	0.375	10
PPARG	x=16; y=16; z=16	x=2.75; y=24.31; z=16.33	8	x=42; y=42; z=42	x=2.75; y=24.31; z=16.33	0.375	10
PRGR	x=16; y=16; z=16	x=-2.57; y=-8.12; z=25.71	8	x=42; y=42; z=42	x=-2.57; y=-8.12; z=25.71	0.375	10
PTN1	x=16; y=16; z=16	x=46.16; y=14.24; z=3.07	8	x=42; y=42; z=42	x=46.16; y=14.24; z=3.07	0.375	10
PUR2	x=16; y=16; z=16	x=74.78; y=22.95; z=32.19	8	x=42; y=42; z=42	x=74.78; y=22.95; z=32.19	0.375	10
PYGM	x=16; y=16; z=16	x=39.78; y=36.15; z=29.59	8	x=42; y=42; z=42	x=39.78; y=36.15; z=29.59	0.375	10
PYRD	x=16; y=16; z=16	x=51.29; y=43.30; z=-3.07	8	x=42; y=42; z=42	x=51.29; y=43.30; z=-3.07	0.375	10

RENI	x=16; y=16; z=16	x=-8.67; y=-14.90; z=-10.39	8	x=42; y=42; z=42	x=-8.67; y=-14.90; z=-10.39	0.375	10
ROCK1	x=16; y=16; z=16	x=52.66; y=101.87; z=29.67	8	x=42; y=42; z=42	x=52.66; y=101.87; z=29.67	0.375	10
RXRA	x=16; y=16; z=16	x=59.66; y=46.22; z=31.74	8	x=42; y=42; z=42	x=59.66; y=46.22; z=31.74	0.375	10
SAHH	x=16; y=16; z=16	x=46.26; y=-19.83; z=101.93	8	x=42; y=42; z=42	x=46.26; y=-19.83; z=101.93	0.375	10
SRC	x=16; y=16; z=16	x=1.76; y=4.64; z=6.96	8	x=42; y=42; z=42	x=1.76; y=4.64; z=6.96	0.375	10
TGFR1	x=16; y=16; z=16	x=14.42; y=66.48; z=5.63	8	x=42; y=42; z=42	x=14.42; y=66.48; z=5.63	0.375	10
THB	x=16; y=16; z=16	x=13.75; y=22.81; z=46.86	8	x=42; y=42; z=42	x=13.75; y=22.81; z=46.86	0.375	10
THRB	x=16; y=16; z=16	x=16.84; y=-11.61; z=21.24	8	x=42; y=42; z=42	x=16.84; y=-11.61; z=21.24	0.375	10
TRY1	x=16; y=16; z=16	x=26.36; y=20.82; z=27.79	8	x=42; y=42; z=42	x=26.36; y=20.82; z=27.79	0.375	10
TRYB1	x=16; y=16; z=16	x=25.42; y=75.74; z=82.91	8	x=42; y=42; z=42	x=25.42; y=75.74; z=82.91	0.375	10
TYSY	x=16; y=16; z=16	x=14.36; y=13.43; z=34.79	8	x=42; y=42; z=42	x=14.36; y=13.43; z=34.79	0.375	10
UROK	x=16; y=16; z=16	x=31.33; y=18.35; z=35.95	8	x=42; y=42; z=42	x=31.33; y=18.35; z=35.95	0.375	10
VGFR2	x=16; y=18; z=16	x=37.42; y=36.08; z=11.98	8	x=42; y=48; z=42	x=37.42; y=36.08; z=11.98	0.375	10
WEE1	x=16; y=16; z=16	x=4.28; y=53.97; z=22.88	8	x=42; y=42; z=42	x=4.28; y=53.97; z=22.88	0.375	10
XIAP	x=16; y=16; z=16	x=10.13; y=13.39; z=-21.84	8	x=42; y=42; z=42	x=10.13; y=13.39; z=-21.84	0.375	10

¹ Box dimensions, center and spacing are given in Å

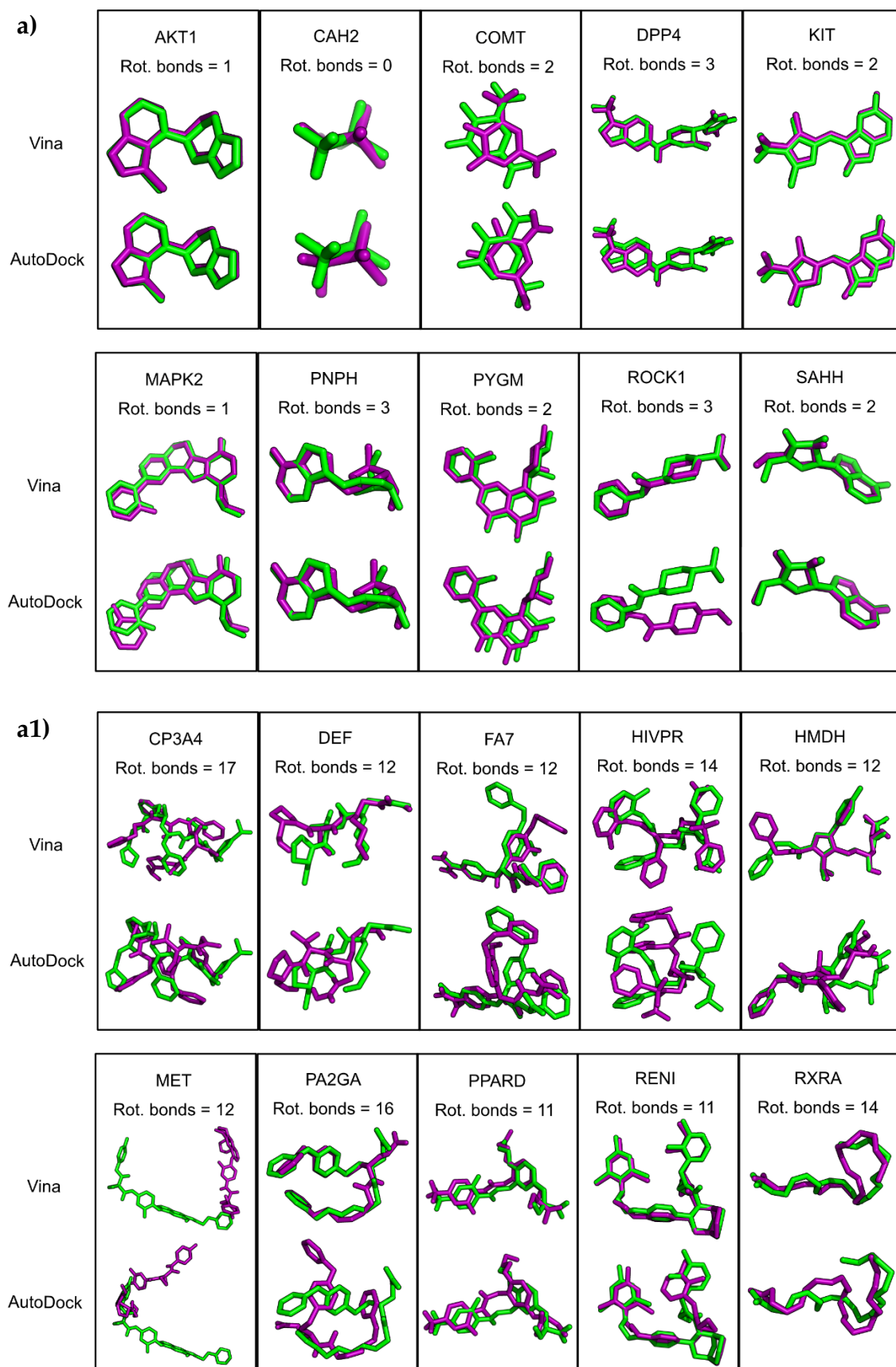


Figure S2. Comparison between the crystallographic (green) and “docked” (purple) poses for Vina and AutoDock, to evaluate the influence of the number of rotational bonds in pose prediction. (a) Ligands with the lowest number of rotational bonds (a1) Ligands with the highest number of rotational bonds.