Angiotensin receptor inhibitors

TerraQSAR-LOGP computed octanol/water partition coefficients (CLOGPs).

For other effect values, such as rat/mouse intravenous LD50, fish (fathead minnow) 96-hr LC50, estrogen receptor binding affinity (RBA), use TerraQSAR-RMIV, TerraQSAR-FHM, and TerraQSAR-E2-RBA programs, or consult TerraBase Inc.

SMILES	CAS	NAME	FORMULA	MW	TerraQSAR- CLOGP
CC1(C)[C@H](O)C[C@@]2(O)[C@H](CI)[C@@H](O)C(CCCCC)=C(C=O)[C@@]2([H])O1		cytosporin B	C17H27ClO5	346.85	1.89
[H][C@]12CCCC[C@]1([H])C[C@]([H])(N2C(=O)[C @@](C)([H])N[C@@]([H])(CCC)C(O)=O)C(O)=O	95153-31-4	perindoprilat	C17H28N2O5	340.42	0.73
O = C(N2c1ccccc1C[C@]2([H])C(O) = O)[C@@](C)([H])C[C@](C)([H])C(=O)OCC	82924-03-6	pentopril	C18H23NO5	333.38	2.46
OC(=O)[C@@H]1CCC[C@]2([H])SCC[C@@]([H])(C(=O)N12)NC(=O)[C@@]([H])(S)Cc1ccccc1	167305-00-2	omapatrilat	C19H24N2O4S2	408.54	1.32
CC(=O)SC[C@](C)([H])C(=O)N1CCC[C@@]1([H]) C(=O)N[C@@](c2cccc2)([H])C(=O)O	74258-86-9	alacepril	C19H24N2O5S	392.47	1.33
c1ccccc1C[C@H](S)C(=O)N[C@@H]2C(=O)N(CC(=O)O)C(C)(C)CCC2	160135-92-2	gemopatrilat	C19H26N2O4S	378.49	-1.09
CCC[C@H](C(=O)OCC)N[C@H](C)C(=O)N1C(C(=O)O)C[C@]2([H])CCCC[C@]12([H])	82834-16-0	perindopril	C19H32N2O5	368.47	1.49
$ \begin{aligned} & OC(=O) c1 ccccc1C(=O) Nc2 ccc(cc2) Cn3c(SCC) nnc \\ & 3C(F)(F)F \end{aligned} $		1,2,4-triazole deriv.; T-6651-013	C20H17F3N4O3S	450.44	2.77
OC(=O)[C@]2([H])CCCN3CCC[C@]([H])(N[C@@]([H])(CC/c1ccccc1)C(O)=O)C(=O)N23	90139-06-3	cilazaprilat	C20H27N3O5	389.45	1.11
CCOC(=O)[C@]([H])(CC/c1ccccc1)N[C@](C)([H])C (=O)N2C(=O)N(C)C[C@@]2([H])C(O)=O	89371-37-9	imidapril	C20H27N3O6	405.45	-0.07
O=C(N1CCC[C@@]1([H])C(O)=O)[C@@](C)([H])N [C@]([H])(CCc2cccc2)C(=O)OCC	75847-73-3	enalapril	C20H28N2O5	376.45	-0.63
OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(SCCC)nnc3C(F)(F)F		1,2,4-triazole deriv.; T-6651-014	021H19F3N4O33	464.47	2.80
OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(SCC)nnc 3COC		1,2,4-triazole deriv.; T-6651-012	C21H22N4O4S	426.49	2.87
c1ccccc1CC[C@@H](C(=O)O)NC2C(=O)N(CC(=O)O)C[C@@H](c3cccs3)SC2	110221-53-9	temocaprilat	C21H24N2O5S2	448.56	1.22
O=C(N2[C@@]1([H])CCC[C@@]1([H])C[C@@]2([H])C(O)=O)[C@@](C)([H])N[C@@]([H])(CC/C3=C/ C=CC=C3)C(O)=O	87269-97-4	ramiprilat	C21H28N2O5	388.46	1.11
O=C(O)[C@@]2([H])N(C(=O)[C@@](C)([H])N[C@ @]([H])(CC/c1ccccc1)C(O)=O)C3([H])CCC2([H])CC 3	90103-92-7	zabiciprilat	C21H28N2O5	388.46	1.11
OC(=0)C1CCCN1C(=0)C(CCCCN)OP(=0)(0)OCC		ceronapril	C21H33N2O7P	456.48	1.21
CCCCc1nc(Cl)c(CO)n1Cc2ccc(cc2)c3ccccc3c4nnn n-]4.[K+]	124750-99-8	losartan-potassium	C22H22CIKN6O	461.01	3.20
O=C(SC[C@@](C)([H])C(=O)N1C[C@]([H])(C[C@@]1([H])C(=O)O)Sc2ccccc2)c3ccccc3	75176-37-3	zofenoprilat	C22H23NO4S2	429.56	2.79
O=C(O)[C@]1([H])C[C@@]([H])(CN1C(=O)[C@@](C)([H])CSC(=O)c2cccc2)SC=3C=CC=CC=3	81872-10-8	zofenopril	C22H23NO4S2	429.56	2.79

O=C2N(CC(O)=O)c1ccccc1CC[C@]2([H])N[C@@]([H])(CCC=3C=CC=CC=3)C(O)=O	86541-78-8	benazeprilat	C22H24N2O5	396.44	0.36
C1CCC[C@]2([H])C[C@@H](C(=O)O)N([C@@]12([H]))C(=O)[C@@H](C)N[C@H](C(=O)O)CC3ccccc		trandolapril	C22H30N2O5	402.49	1.11
3 O=C(N1C[C@]2(C[C@@]1([H])C(O)=O)SCCS2)[C @@](C)([H])N[C@]([H])(CC/C3=C/C=CC=C3)C(=O)OCC	83602-05-5	spiraprilat	C22H30N2O5S2	466.62	1.37
O=C(N1C[C@@]2(C[C@]1([H])C(=O)O)SCCS2)[C @](C)([H])N[C@@]([H])(CC/C3=C/C=CC=C3)C(=O)OCC	83647-97-6	spirapril	C22H30N2O5S2	466.62	1.37
c1cc(C(C)C)ccc1Cn2cncc2C[C@@H](C(=O)O)NC(C(=O)O)CC(C)C		ACE2	C22H31N3O4	401.51	-0.08
c1ccccc1CC[C@](C(=O)OCC)(NC2C(=O)N3[C@H] (C(=O)O)CCCN3CCC2)([H])	92077-78-6	cilazapril [monohydrate]	C22H31N3O5	417.51	-0.65
c1ccccc1CCC(C(=O)OCC)NC(C)C(=O)N2N=C(C(C)(C)C)SC12C(=O)O	109683-61-6	utibapril	C22H31N3O5S	449.57	1.26
c1ccccc1CC[C@@H](C(=O)OCC)N[C@@H](C)C(= O)N2[C@H](C(=O)O)SC(=N2)C(C)(C)C	109003-79-0	utibapril	C22H31N3O5S	449.57	1.26
O=C2CCc1c(nc(C)nc1C)N2C/c3ccc(cc3)c4ccccc4/c5nnnn5	145733-36-4	tasosartan	C23H21N7O	411.47	1.87
O=C5NN4C(C)=NC(CCC)=C(Cc1ccc(cc1)C2=CC= C/C=C2/C=3NN=NN=3)C4=N5	148504-51-2	ripisartan	C23H22N8O	426.48	1.54
C[C@]([H])(NC(=O)[C@](C)(CC=2C=C1OCOC1=C C=2)SC(=O)C)C(=O)OCC=3C=CC=CC=3	135038-57-2	fasidotril	C23H25NO6S	443.52	3.09
OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(CCCC)nnc3SCCO		1,2,4-triazole deriv.; T-6651-017	C23H26N4O4S	454.55	2.95
CCCC/C1=N/C(=NN1CC=2C=CC(=NC=2)C3=CC=C/C=C3/C=4NN=NN=4)CCCC	145216-43-9	forasartan	C23H28N8	416.53	2.68
O=C(O)[C@@]2([H])N(C(=O)[C@@](C)([H])N[C@ @]([H])(CC/c1ccccc1)C(=O)OCC)C3([H])CCC2([H]) CC3	83059-56-7	zabicipril	C23H32N2O5	416.52	0.73
c1ccccc1CC[C@](C(=O)OCC)([H])N[C@@H](C)C(=O)N2[C@@]([H])(C(=O)O)C[C@@]3([H])CCC[C@ @]23([H])	87333-19-5	ramipril	C23H32N2O5	416.52	0.70
O=C(CP(O)(=O)CCCCc1ccccc1)N2C[C@@]([H])(C [C@@]2([H])C(O)=O)[C@]3([H])CCCCC3	95399-71-6	fosinoprilat	C23H34NO5P	435.50	5.22
CCC[C@H](C(=O)OCC)N[C@H](C)C(=O)N1C(C(= O)[O-])C[C@]2([H])CCCC[C@]12([H]).[N+]C(C)(C)C	107133-36-8	perindopril erbumine	C23H43N3O5	441.61	-0.63
CIC=5/N=C(/CCCC)N(C/C1=C/C2=C(C=C1)O/C(=C 2/Br)C3=CC=C/C=C3/C4=N/N=NN4)C=5C(=O)O	145/81-32-4	zolasartan	C24H20BrCIN6O3	555.82	3.32
O=C(O)C5=CC=CC=4/N=C(/OCC)N(Cc1ccc(cc1)c2cccc2/C3=N/N=NN3)C=45	139481-59-7	candesartan	C24H20N6O3	440.46	4.33
OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(CCCC)nnc3SCC(=O)OC		1,2,4-triazole deriv.; T-6651-015	C24H26N4O5S	482.56	3.00
CCCc1nc(C(C)(C)O)c(C(=O)O)n1Cc2ccc(cc2)c3ccccc3c4nnnn4	144689-24-7	olmesartan	C24H26N6O3	446.51	3.65
OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(CCCC)nnc3SCC(=O)NC		1,2,4-triazole deriv.; T-6651-016	C24H27N5O4S	481.57	2.82
c1cccc(c2nnnn2)c1c3ccc(cc3)CN(C(=O)CCCC)[C@](C(C)C)(C(=O)O)([H])	137862-53-4	valsartan	C24H29N5O3	435.53	1.77
O=C(N2[C@]1([H])CCCC[C@@]1([H])C[C@@]2([H])C(O)=O)[C@](C)([H])N[C@@]([H])(CC/C3=C/C=CC=C3)C(=O)OCC	80876-01-3	indolapril	C24H34N2O5	430.54	0.98
n1c2cccc(C(=O)O)c2n(c1OCC)Cc3ccc(cc3)c4ccccc 4c5nc(O)on5	147403-03-0	azilsartan	C25H20N4O5	456.46	4.17

NC(=O)C1=C(/N=C(/CC)N1Cc2cc3c(cc2)oc(c3Br)c 4ccccc4/NS(=O)(=O)C(F)(F)F)C5([H])CC5	146623-69-0	sapropterin, [saprisartan]	C25H22BrF3N4O4 S	611.44	5.37
OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(SCC)nnc3c4ccccc4		1,2,4-triazole deriv.; T-6651-002	C25H22N4O3S	458.54	2.59
O=C(OC)C4=CC(=O)N(C/c1ccc(cc1/F)c2cccc2/c3 nnnn3)C(=C4)CCCC	156001-18-2	embusartan	C25H24FN5O3	461.50	2.93
OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(CCCC)nn c3c4occc4		1,2,4-triazole deriv.; T-6651-006	C25H24N4O4	444.49	2.77
C1CCCC(=O)c2n(c(CCC)nc12)Cc3ccc(cc3)c4ccccc4c5nnnn5	153804-05-8	pratosartan	C25H26N6O	426.52	3.88
C1CCCC12N=C(CCCC)N(C2=O)Cc3ccc(cc3)c4c(c5nnnn5)cccc4	138402-11-6	irbesartan	C25H28N6O	428.54	3.17
c1cccc2C[C@@]([H])(C(=O)O)N(Cc12)C(=O)[C@H](C)N[C@@]((C(=O)OCC)CC3ccccc3)[H]	85441-61-8	quinapril	C25H30N2O5	438.52	1.16
c1c(OC)c(OC)cc2C[C@H](C(=O)O)N(Cc12)C(=O)[C@H](C)N[C@H](C(=O)O)CC3ccccc3	103775-14-0	moexiprilat	C25H30N2O7	470.52	0.68
OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(SCCC)nnc3c4ccccc4		1,2,4-triazole deriv.; T-6651-003	U20H24IN4U3S	472.57	2.63
OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(SCC)nnc 3Cc4cccc4		1,2,4-triazole deriv.; T-6651-007		472.57	2.61
OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(CCCC)nn c3c4ccncc4		1,2,4-triazole deriv.; T-6651-004	C26H25N5O3	455.52	2.55
OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(CCCC)nn c3c4cnccc4		1,2,4-triazole deriv.; T-6651-005	G2011231N3O3	455.52	2.55
$ \begin{array}{lll} OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(CCCC)nn \\ c3SC(CC)C(=O)OC \end{array} $		1,2,4-triazole deriv.; T-6651-018	C26H30N4O5S	510.61	3.07
CCCC(=O)N(CC1(CCCC1)C(O)=O)C/C2=C/C=C(C=C2)C3=CC=C/C=C3/C4=N/N=NN4	137882-98-5	abitesartan	C26H31N5O3	461.57	2.03
O=C(O)C[C@]([H])(NC(=O)[C@@]([H])(NS(=O)(=O)C)CCCCN)C[C@]1(CCCC1)C(=O)N[C@@]([H])(CC=2C=CC(O)=CC=2)C(=O)O	129981-36-8	sampatrilat	C26H40N4O9S	584.69	0.86
OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(CCCC)nn c3c4ccccc4		1,2,4-triazole deriv.; T-6651-001		454.53	2.54
OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(SCCC)nnc3Cc4ccccc4		1,2,4-triazole deriv.; T-6651-008		486.59	2.65
OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(CCCC)nn c3Sc4cccc4		1,2,4-triazole deriv.; T-6651-020		486.59	2.81
OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(CCC)nnc 3SCc4cccc4		1,2,4-triazole deriv.; T-6651-023		486.59	2.67
OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(SCCC)nn c3CSc4ccccc4		1,2,4-triazole deriv.; T-6651-011	C27H26N4O3S2	518.66	2.87
n1nnnc1c2cccc2c3ccc(cc3)Cn4c(CCCC)nc(Cl)c4C (=O)O[C@H](C)OC(=O)OCC		elisartan [both enantiomers]	C27H29CIN6O5	553.02	4.14
CCCCC1=NC(C)=C(CC(=S)N(C)C)C(=O)N1Cc2ccc (cc2)c3ccccc3c4nnnn4	247257-48-3	fimarsatan	C27H31N7OS	501.66	2.91
c1c(OC)c(OC)cc2C[C@H](C(=O)O)N(Cc12)C(=O)[C@H](C)N[C@H](C(=O)OCC)CCc3ccccc3	103775-10-6	moexipril	C27H34N2O7	498.58	2.07
OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(CCCC)nnc3SCc4ccccc4Cl		1,2,4-triazole deriv.; T-6651-027		535.07	2.79
OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(CCCC)nn c3SCc4cc(Cl)ccc4		1,2,4-triazole deriv.; T-6651-028		535.07	2.79
OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(CCCC)nn c3SCc4ccc(Cl)cc4		1,2,4-triazole deriv.; T-6651-029		535.07	2.79
OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(SCCC)nnc3CCc4ccccc4		1,2,4-triazole deriv.; T-6651-009	C28H28N4O3S	500.62	2.68

OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(CCCC)nn c3SCc4cccc4		1,2,4-triazole deriv.; T-6651-021	C28H28N4O3S	500.62	2.70
OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(CCCC)nn c3SCc4ccc(C(F)(F)F)cc4		1,2,4-triazole deriv.; T-6651-034		568.62	2.78
OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(CCCC)nn c3SCc4ccccc4C#N		1,2,4-triazole deriv.; T-6651-033	C29H27N5O3S	525.63	3.09
OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(CCCC)nn		1,2,4-triazole deriv.;		528.63	2.86
c3SCC(=0)c4cccc4 OC(=0)c1ccccc1C(=0)Nc2ccc(cc2)Cn3c(SCCC)nn c3CCCc4cccc4		1,2,4-triazole deriv.;		514.65	2.71
OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(CCCC)nn		1,2,4-triazole deriv.;		514.65	2.73
c3SCCc4ccccc4 OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(CCCC)nn		1,2,4-triazole deriv.;		514.65	2.74
c3SCc4cccc4C OC(=0)c1ccccc1C(=0)Nc2ccc(cc2)Cn3c(CCCC)nn		1,2,4-triazole deriv.;		514.65	2.74
c3SCc4cc(C)ccc4 OC(=0)c1ccccc1C(=0)Nc2ccc(cc2)Cn3c(CCCC)nn		1,2,4-triazole deriv.;		514.65	2.74
c3SCc4ccc(C)cc4 OC(=0)c1ccccc1C(=0)Nc2ccc(cc2)Cn3c(CCCC)nn		1,2,4-triazole deriv.;		530.65	2.90
c3SCc4cc(OC)ccc4 OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(CCCC)nn		1,2,4-triazole deriv.;		530.65	2.90
c3SCc4ccc(OC)cc4 OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(CCCC)nn		1,2,4-triazole deriv.;		546.65	2.96
c3S(=0)Cc4ccc(OC)cc4 CCCc1nc(C(C)(C)O)c(C(=O)OCC5=C(C)OC(=O)O5		T-6651-032 olmesartan		040.00	2.00
)n1Cc2ccc(cc2)c3ccccc3c4nnn4	144689-63-4	medoximil	C29H30N6O6	558.59	4.60
O1C(=O)OC(=C1C)COC(=O)c2cccc3nc(OCC)n(c23)Cc4ccc(cc4)c5ccccc5c6nc(O)on6	863031-24-7	azilsartan medoxomil	C30H24N4O8	568.54	3.99
OC(=0)c1ccccc1C(=0)Nc2ccc(cc2)Cn3c(CCCC)nn c3SC(C(=0)OC)c4ccccc4		1,2,4-triazole deriv.; T-6651-036		558.66	3.03
OC(=0)c1cccc1C(=0)Nc2ccc(cc2)Cn3c(CCCC)nn c3SCc4cccc4C(=0)OC		1,2,4-triazole deriv.; T-6651-037	C30H30N4O5S	558.66	3.05
OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(CCCC)nn c3SCc4cc(C(=O)OC)ccc4		1,2,4-triazole deriv.; T-6651-038	C30H30N4O5S	558.66	3.05
O=C1N(Cc2sccc2C(=O)OC)C(C)=NC(CCCC)=C1C c2ccc(cc2)c3ccccc3c4nnnn4	148564-47-0	milfasartan	C30H30N6O3S	554.67	3.11
c1n2CCCCc2nc1c3cc4n(Cc5ccc(cc5)c6cccc6C(= O)O)c(CC)nc4c(C)c3	144702-17-0	pomisartan	C31H30N4O2	490.61	5.10
OC(=O)c1ccccc1C(=O)Nc2ccc(cc2)Cn3c(CCCC)nn c3SCc4cc5cccc5cc4		1,2,4-triazole deriv.; T-6651-035	C32H30N4O3S	550.68	2.79
OC(=O)c1ccccc1c2ccc(cc2)Cn3c(CCC)nc4c(C)cc(c c34)c5n(C)c6cccc6n5	144701-48-4	telmisartan	C33H30N4O2	514.63	5.10
O=C(N1CCC[C@]1([H])C(=O)N[C@@](C)([H])C(O) =O)[C@@]([H])(Cc2cncn2)NC(=O)[C@@]([H])(NC(=O)[C@@]([H])(NC(=O)[C@@]([H])(N C(=O)[C@@]([H])(NC(=O)CNC)CCCNC(N)=N)C(C) C)C(C)C	34273-10-4	saralasin	C42H65N13O10	912.06	2.16
O=C(N1CCC[C@]1([H])C(=O)N[C@]([H])(CCCNC(N)=N)C(=O)N2CCC[C@@]2([H])C(=O)N[C@]([H])(CCC(N)=O)C(=O)N[C@]([H])(C(=O)N3CCC[C@@]3([H])C(=O)N4CCC[C@@]4([H])C(O)=O)[C@@](C([H])CC)[C@@]([H])(C/C5=C/NC=6C=CC=CC5=6)NC(=O)[C@@]7([H])CCC(=O)N7	35115-60-7	teprotide	C53H76N14O12	1101.28	2.16

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