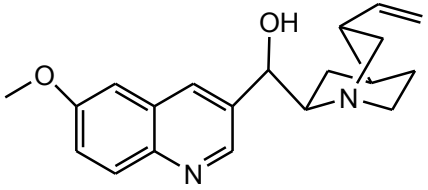
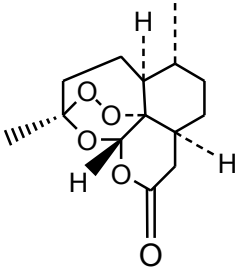
Material Suplementario 1: Estructuras antimaláricas de referencia utilizadas para el estudio de similitud molecular.

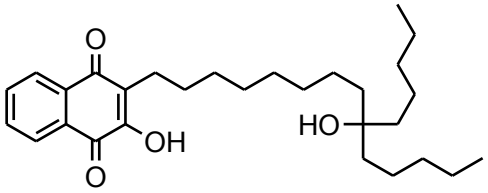
QUININA



ARTEMISINA



LAPINONE



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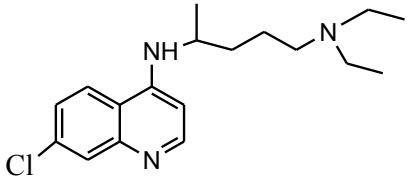
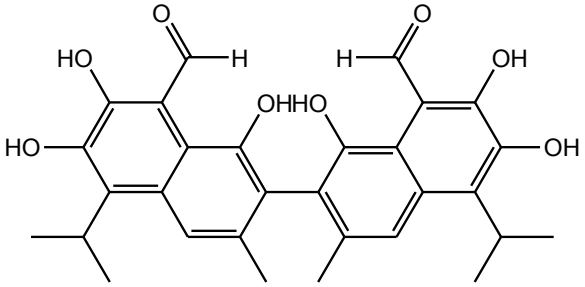
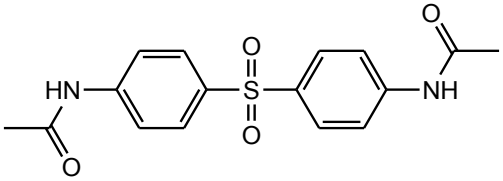


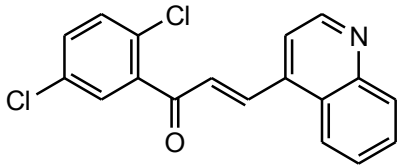
GOSSYPOL

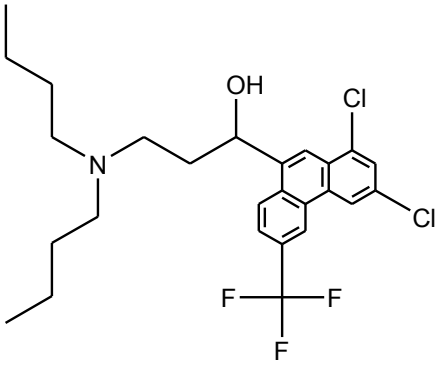
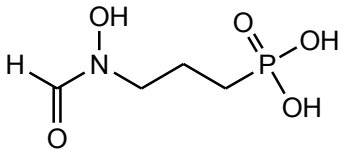
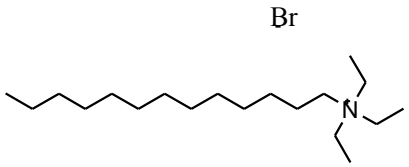
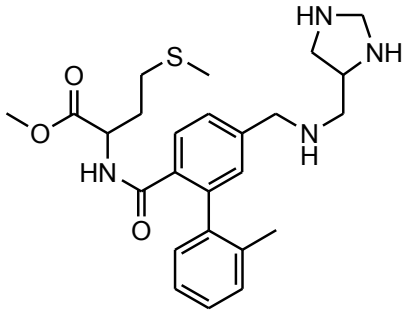


ACEDAPSONE



CHALCONE



HALOFANTRINA	FOSMIDOMYCIN	CALAS97-E10	FTI 2153
			
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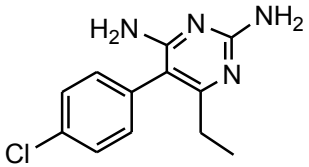
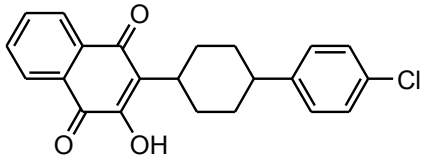
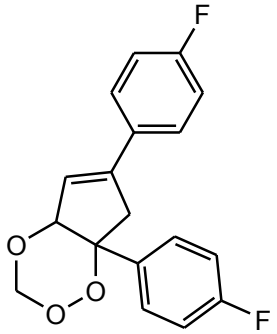
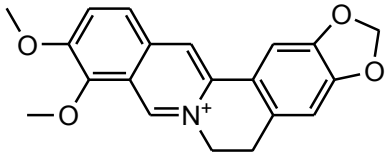
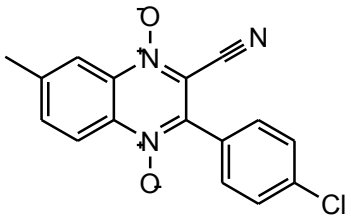
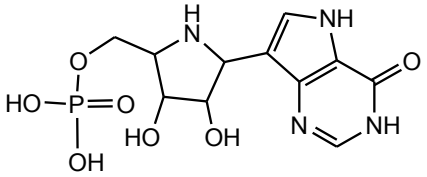
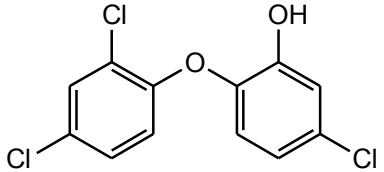
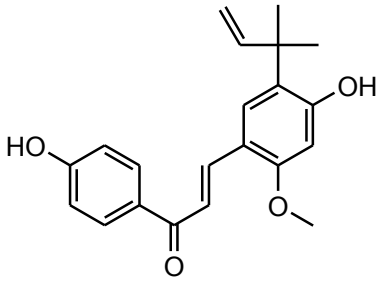
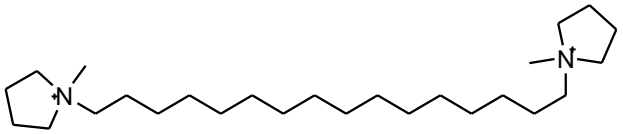
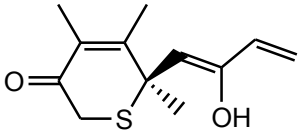
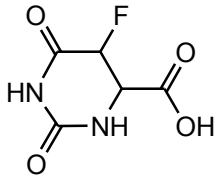
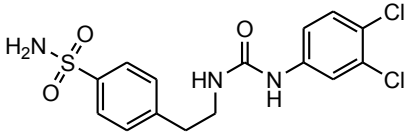
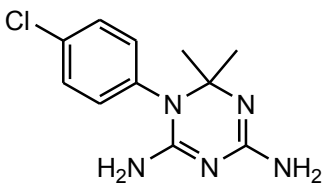
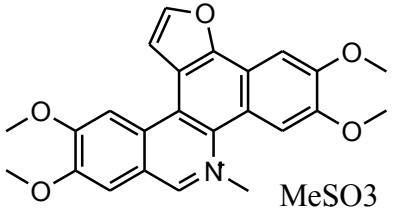
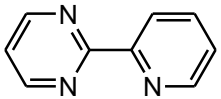
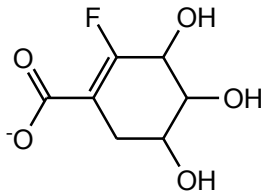
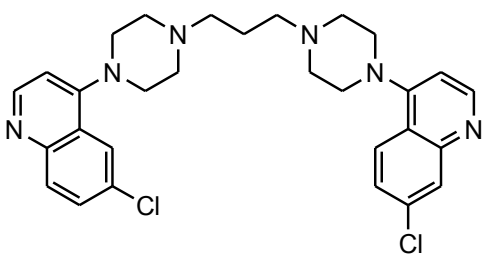
			

VICENTE ESTHER08-7	INMUNCILLIN HP	TRICLOSAN	LICOCHALCONE-A
			

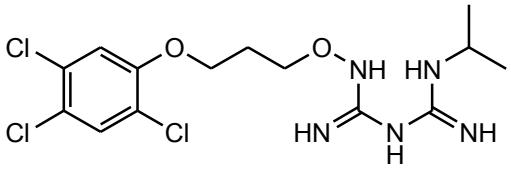
GALVEZ05-G25	TIALACTOMICINA	5-FLUOROOATE	KRUNGKRAI04-18
			

CYCLOGUANIL	NYANGULU05-7	2-(2-PYRIDINYL)-PYRIMIDINE	6-R FLUOROSHIKIMATE
	 MeSO3		

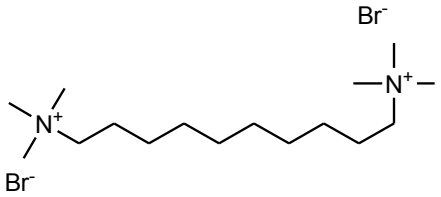
PIPERAQUINA



PS-15



DECAMETONIUM BROMIDE



Material Suplementario 2: SMILES de los 154 compuestos seleccionados por similitud molecular con un *score fusionado* (*sf*)> 66%.

Smiles	Nombre
C1(=C[C@H]([C@H]([C@@H](C1)O)O)O)C(=O)O	SHIKIMIC ACID
[nH]1c(=O)c(c[nH]c1=O)F	FLUOROURACIL
c1(cc(c(c(c1)O)C(=O)/C=C/c1cc(c(cc1)O)OC)OC)OC	2',4-DIHYDROXY-3,4',6'-TRIMETHOXYCHALCONE
c1(cc(c(c(c1)O)C(=O)/C=C/c1cc(c(cc1)OC)O)OC)OC	2',3-DIHYDROXY-4,4',6'-TRIMETHOXYCHALCONE
N1C(=O)C(=O)C(=O)NC1=O	ALLOXAN
c12c(c(c(=O)oc1c(c1c(c2OC)C=CC(O1)(C)C)CC=C(C)C)c1ccc(cc1)O)O	LONCHOCARPIC ACID
c1(c(c(cc(c1)Cl)Cl)[O-])Sc1c(c(cc(c1)Cl)Cl)[O-]	BITHIONATE SODIUM
[C@@]12(C3=CC(=O)O[C@H]([C@@]3(CCC1C1(C(=O)[C@@H](C(=O)C([C@@H]1CC(=O)O)(C)C)C2)C)C)c1cocc1)O	8-HYDROXYCARAPINIC ACID
c12c(=O)c(coc1c1c(c(c2O)CC=C(C)C)OC(C=C1)(C)C)c1cc(c(cc1)O)O	POMIFERIN
c1(ccc(c(c1)O)C(=O)/C=C/c1cc(c(cc1)OC)OC)O	2',4'-DIHYDROXY-3,4-DIMETHOXYCHALCONE
c1(Cc2c(c(cc(c2O)Cl)Cl)Cl)c(c(cc(c1O)Cl)Cl)Cl	HEXACHLOROPHENE
c1(Cc2c(ccc(c2)Cl)O)c(ccc(c1)Cl)O	DICHLOROPHENE
[C@@]12(C[C@H](OC(=O)[C@@H]1CC[C@@]1(C2C(=O)[C@H](CC1C(=O)OC)OC(=O)C)C)c1cocc1)C	SALVINORIN A
c1(C(=O)[C@@H](c2ccc(cc2)OC)C)c(cc(cc1)O)O	ANGOLENSIN (R)
c12C(=O)c3c(C(=O)c1ccc(c2O)O)cccc3	ALIZARIN
c12c(C(=O)c3c(C1=O)c(c(cc3O)C)O)c(c(cc2O)C)O	1,4,5,8-TETRAHYDROXY-2,6-DIMETHYLANTHROQUINONE
c12C(=O)c3c(C(=O)c1ccc(c2O)O)c(ccc3O)O	QUINALIZARIN
c1(ccc(c(c1)O)C(=O)/C=C/c1ccc(cc1)OC)O	2',4'-DIHYDROXY-4-METHOXYCHALCONE
c12c(c3c(cc1CC[N+](=C2)C)OCO3)OC	COTARNINE CHLORIDE

Smiles	Nombre
S(=O)(=O)(NC(=O)NCCC)c1ccc(cc1)Cl	CHLORPROPAMIDE
C(=O)(c1c(cc(cc1)OC)O)c1c(O)cccc1	DIOXYBENZONE
c1(c(c2c(c3c(cc2oc1=O)OC(C=C3)(C)C)OC)O)c1ccc(cc1)OC	ROBUSTIC ACID
c1(C(=O)Oc2c(c(c(c(c2)C)C(=O)OC)O)C)c(c(c(cc1C)O)C=O)O	ATRANORIN
c1(C(=O)Oc2cc(c(c(c2)C)C(=O)O)O)c(cc(cc1C)OC)O	EVERNIC ACID
n1(C2C([C@@H]([C@H](O2)C)O)O)c(=O)[nH]c(=O)c(c1)F	5-FLUORO-5'-DEOXYURIDINE
c1(C(=O)Oc2c(c(c(c(c2)C)C(=O)O)O)C)c(c(c(cc1C)OC)C)OC	DIFFRACTAIC ACID
c1(C(=O)Oc2c(c(c(c(c2)C)O)C(=O)O)C)c(c(c(cc1C)OC)C=O)O	BAEOMYCESIC ACID
S(=O)(=O)(NC(=O)c1ccccc1)c1ccc(N)cc1	SULFABENZAMIDE
C12(C(C(=C)C[C@@H](C1C(CCC2)(C)C)O)CC[C@@](C=C)(O)C)C	LARIXOL
C1(=CC(=O)C(=CC1=O)OC)C(c1ccc(cc1)O)C=C	DALBERGIONE, 4-METHOXY-4'-HYDROXY-
C1(=CC(=O)C(=CC1=O)OC)C(c1ccc(cc1)OC)C=C	4,4'-DIMETHOXYDALBERGIONE
c12c(c3c(c(c2O)CC=C(C)C)OC(C=C3)(C)C)occ(c1=O)c1ccc(cc1)O	OSAJIN
[C@]12([C@](C(=CC(=O)C1C(CCC2)(C)C)C)(CCc1cocc1)O)C	SOLIDAGENONE
c12c(C(=O)c3c(C1=O)cccc3)c(c(cc2O)O)O	PURPURIN
c12c(=O)c3c(c(c(cc3oc2cc(c(c1O)CC=C(C)C)OC)OC)O)CC=C(C)C	beta-MANGOSTIN
C12=CCc3c(C2CCC2(C1CCC2=O)C)ccc(c3)O	EQUILIN
C1(=Nc2c(Nc3c1cccc3)ccc(c2)Cl)N1CCN(CC1)C	CLOZAPINE
c1(c(c(c(c(c1Cl)O)Cl)Cl)Cl)Cl	PENTACHLOROPHENOL
[C@@]12(C[C@H](OC(=O)[C@@H]1CC[C@@]1(C2C(=O)[C@H](CC1C(=O)OC)O)C)c1cocc1)C	SALVINORIN B
c1(C(=O)c2ccccc2)c(cc(c(c1)O)OC)O	CEAROIN
c1cc(c2c(c1)C(=O)C(=CC2=O)C)O	PLUMBAGIN
[C@]12(C([C@@]([C@@H](CC2)O)(CO)C)CCC(=C)[C@H]1C/C=C\1/C(=O)OC[C@H]1O)C	ANDROGRAPHOLIDE
c12C(=O)O[C@@H]([C@H]3c4c(c5c(cc4CCN3C)OCO5)OC)c1ccc(c2OC)OC	NOSCAPINE HYDROCHLORIDE
[n+]12c(c3cc(c(cc3cc2)OC)OC)cc2c(c1C)cc(c(c2)OC)OC	CORALYNE CHLORIDE

Smiles	Nombre
c12c(c(c(cc2O)OC)CC=C(C)C)oc(cc1=O)C	HETEROPEUCENIN, METHYL ETHER
c1(c(cc(cc1OC)OC)O)C(=O)C	XANTHOXYLIN
c1(c(cc(c(c1O)C)OC)OC)C(=O)C	METHYLXANTHOXYLIN
c12c(=O)cc(oc2cc(c(c1O)OC)OC)c1cc(c(cc1)OC)O	EUPATORIN
S(=O)(=O)(NC(=O)C)c1ccc(N)cc1	SULFACETAMIDE
c1c(ccc(c1)S(=O)(=O)c1ccc(cc1)NC(=O)N)N	AMIDAPSONE
c12C(=O)C3c4c(OCC3Oc2cc2c(c1O)C=CC(O2)(C)C)cc(c(c4)OC)OC	beta-TOXICAROL
c1c(c(nc(=O)[nH]1)N)F	FLUCYTOSINE
C12(C([C@H](CC(=C)C1CC[C@@](C=C)(O)C)OC(=O)C)C(CCC2)(C)C)C	LARIXOL ACETATE
[C@]12(c3c(c(c(cc3CCC1C(CCC2)(C)C)C(C)C)O)O)C(=O)O	CARNOSIC ACID
c12C(=O)O[C@@H](c1ccc(c2OC)OC)[C@@H]1c2c(cc3c(c2)OCO3)CCN1C	HYDRASTINE (1S,9R)
c1(nnc(c(n1)N)c1c(c(ccc1)Cl)Cl)N	LAMOTRIGINE
[C@@]1(C[C@H]([C@H]([C@@H](C1)O)O)O)(C(=O)O)O	QUINIC ACID
C1(=CC(=O)C(=C(C1=O)OC)OC)[C@H](C=C)c1ccccc1	3,4-DIMETHOXYDALBERGIONE
C1(=O)c2c(C(=O)c3c1c(cc(c3)C)O)cc(cc2O)OC	PHYSCION
c1(c(cc(/C=C/C(=O)O)cc1OC)OC)OC	SINAPIC ACID METHYL ETHER
c12c(c(c(c(c1O)C/C=C(/CCC(=O)O)\C)OC)C)COC2=O	MYCOPHENOLIC ACID
c12c(c(c(cc2oc(cc1=O)C)O)CC=C(C)C)O	PEUCENIN
C12(c3c(c(c(c(c3O)C)O)C(=O)C)OC1=CC(=O)C(C2=O)C(=O)C)C	USNIC ACID
c12[C@H]([C@H](C(Oc2ccc2c1oc(=O)cc2)(C)C)OC(=O)C)OC(=O)/C(=C/C)/C	PTERYXIN
c1(c(ccc(c1)O)Cl)C	CHLOROCRESOL
N1(c2ncccc2)CCN(CC1)CCCC(=O)c1ccc(cc1)F	AZAPERONE
c1cc(c2c(c1O)C(=O)C(=C(C2=O)Cl)Cl)O	2,3-DICHLORO-5,8-DIHYDROXYNAPTHOQUINONE

Smiles	Nombre
c12C(=O)c3c(C(=O)c1cc(cc2O)C)cccc3O	CHRYSOPHANOL
c1(c(cc(cc1OC)C(=O)C)OC)O	ACETOSYRINGONE
c1(c(cc(cc1O)OC)O)C(=O)C	4-O-METHYLPHLORACETO PHENONE
c1(c(cc(cc1C)OC)OC)C(=O)O	ORSELLINIC ACID DIMETHYL ETHER
c1(c(cc(cc1C)OC)O)C(=O)OC	METHYL EVERNINATE
c1(c(cc2OC(C=Cc2c1)(C)C)O)C(=O)C	EUPATORIOCHROMENE
c12oc(cc(=O)c1ccc(c2O)O)c1ccccc1	7,8-DIHYDROXYFLAVONE
c1(c(c(=O)c2c(o1)cc(cc2)O)O)c1cc(c(cc1)O)O	FISETIN
c1ccc2c(c1)oc(cc2=O)c1ccc(c(c1)O)O	3',4'-DIHYDROXYFLAVONE
[N+](CCOC(=O)C)(C)(C)C	ACETYLCHOLINE
C\1(=C\c2cc(c(cc2)OC)O)/C(=O)c2c(OC1)cc(cc2)OC	SAPPANONE A DIMETHYL ETHER
c1(c(=O)c2c(oc1)cc1OC(C(Cc1c2)O)(C)C)c1c(c2c(OC(C=C2)(C)C)cc1)OC	MUNDULONE
[C@@H]1(CCC(C2[C@@]31[C@H]1[C@@]4([C@@](C2O)(O)OC3)C([C@@H](CC1)C(=C)C4=O)O)(C)C)O	RUBESCENSIN A
C12=CO[C@@H]([C@H](C1=C(C(=O)C(=C2O)C(=O)O)C)C)C	CITRININ
c1(C(=O)Oc2cc(c(c(c2)C)C(=O)O)O)c(cc(cc1C)O)O	LECANORIC ACID
c12c(C(=O)[C@H]3c4c(OC[C@H]3O1)cc(c(c4)OC)OC)ccc1c2C=CC(O1)(C)C	DEGUELIN(-)
C(=C(\c1ccccc1)/O)/C(=O)c1c(O)cccc1	2',beta-DIHYDROXYCHALCONE
C(C(=O)c1ccc(C(C)(C)C)cc1)C(=O)c1ccc(cc1)OC	AVOBENZONE
c12c(=O)c(coc1c(c(cc2O)OC)OC)c1ccc(cc1)OC	ISOTECTORIGENIN, 7-METHYL ETHER
c1(c(=O)c2c(oc1)cc(cc2)O)c1c(c(c(cc1)OC)O)O	KOPARIN
c1(c(oc2c(c1=O)c(cc(c2)OC)OC)c1cc(c(cc1)OC)OC)O	QUERCETIN TETRAMETHYL (5,7,3',4') ETHER

Smiles	Nombre
c1(c(oc2c(c1=O)c(cc(c2)OC)O)c1cc(c(cc1)O)O)O	RHAMNETIN
c12c(oc(cc2=O)c2cc(c(cc2)OC)OC)c(c(c(c1O)OC)OC)OC	DEMETHYLNOBILETIN
c12c(oc(cc2=O)c2ccc(cc2)OC)c(c(c(c1O)OC)OC)OC	GARDENIN B
c1(cc(c2c(c1OC)oc(cc2=O)c1c(cc(cc1)OC)OC)O)OC	5-HYDROXY-2',4',7,8-TETRAMETHOXYFLAVONE
c1(C(=O)c2ccccc2)c(cc(cc1)OC)O	OXYBENZONE
c1(c(cc(c(c1)C(C)(C)C)O)C(C)(C)C)OC	2,5-DI-t-BUTYL-4-HYDROXYANISOLE
[N+](CCO)(C)(C)C	CHOLINE CHLORIDE
S(=O)(=O)(Nc1ccc([N+](=O)[O-])cc1)c1ccc(NC(=O)C)cc1	SULFANITRAN
N1C(=O)NC(C1=O)NC(=O)N	ALLANTOIN
N(CCCl)(CCCl)C	MECHLORETHAMINE
c12c(c3c(cc1CCN(C2)C)OCO3)OC	HYDROCOTARNINE HYDROBROMIDE
[C@@]123[C@@H]([C@@](C(=O)O1)([C@H](C=C3)O)C)[C@@H]([C@]13[C@H]2CC[C@](C1)(C(=C)C3)O)C(=O)O	GIBBERELLIC ACID
[N+]1(CCCCC[N+]2(C)CCCC2)(C)CCCC1	PENTOLINIUM TARTRATE
[C@]12([C@@](C(=O)CO)(CCC1C1C([C@@]3(C(=CC(=O)CC3)CC1)C)[C@H](C2)O)O)C	HYDROCORTISONE
[C@]12([C@@](C(=O)CO)(CCC1C1C([C@@]3(C(=CC(=O)C=C3)CC1)C)[C@H](C2)O)O)C	PREDNISOLONE
[C@]12([C@@](C(=O)CO)(CCC1C1C([C@@]3(C(=CC(=O)C=C3)CC1)C)C(=O)C2)O)C	PREDNISONE
[C@]12([C@@](C(=O)CO)(CCC1C1C([C@@]3(C(=CC(=O)CC3)CC1)C)C(=O)C2)O)C	CORTISONE
[C@]12([C@@](C(=O)COC(=O)C)(CCC1C1C([C@@]3(C(=CC(=O)CC3)CC1)C)[C@H](C2)O)O)C	HYDROCORTISONE ACETATE
[C@@]12(C(=CC(=O)C=C2)[C@H](CC2C1[C@H](C[C@@]1([C@@](C(=O)CO)(CCC21O)C)O)C)C	METHYLPREDNISOLONE
[C@]12([C@@](C(=O)COC(=O)C)(CCC1C1C(C3(C(=CC(=O)C=C3)CC1)C)[C@H](C2)O)O)C	PREDNISOLONE ACETATE
[C@@]12(C(=CC(=O)CC2)C=CC2C1CC[C@]1(C2CC[C@]1(CCC(=O)[O-])O)C)C	CANRENOIC ACID, POTASSIUM SALT
C12=CC(=O)C3[C@]([C@@]1(CC[C@@]1([C@@H]2C[C@@](C(=O)O)(CC1)C)C)C)(CCC1[C@@]3(CC[C@@H](C1(C)C)O)C)C	18alpha-GLYCYRRHETINIC ACID

Smiles	Nombre
[C@]12([C@@](C(=O)CO)(CCC1[C@H]1C([C@@]3(C(=CC(=O)CC3)CC1)C)[C@H](C2)O)OC(=O)CC)C	HYDROCORTISONE BUTYRATE
C1=C[C@]2(C(=CC1=O)CCC1C2[C@H](C[C@]2(C1CC[C@@]2(C(=O)COC(=O)CC(C)(C)C)O)C)O)C	PREDNISOLONE TEBUTATE
[C@]12([C@](CCC1C1C([C@@]3(C(=CC(=O)CC3)CC1)C)CC2)(C(=O)C)O)C	HYDROXYPROGESTERONE
[C@]12([C@@](C(=O)COC(=O)C)(CCC1C1C([C@@]3(C(=CC(=O)CC3)CC1)C)C(=O)C2)O)C	CORTISONE ACETATE
C12=CCC3[C@]([C@@]1(CC[C@@]1([C@H]2[C@H]([C@@H](CC1)C)C)C(=O)O)C)(C[C@H](C1[C@@]3(C[C@H]([C@@H]([C@]1(CO)C)O)O)C)O)C	MADECASSIC ACID
C12([C@@]3(C(C4[C@@]([C@](CC4)(C(=O)C)O)(C[C@@H]3O)C)C[C@@H](C1=CC(=O)C=C2)C)F)C	FLUOROMETHOLONE
[C@]12([C@@]3(C([C@@]4([C@H]([C@@H]([C@@H](CC4)O)C)CC3)C)[C@@H](C[C@H]1/C(=C(\C(=O)O)/CCC=C(C)C)/[C@H](C2)OC(=O)C)O)C)C	FUSIDIC ACID
[C@@]12(C(=CC(=O)CC2)[C@H](CC2C1[C@H](C[C@]1(C2CC[C@@H]1C(=O)C)C)O)C)C	MEDRYSONE
[C@@]12(C(C3C([C@@]4(C(=CC3)C[C@H](CC4)O)C)CC2)CC[C@@H]1C(=O)COC(=O)C)C	21-ACETOXYPREGNENOLONE
[C@@]12(C(C3[C@@]([C@@]4(C(=CC(=O)C=C4)CC3)C)([C@H](C2)O)F)C[C@@H]([C@@]1(C(=O)CO)O)C)C	BETAMETHASONE
[C@@]12(C(C3[C@@]([C@@]4(C(=CC(=O)C=C4)CC3)C)([C@H](C2)O)F)C[C@H]([C@@]1(C(=O)COC(=O)C)O)C)C	DEXAMETHASONE ACETATE
[C@]12([C@@](C(=O)COC(=O)C)(CCC1C1[C@@]([C@@]3(C(=CC(=O)CC3)CC1)C)([C@H](C2)O)F)O)C	FLUDROCORTISONE ACETATE
[C@]12([C@]([C@@H](CC1C1[C@@]([C@@]3(C(=CC(=O)C=C3)CC1)C)([C@H](C2)O)F)O)(C(=O)CO)O)C	TRIAMCINOLONE
[C@]12([C@]([C@@H](CC1C1[C@@]([C@@]3(C(=CC(=O)C=C3)CC1)C)([C@H](C2)O)F)OC(=O)C)(C(=O)COC(=O)C)O)C	TRIAMCINOLONE DIACETATE
[C@@]12(C(=CC(=O)CC2)CCC2C1CC[C@]1(C2CC[C@@H]1O)C)C	TESTOSTERONE
[C@]12([C@@](C(=O)CO)(CCC1C1C([C@@]3([C@H](CC1)C[C@@H](CC3)O)C)C(=O)C2)O)C	TETRAHYDROCORTISONE
C123C(O3)C(=O)O[C@H]([C@@]2(CCC2[C@]1([C@@H](CC1[C@@]2(CCC(=O)C1(C)C)C)OC(=O)C)C)C)c1cocc1	DIHYDROGEDUNIN

Smiles	Nombre
[C@@]123[C@H](O3)C(=O)O[C@H]([C@@]2(CCC2[C@]1([C@@H](CC1[C@@]2(CC[C@@H](C1(C)C)OC(=O)C)C)OC(=O)C)C)C)c1cocc1	3beta-ACETOXYDEOXODIHYDROGEDUNIN
[C@@]12(C(C3C([C@@H]4C(=CC(=O)CC4)CC3)CC2)CC[C@]1(C#C)O)CC	NORGESTREL
C12(C(=CC(=O)CC2)CCC2C1CCC1(C2CCC1(C#C)O)C)C	ETHISTERONE
[C@@]123[C@H](O3)C(=O)O[C@H]([C@@]2(CC[C@H]2[C@]1(C(=O)C[C@@H]1[C@@]32[C@@H](OC1(C)C)CC(=O)OC3)C)C)c1cocc1	LIMONIN
[C@@]123[C@H](O3)C(=O)O[C@H]([C@@]2(CCC2[C@]1(C(=O)CC1[C@@]2(C=CC(=O)C1(C)C)C)C)c1cocc1	DEACETOXY-7-OXOGEDUNIN
[C@@]123[C@H](O3)C(=O)O[C@H]([C@@]2(CCC2[C@]1(C(=O)CC1[C@@]2([C@H](C[C@H](C1(C)C)OC(=O)C)OC(=O)C)C)C)c1cocc1	7-DEACETOXY-7-OXOKHIVORIN
C123C(O3)C(=O)O[C@H]([C@@]2(CCC2[C@]1([C@@H](CC1[C@@]2(C2C(O2)C(=O)C1(C)C)C)OC(=O)C)C)C)c1cocc1	EPOXYGEDUNIN
C123C(O3)C(=O)O[C@H]([C@@]2(CCC2[C@]1(C(=O)CC1[C@@]2(C(=O)C=CC1(C)C)C)C)C)c1cocc1	DEACETOXY-7-OXISOGEDUNIN
C123C(O3)C(=O)O[C@H]([C@@]2(CCC2[C@]1(C(=O)CC1[C@@]2(C(=O)C[C@H](C1(C)C)OC(=O)C)C)C)C)c1cocc1	1,7-DIDEACETOXY-1,7-DIOXOKHIVORIN
[C@@]123[C@H](O3)C(=O)O[C@H]([C@@]2(CCC2[C@]1(C(=O)CC1[C@@]2([C@@H](CC(=O)OC1(C)C)OC(=O)C)C)C)C)c1cocc1	NOMILIN
[C@]12(C(C3C([C@@]4([C@H](CC3)C[C@@H](CC4)O)C)C[C@@H]1O)CC[C@@H]2[C@@H](CCC(=O)O)C)C	DEOXYCHOLIC ACID
[C@]12(C3C(C4[C@@]([C@H](CC4)[C@@H](CCC(=O)O)C)(CC3)C)C[C@@H]([C@@H]1C[C@@H](CC2)O)O)C	alpha-HYDROXYDEOXYCHOLIC ACID
[C@@]12(C(C3C([C@@]4([C@H](C[C@@H]3O)C[C@@H](CC4)O)C)CC2)CC[C@@H]1C(CCC(=O)O)C)C	URSODIOL
[C@]12(C(C3C([C@@]4([C@H](C[C@H]3O)C[C@@H](CC4)O)C)C[C@@H]1O)CC[C@@H]2[C@@H](CCC(=O)O)C)C	CHOLIC ACID

Smiles	Nombre
[C@]12([C@@]3(C(C4[C@@]([C@]([C@@H](C4)C)(C(=O)CO)O)(C[C@@H]3O)C)C[C@@H](C1=CC(=O)C=C2)F)F)C	FLUMETHASONE
[C@]12([C@]([C@H](CC1C1[C@@]([C@@]3(C(=CC(=O)C=C3)CC1)C)([C@H](C2)O)F)C)(C(=O)CCl)OC(=O)CC)C	CLOBETASOL PROPIONATE
C12(C(C3C(C4([C@H](CC(OC(=O)C)CC4)CC3)C)CC2=O)CC2C1[C@@H](C1(O2)OCC(CC1)C)C)C	HECOGENIN ACETATE
C12=C(CC(=O)CC2)CCC2C3[C@@]([C@](C#C)(CC3)O)(CCC12)C	NORETHYNODREL
[C@@]12(C(C3C([C@@]4(C(=CC3)C[C@H](CC4)O)C)CC2)CC[C@@H]1C(=O)C)C	PREGNENOLONE
[C@@]123[C@H](O3)C(=O)O[C@H]([C@@]2(CCC2[C@]1([C@@H](CC1[C@@]2(C=CC(=O)C1(C)C)C)OC(=O)C)C)C)c1cocc1	GEDUNIN
C123C(O3)C(=O)O[C@H]([C@@]2(CCC2[C@]1([C@@H](CC1[C@@]2(C(=O)C=CC1(C)C)C)OC(=O)C)C)C)c1cocc1	ISOGEDUNIN
C12=CC(=O)O[C@H]([C@@]2(CCC2C1([C@@H](CC1C2(CC[C@@H](C1(C)C)O)C)OC(=O)C)C)C)c1cocc1	3beta-HYDROXYDEOXODIHYDRODEOXYGEDUNIN
[C@]12([C@@]3(C(C4[C@@]([C@]([C@@H](C4)C)(C(=O)COC(=O)C(C)(C)C)O)(C[C@@H]3O)C)C[C@@H](C1=CC(=O)C=C2)F)F)C	FLUMETHAZONE PIVALATE
[C@@]12(C(=CC(=O)CC2)CCC2C1CC[C@]1(C2CC[C@@H]1OC(=O)CC)C)C	TESTOSTERONE PROPIONATE
[C@@]12(C(=CC(=O)CC2)[C@H](CC2C1CC[C@@]1([C@@](CCC21)(OC(=O)C)C(=O)C)C)C)C	MEDROXYPROGESTERONE ACETATE
C12=CC(=O)CCC1(C1C(C=C2C)C2C([C@@](CC2)(OC(=O)C)C(=O)C)(CC1)C)C	MEGESTROL ACETATE
[C@]12(C3=CCC4[C@@](C3CC[C@]1([C@H]([C@H](C1OC(C(C1O)O)(C)C)C)CC2)C)(CCC(=O)C4(C)C)C)C	ODORATONE

Material Suplementario 3: Desempeño de los 37 modelos QSAR obtenidos por ADL.

Modelo	*C*	Q	Sens	Spec	FAR	λ Wilks	D^2	F
1	0,73 [0,74]	86,86 [87,56]	89,03 [80,26]	78,24 [87,79]	14,40 [7,5]	0,47	4,90	281,3377
2	0,77 [0,77]	89,28 [88,95]	89,50 [81,70]	82,75 [90,14]	10,85 [6,10]	0,45	5,32	305,3036
3	0,77 [0,74]	89,11 [87,74]	89,81 [80,08]	82,21 [88,73]	11,30 [7,00]	0,43	5,61	322,1649
4	0,79 [0,78]	90,03 [89,81]	89,81 [84,68]	84,14 [88,26]	9,85 [7,00]	0,43	5,73	329,1215
5	0,80 [0,81]	90,66 [91,02]	91,69 [85,15]	84,29 [91,55]	9,94 [5,14]	0,42	5,96	342,4944
6	0,73 [0,73]	87,09 [87,05]	88,71 [80,80]	78,83 [84,98]	13,86 [9,01]	0,48	4,59	263,4684
7	0,76 [0,73]	88,88 [87,22]	87,77 [80,35]	82,96 [86,38]	10,48 [8,29]	0,46	5,10	292,9673
8	0,76 [0,74]	88,59 [87,74]	88,24 [82,87]	82,07 [84,04]	11,21 [9,37]	0,46	4,97	221,5716
9	0,80 [0,80]	90,37 [90,85]	89,34 [86,36]	85,20 [89,20]	9,02 [6,41]	0,42	5,89	262,8651
10	0,79 [0,81]	90,26 [90,85]	89,66 [86,04]	84,74 [89,67]	9,39 [6,16]	0,43	5,77	331,5598
11	0,75 [0,74]	88,07 [87,74]	89,66 [80,08]	80,22 [88,73]	12,85 [7,00]	0,46	5,00	287,3787
12	0,77 [0,76]	88,82 [88,43]	89,50 [82,02]	81,81 [87,79]	11,58 [7,41]	0,46	5,07	291,2286
13	0,73 [0,72]	87,32 [86,87]	87,30 [80,44]	80,03 [84,98]	12,67 [9,04]	0,47	4,85	278,3801
14	0,77 [0,77]	89,16 [89,12]	88,71 [82,89]	82,99 [88,73]	10,57 [6,84]	0,45	5,22	299,4637
15	0,79 [0,77]	89,97 [89,29]	88,24 [83,56]	85,05 [88,26]	9,02 [7,06]	0,43	5,71	327,9478
16	0,77 [0,75]	89,05 [88,08]	89,18 [81,03]	82,46 [88,26]	11,03 [7,20]	0,43	5,68	326,1627
17	0,78 [0,75]	89,57 [88,43]	89,97 [82,88]	83,07 [86,38]	10,67 [8,12]	0,42	5,91	263,8623
18	0,81 [0,81]	91,18 [91,02]	90,91 [86,76]	85,93 [89,20]	8,66 [6,39]	0,42	6,04	347,0380
19	0,76 [0,75]	88,59 [87,91]	89,03 [79,92]	81,61 [89,67]	11,67 [6,47]	0,47	4,90	281,5600
20	0,77 [0,74]	89,05 [87,74]	89,66 [80,08]	82,18 [88,73]	11,30 [7,00]	0,45	5,33	305,9011
21	0,77 [0,77]	89,22 [88,95]	89,97 [82,53]	82,35 [88,73]	11,21 [6,86]	0,43	5,60	321,6680
22	0,77 [0,79]	89,28 [90,33]	88,24 [85,84]	83,53 [88,26]	10,12 [6,94]	0,44	5,27	303,0869
23	0,79 [0,79]	90,09 [89,81]	89,97 [82,91]	84,16 [91,08]	9,85 [5,51]	0,42	5,71	255,1377
24	0,71 [0,73]	86,05 [87,39]	85,11 [81,82]	78,70 [84,51]	13,40 [9,19]	0,50	4,21	241,9065

Modelo	*C*	Q	Sens	Spec	FAR	λ Wilks	D^2	F
25	0,73 [0,73]	87,09 [86,87]	87,30 [79,40]	79,57 [86,85]	13,04 [8,09]	0,48	4,59	230,6731
26	0,74 [0,71]	87,78 [86,18]	87,77 [78,79]	80,69 [85,45]	12,22 [8,91]	0,46	4,96	285,2241
27	0,74 [0,80]	87,55 [90,33]	88,40 [83,69]	79,89 [91,55]	12,94 [5,20]	0,45	5,09	292,5573
28	0,78 [0,76]	89,39 [88,60]	89,50 [83,26]	82,99 [86,38]	10,67 [8,10]	0,45	5,22	299,9503
29	0,72 [8,10]	86,80 [86,70]	86,68 [80,09]	79,34 [84,98]	13,13 [9,07]	0,49	4,32	248,6270
30	0,73 [0,76]	87,26 [88,43]	87,46 [80,93]	79,83 [89,67]	12,85 [6,41]	0,49	4,45	255,8101
31	0,74 [0,79]	87,67 [89,98]	87,93 [84,44]	80,37 [89,20]	12,49 [6,50]	0,47	4,77	274,0049
32	0,73 [0,75]	87,03 [88,08]	86,68 [81,58]	79,80 [87,32]	12,76 [7,69]	0,47	4,73	269,3719
33	0,74 [0,72]	87,55 [86,53]	87,62 [78,72]	80,32 [86,85]	12,49 [8,14]	0,48	4,60	264,4024
34	0,74 [0,74]	87,72 [87,56]	87,77 [80,26]	80,58 [87,79]	12,31 [7,51]	0,47	4,73	271,6514
35	0,78 [0,78]	89,45 [89,29]	89,66 [82,40]	83,02 [90,14]	10,67 [6,07]	0,43	5,55	221,0526
36	0,79 [0,78]	90,03 [89,81]	89,97 [84,07]	84,04 [89,20]	9,94 [6,52]	0,40	6,20	276,9992
37	0,82 [0,82]	91,41 [91,36]	91,69 [85,28]	85,90 [92,49]	8,75 [4,60]	0,38	6,82	304,4584

Leyenda: [ ] Parámetros estadísticos obtenidos para a SP.