

SP18 Chemical ligands for FKBP12 secondary assays

ID	Mol Weight	Mol Formula	Mol Name	Team 1	Team 2
97594191	373.5	C ₂₀ H ₂₁ N ₃ O ₂	1-(3-aminopropanoyl)-N-(pyridin-2-ylmethyl)-1,4-dihydropyridine-3-carboxamide	T/R Red Team	W/F Pink Team
74694438	368.5	C ₂₀ H ₂₀ N ₄ O	1-(6-(4-aminocyclohexyl)-N-(3-(4,3-dihydro-1H-indol-1-yl)propyl)-1H-1,2,3-triazole-4-carboxamide	W/F Pink Team	W/F Orange Team
76677434	369.4	C ₂₀ H ₂₀ N ₄ O ₂	4-hydroxy-N-(3R*,4R*)-4-piperidin-1-ylretarydroluran-3-yl-2-pyridin-2-ylpyrimidine-5-carboxamide	T/R Red Team	T/R Pink Team
97430942	312.4	C ₁₈ H ₂₀ N ₄ O	2-(4-(6-(isopropylamino)pyrimidin-4-yl)-1H-pyridin-2,3-dipyridin-6-ylamino)ethanol		T/R Pink Team
66267745	372.5	C ₂₀ H ₂₀ N ₄ O	(3R*,6aR*)-2-cyclopropyl-N-(6,7,8,9-tetrahydro-5H-[1,2,4]triazolo[4,3-a]azepin-3-ylmethyl)neohydroxypropyl 3-(4-chloro-3a(1H)-carboxamide	T/R Yellow Team	
40096953	323.5	C ₁₈ H ₂₁ N ₃ O ₂ S	[(3R*,4R*)-1-(2-methyl-1,3-thiazol-4-yl)carbamoyl-4-(piperidin-1-ylmethyl)pyrrolidin-3-yl]methanone	T/R Silver	
34120495	357.4	C ₂₁ H ₂₁ N ₃ O ₂ S	4-[[1-(piperidin-3-ylmethyl)-1H-1,2,3-triazol-4-yl]carbamoyl]piperazine-1-sulfonamide	T/R Pink Team	T/R Orange Team
13742946	356.5	C ₂₀ H ₂₀ N ₄ O ₂	3-[6-(2-hydroxyethyl)(methylamino)pyridazin-3-yl]-5-(2-piperidin-2-ylthyl)phenol		
16210766	373.4	C ₂₀ H ₂₁ N ₃ O ₂	[(3R*,4R*)-1-[[5-(1,5-dimethyl-1H-pyrazol-4-yl)isoxazol-3-yl]carbamoyl-4-(pyrrolidin-1-ylmethyl)pyrrolidin-3-yl]methanone		
53106246	322.4	C ₁₈ H ₂₁ N ₄ O ₂	[(3R*,4R*)-1-[[2-methoxyethyl(methylamino)methyl]-1-(quinolin-6-yl)propanoyl]pyrrolidin-3-yl]methanone	T/R Blue Team	
31064975	357.5	C ₂₁ H ₂₁ N ₃ O ₂	[(3S*,5R*)-5-[[2-methoxyethyl(methylamino)methyl]-1-(quinolin-6-ylmethyl)pyrrolidin-3-yl]methanone	W/F Silver Team	
36421524	340.5	C ₁₈ H ₂₂ N ₄ O ₄	N-cyclooctyl-N'-[(3S*,4R*)-4-ethoxytetrahydrofuran-3-yl]succinamide	T/R Yellow Team	T/R Blue Team
73410334	361.5	C ₂₀ H ₂₃ N ₃ O	[(3R*,4R*)-1-(5-ethyl-2,6-dimethylpyrimidin-4-yl)-4-(4-ethyl)piperazin-1-yl]methylpyrrolidin-3-yl]methanone		W/F Blue Team
89765560	357.9	C ₁₈ H ₂₀ ClN ₃ O ₂ S	[(3R*,4R*)-1-(3-chloro-2-thienyl)carbamoyl-4-(4-methyl)piperazin-1-yl]methylpyrrolidin-3-yl]methanone	T/R Orange Team	W/F Orange Team
71743940	335.4	C ₁₈ H ₂₁ N ₃ O ₂	1-(6-(4-aminocyclohexyl)-N-(2-(2-amino-1,3-thiazol-4-yl)ethyl)-1H-1,2,3-triazole-4-carboxamide		
77248815	357.5	C ₂₁ H ₂₁ N ₃ O ₂	4-(1-piperidinylmethyl)-N-[(3R*,4R*)-4-(1-pyrrolidinyl)butyl]dipyrro-3-furanyl]benzamide	T/R Purple Team	
95189130	386.5	C ₂₂ H ₂₆ N ₄ O ₂	[(3R*,4R*)-4-[[2-methoxyethyl(methylamino)methyl]-1-(4-(5-methyl-2-furyl)benzoyl)pyrrolidin-3-yl]methanone]	T/R White Team	W/F Green
67060995	319.4	C ₁₈ H ₂₀ N ₄ O ₂	1-(5-[[[(3R*,4R*)-1-(3-hydroxyethyl)-4-(pyrrolidin-1-ylmethyl)pyrrolidin-1-yl]methyl]-1-methyl-1H-pyridin-3-yl]ethanone		
90202210	364.5	C ₁₈ H ₂₀ N ₄ O ₂ S	[(3S*,5R*)-1-(2,1,3-benzoxadiazol-5-ylmethyl)-5-[[2-methoxyethyl(methylamino)methyl]pyrrolidin-3-yl]methanone	W/F Silver Team	W/F Blue Team
15018940	379.5	C ₂₀ H ₂₃ N ₃ O	1-(6-(4-aminocyclohexyl)-N-(4-(2-methyl-1H-indazol-1-yl)benzyl)-1H-1,2,3-triazole-4-carboxamide		

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75867752	352.5 C ₂₁ H ₂₈ N ₄ O	3-(3R*,3AR*,7AR*,11-(1-ethyl-1H-pyrazol-4-yl)methyl)octahydro-4,7-ethanopyrrolid[3,2-b]pyridin-3-yl)methanol	T/R Green	
48960545	324.5 C ₁₉ H ₂₄ N ₂ O ₂ S	(3R*,4S*,7-(4-ethyl[4-(piperidin-1-yl)methyl]-2-phenyl)methyl)amino)tetrahydrofuran-3-ol		W/F Purple
10093888	333.5 C ₂₄ H ₃₁ N ₄ O	5-(4-{[2R*,5S*,7-(5,7-dimethylmorpholin-4-yl)piperidin-1-yl]methyl}N-ethyl)pyrimidin-2-amine		
25940613	308.4 C ₂₀ H ₂₄ N ₂ O ₂ S	[(3R*,4R*,1-(piperidin-1-yl)methyl)-1-(2-thienylcarbonyl)pyrrolidin-3-yl]methanol	T/R Silver	W/F Red Team
87334226	331.5 C ₂₄ H ₂₉ N ₃ O ₂	(3S*,4R*,1-[2-methyl-2-(1-piperidinyl)propyl]-4-(3-pyridinyl)-3-pyrrolidinecarboxylic acid	W/F Green	
58639227	245.4 C ₁₈ H ₂₃ N ₃ O ₂ S	(1R*,3S*,7-[3-(methylthio)propyl]-7-azaspiro[3.5]nonane-1,3-diol	T/R White Team	W/F Red Team
68750344	321.5 C ₁₉ H ₂₁ N ₄ O	[(3R*,4R*,1-[(2-(dimethylamino)ethyl)(methyl)amino]methyl)-1-(3,6-dimethyl-2-pyrazinyl)-3-pyrrolidinyl]methanol		
81525945	347.5 C ₂₄ H ₃₁ N ₄ O	1-(2-{4-[(4-allylpiperazin-1-yl)methyl]-3-methyl-1H-pyrazol-5-yl}ethyl)piperidin-4-ol		W/F Purple
80376416	380.5 C ₂₇ H ₃₆ N ₄ O ₂	1-isopropyl(methyl)amino]-3-(2-methoxy-4-[(4-methoxy)piperidin-1-yl]ethyl)piperidin-4-ol		
83302777	374.5 C ₂₆ H ₃₆ N ₄ O ₂	1-[2-[(methyl)(5-methyl-1,3,4-oxadiazol-2-yl)methyl]amino)methyl]phenoxyl-3-piperidin-1-yl]propan-2-ol	T/R Green	
11067284	366.5 C ₂₆ H ₃₄ N ₄ O ₂	1-(4-[3-(diethylamino)-2-hydroxypropoxy]-3-methoxybenzyl)piperidin-4-ol		

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