

Supplementary

Table S1 Compounds tested against the protein target Chain A, kinesin-like protein KIF11

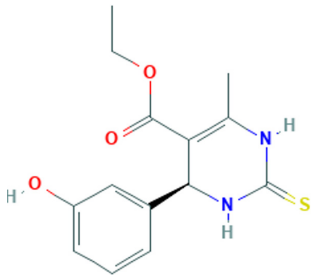
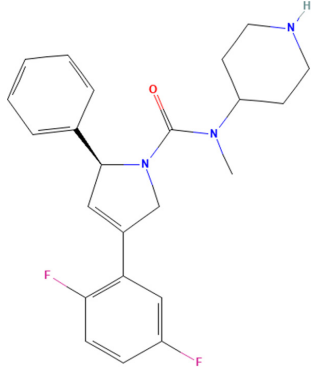
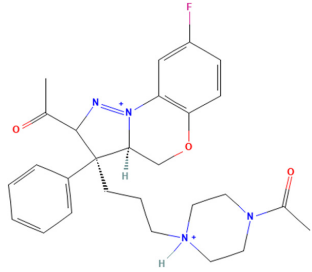
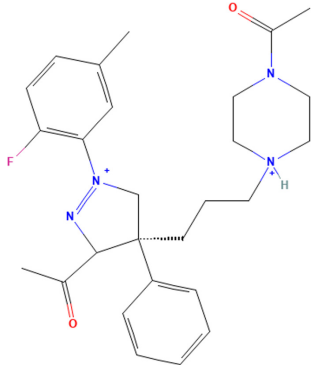
Compound CID	Name	2D structure
794323	(S)-Monastrol	
11675645	(2S)-4-(2,5-Difluorophenyl)-N-methyl-2-phenyl-N-piperidin-4-yl-2,5-dihydro-1H-pyrrole-1-carboxamide	
24916959	1-[(3S,3aR)-3-[3-(4-acetylpiperazin-1-ium-1-yl)propyl]-8-fluoro-3-phenyl-3a,4-dihydro-2H-pyrazolo[5,1-c][1,4]benzoxazin-10-ium-2-yl]ethanone	
24916961	1-[(4R)-4-[3-(4-acetylpiperazin-1-ium-1-yl)propyl]-1-(2-fluoro-5-methylphenyl)-4-phenyl-3,5-dihydropyrazol-1-ium-3-yl]ethanone	

Table S1 (continued)

Table S1 (continued)

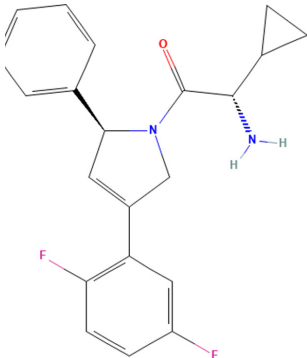
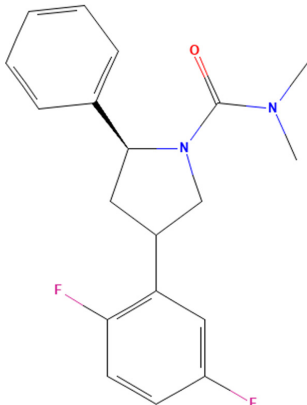
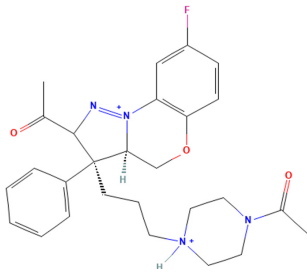
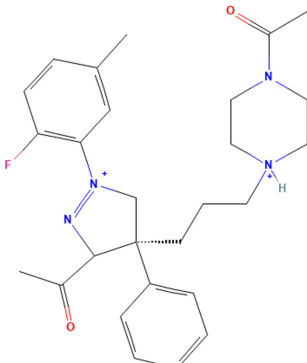
Compound CID	Name	2D structure
6102824	(1S)-1-Cyclopropyl-2-[(2S)-4-(2,5-difluorophenyl)-2-phenyl-2,5-dihydro-1H-pyrrol-1-yl]-2-oxoethanamine	
6102825	(2S)-4-(2,5-difluorophenyl)-N,N-dimethyl-2-phenylpyrrolidine-1-carboxamide	
24916959	1-[(3S,3aR)-3-[3-(4-acetylpiperazin-1-ium-1-yl)propyl]-8-fluoro-3-phenyl-3a,4-dihydro-2H-pyrazolo[5,1-c][1,4]benzoxazin-10-ium-2-yl]ethanone	
24916961	1-[(4R)-4-[3-(4-acetylpiperazin-1-ium-1-yl)propyl]-1-(2-fluoro-5-methylphenyl)-4-phenyl-3,5-dihydropyrazol-1-ium-3-yl]ethanone	

Table S1 (continued)

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Compound CID	Name	2D structure
44629684	(5S)-3-(2,5-difluorophenyl)-N-[(3R,4S)-3-fluoro-1-methylpiperidin-1-ium-4-yl]-5-(hydroxymethyl)-N-methyl-5-phenyl-2H-pyrrole-1-carboxamide	
15942673	[(4R)-4-(3-Hydroxyphenyl)-1,6-dimethyl-2-thioxo-1,2,3,4-tetrahydropyrimidin-5-yl](phenyl) methanone	