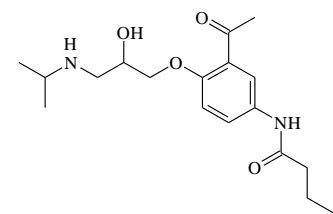
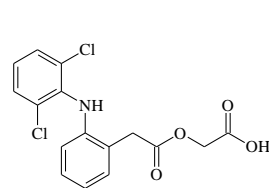


Table S2. The structures of 181 APIs

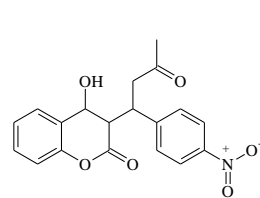
1. acebutolol



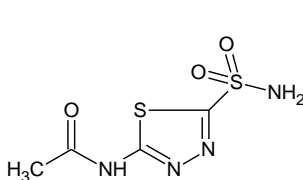
2. aceclofenac



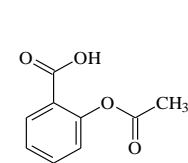
3. acenocumarol



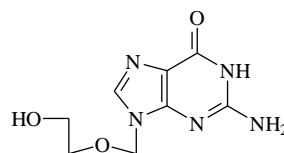
4. acetazolamid



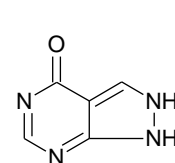
5. acetylsalicylic acid



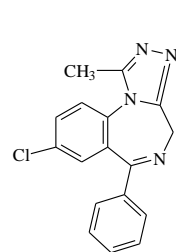
6. acyclovir



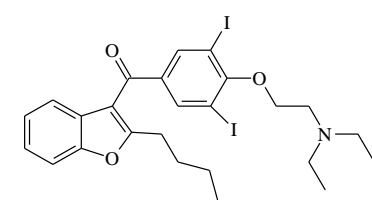
7. allopurinol



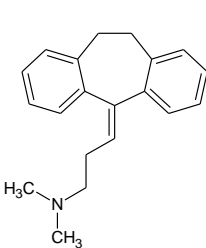
8. alprazolam



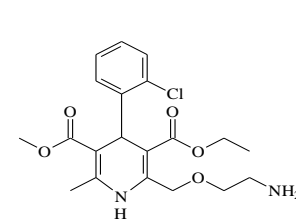
9. amiodarone



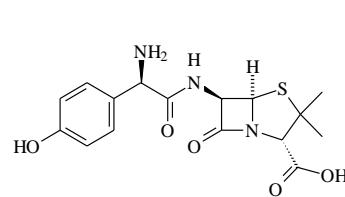
10. amitriptyline



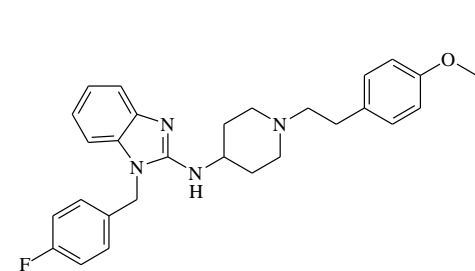
11. amlodipine



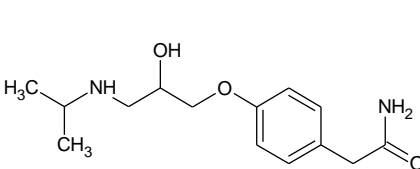
12. amoxicillin



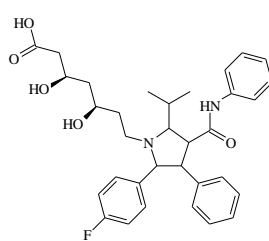
13. astemizol



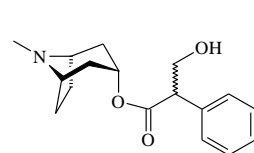
14. atenolol



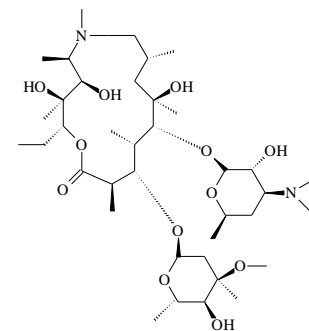
15. atorvastatin



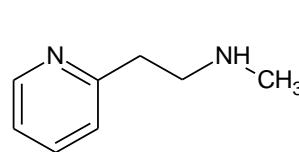
16. atropine



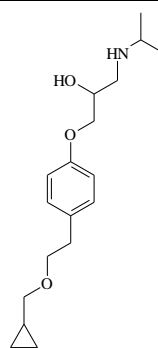
17. azithromycin



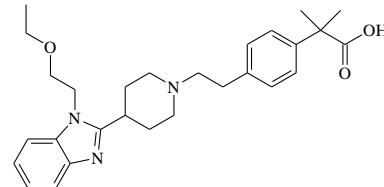
18. betahistine



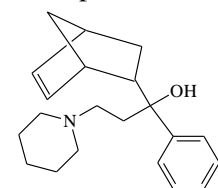
19. betaxolol



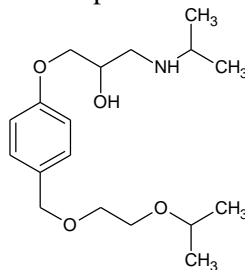
20. bilastine



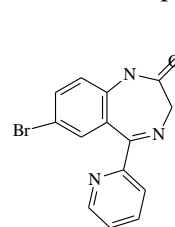
21. biperiden



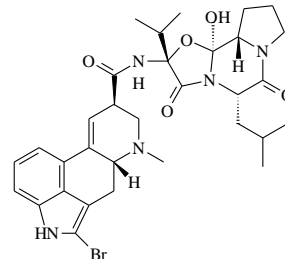
22. bisoprolol



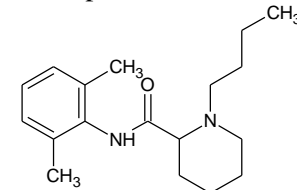
23. bromazepam



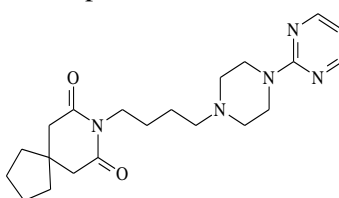
24. bromocriptine



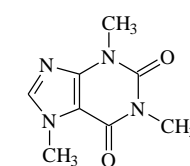
25. bupivacaine



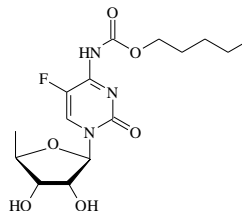
26. buspirone



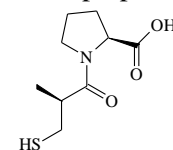
27. caffeine



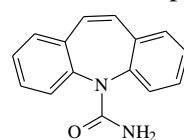
28. capecitabine



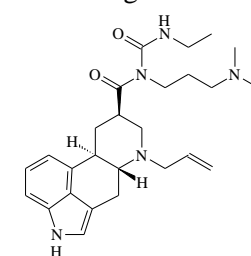
29. captopril



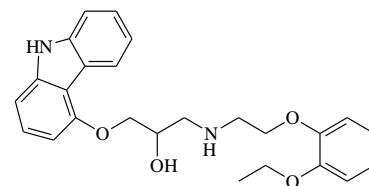
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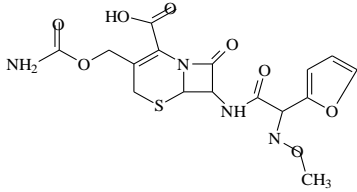
31. carbegoline



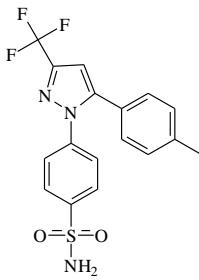
32. carvedilol



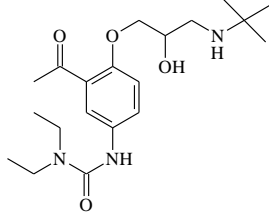
33. cefuroxime



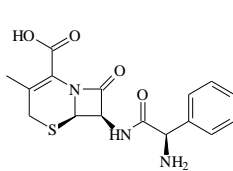
34. celecoxib



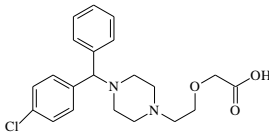
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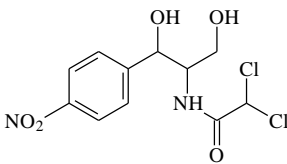
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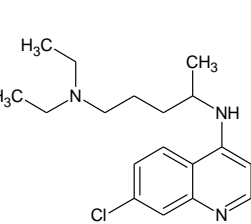
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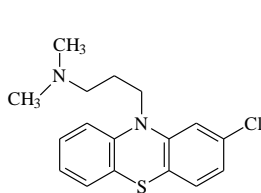
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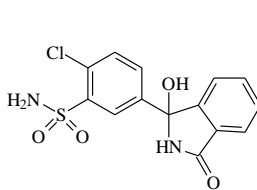
39. chloroquine



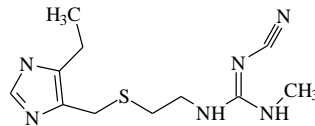
40. chlorpromazine



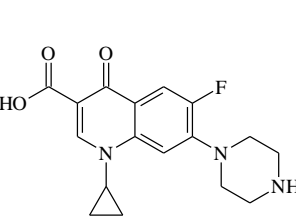
41. chlortalidone



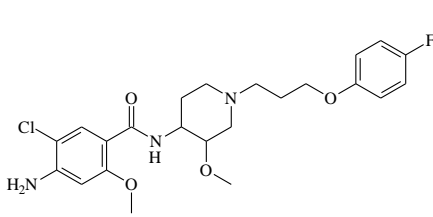
42. cimetidine



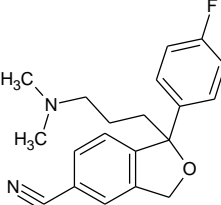
43. ciprofloxacin



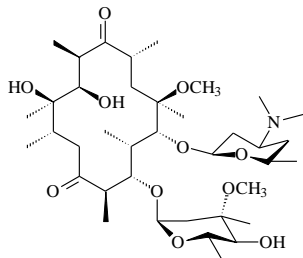
44. cisapride



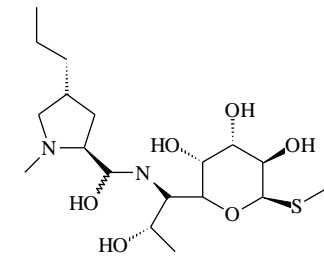
45. citalopram



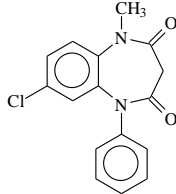
46. clarithromycin



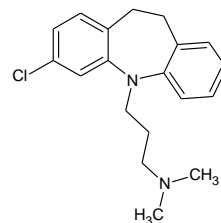
47. clindamycin



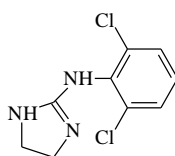
48. clobazam



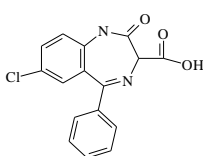
49. clomipramine



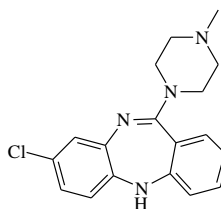
50. clonidine



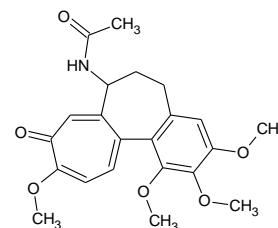
51. clorazepate



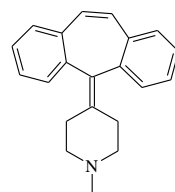
52. clozapine



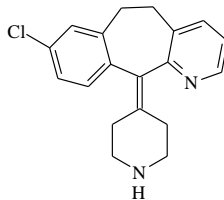
53. colchicine



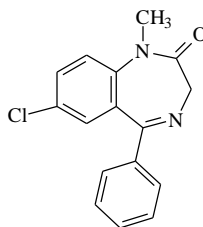
54. cyproheptadine



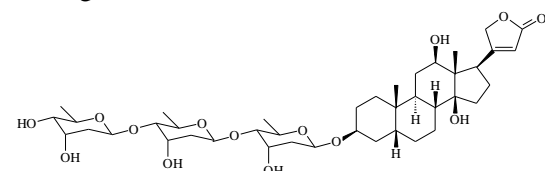
55. desloratidine



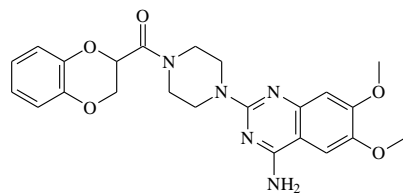
56. diazepam



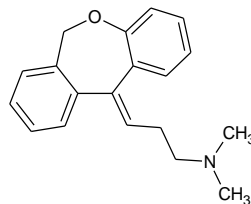
57. digoxin



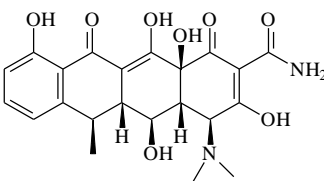
61. doxazosin



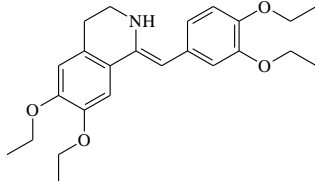
62. doxepin



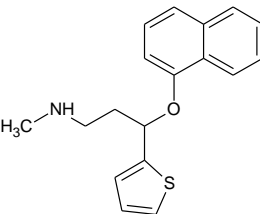
63. doxycycline



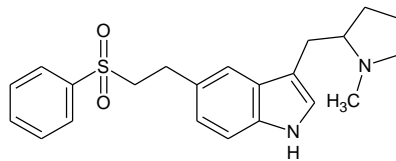
64. drotaverine



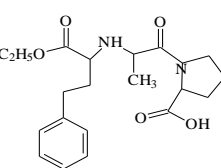
65. duloxetine



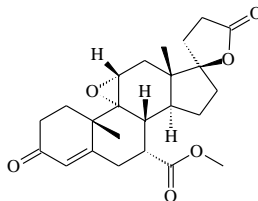
66. eletriptan



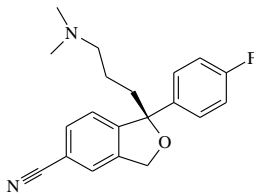
67.enalapril



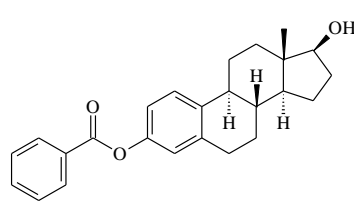
68. eplerenone



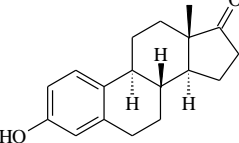
69. escitalopram



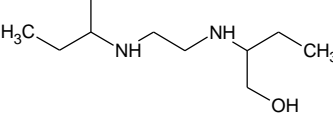
70. estradiol benzoate



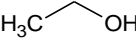
71. estrone



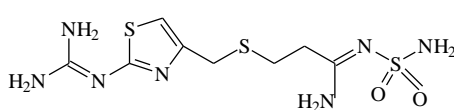
72. ethambutol



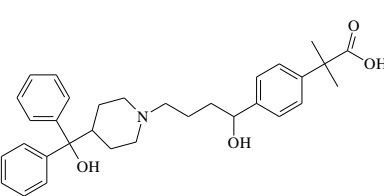
73. ethanol



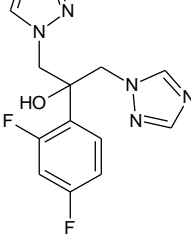
74. famotidine



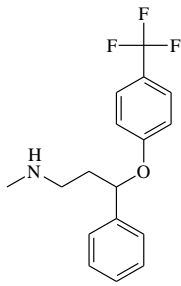
75. fexofenadine



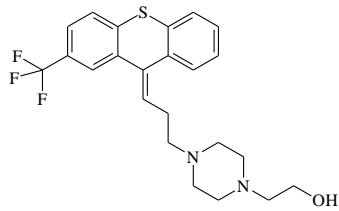
76. fluconazole



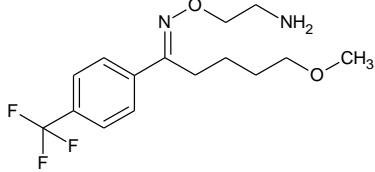
77. fluoxetine



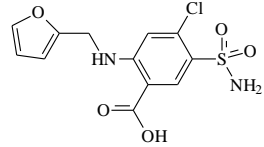
78. flupenthixol



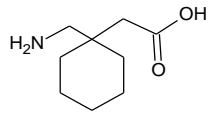
79. fluvoxamine



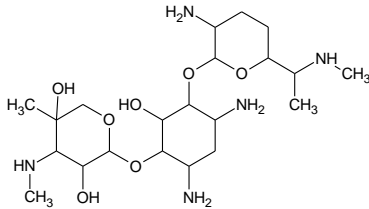
80. furosemide



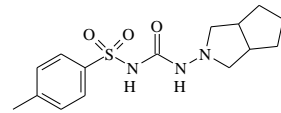
81. gabapentin



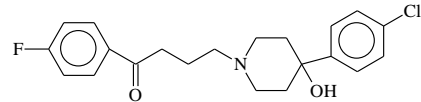
82. gentamycin



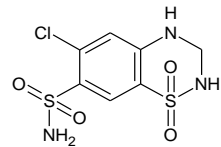
83. gliclazide



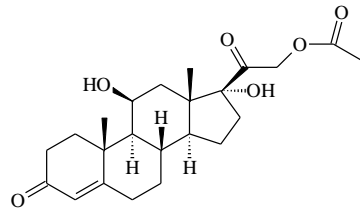
84. haloperidol



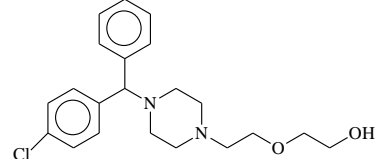
85. hydrochlorothiazide



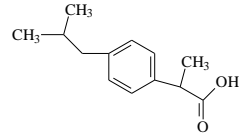
86. hydrocortisone acetate



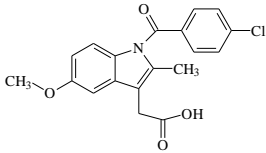
87. hydroxyzine



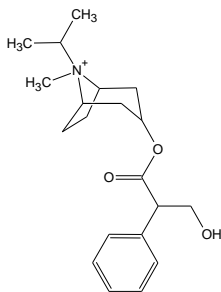
88. ibuprofen



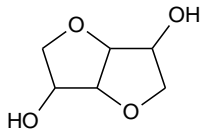
89. indomethacin



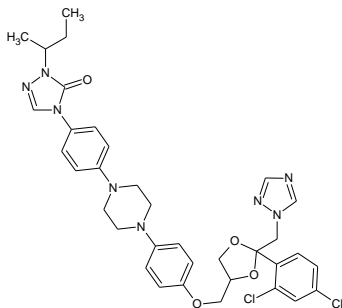
90. ipratropium



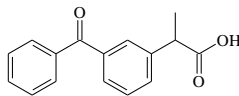
91. isosorbide



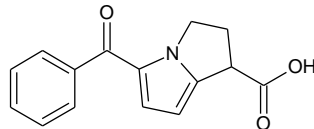
92. itraconazole



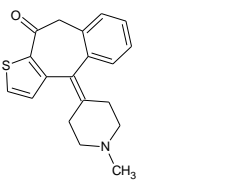
93. ketoprofen



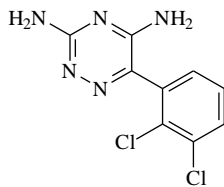
94. ketorolac



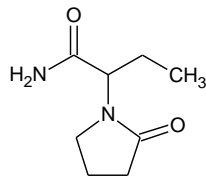
95. ketotifen



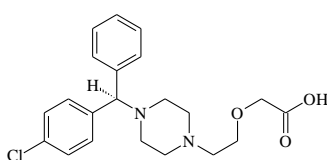
96. lamotrigine



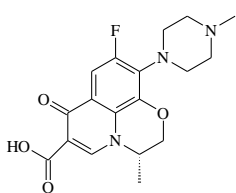
97. levetiracetam



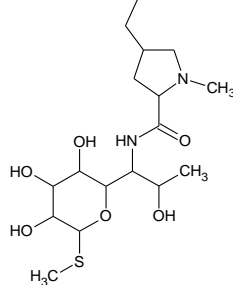
98. levocetizine



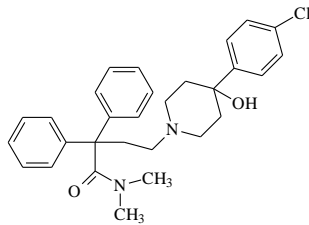
99. levofloxacin



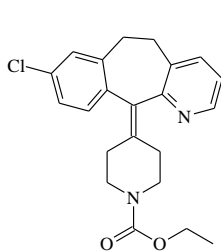
100. lincomycin



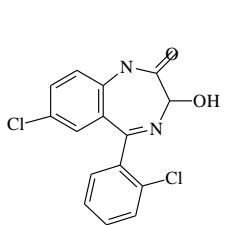
101. loperamide



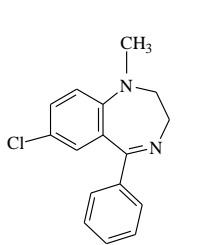
102. loratadine



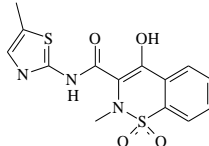
103. lorazepam



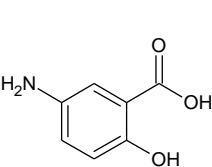
104. medazepam



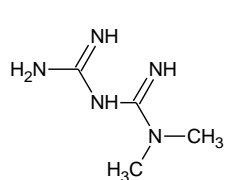
105. meloxicam



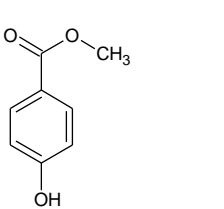
106. mesalazine



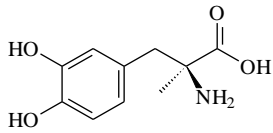
107. metformin



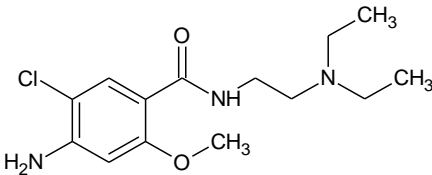
108. methyl paraben



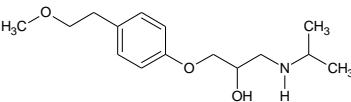
109. methyl dopa



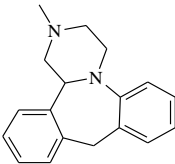
110. metoclopramide



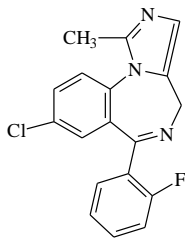
111. metoprolol



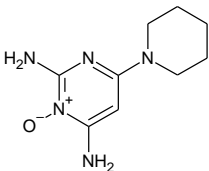
112. mianserin



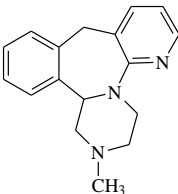
113. midazolam



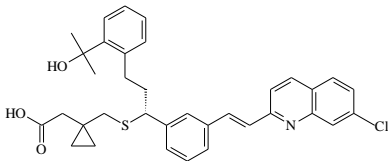
114. minoxidil



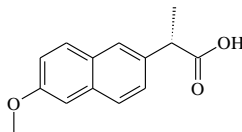
115. mirtazapine



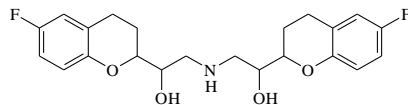
116. montelukast



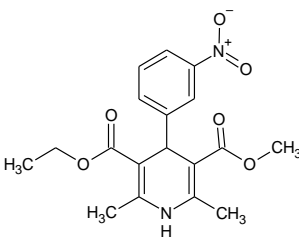
117. naproxen



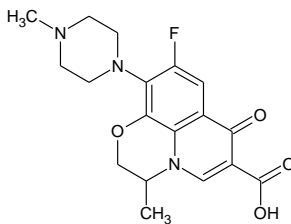
118. nebivolol



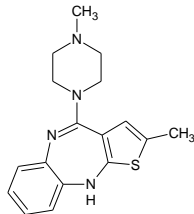
119. nitrendipine



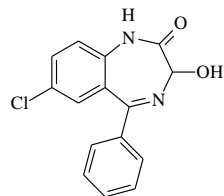
120. ofloxacin



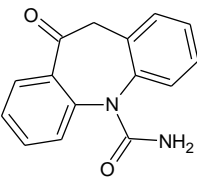
121. olanzapine



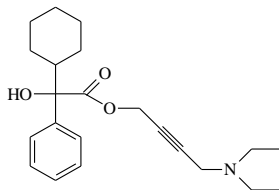
122. oxazepam



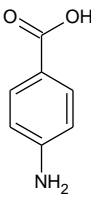
123. oxcarbamazepine



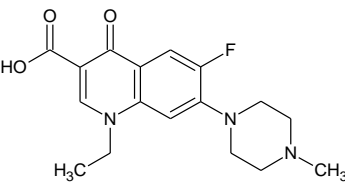
124. oxybutynin



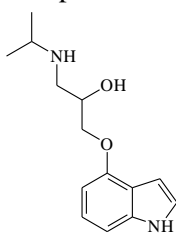
125. PABA



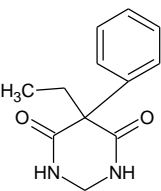
129. pefloxacin



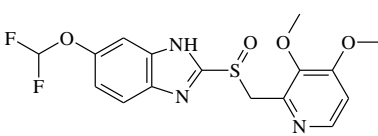
133. pindolol



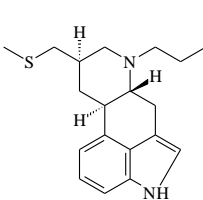
137. primidone



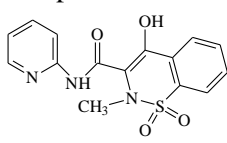
126. pantoprazole



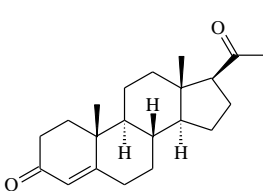
130. pergolide



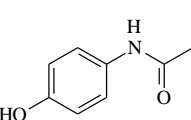
134. piroxicam



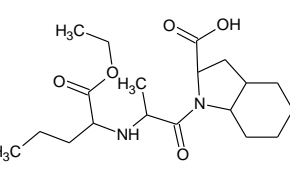
138. progesterone



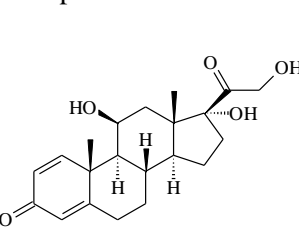
127. paracetamol



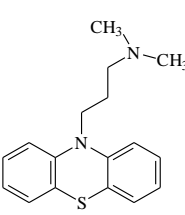
131. perindopril



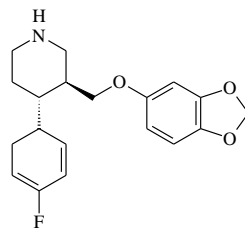
135. prednisolone



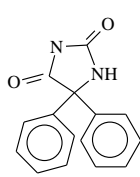
139. promazine



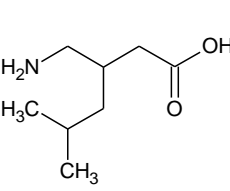
128. paroxetine



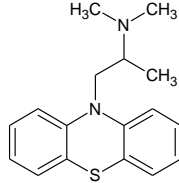
132. phenytoin



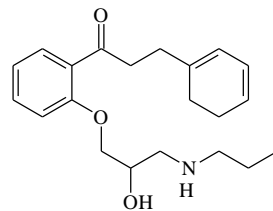
136. pregabalin



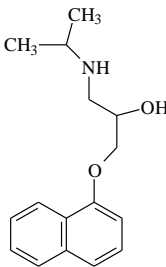
140. promethazine



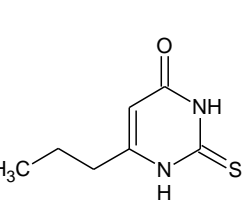
141. propafenone



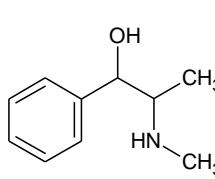
142. propranolol



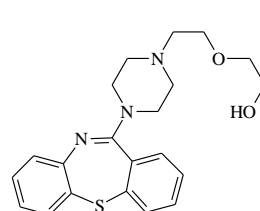
143. propylthiouracil



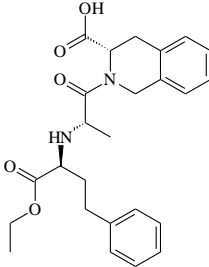
144. pseudoephedrine



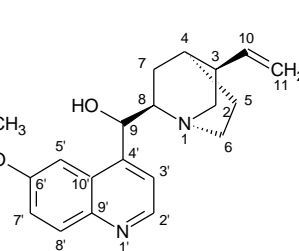
145. quetiapine



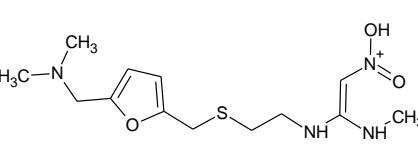
146. quinapril



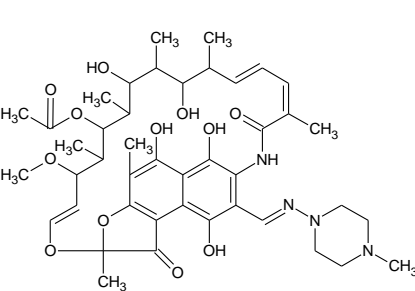
147. quinine



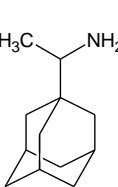
148. ranitidine



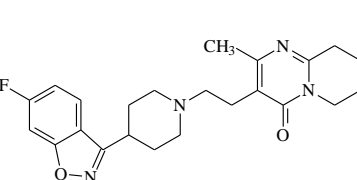
149. rifampicin



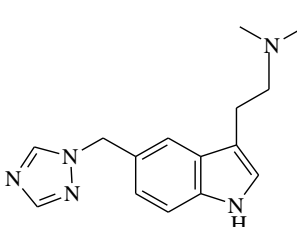
150. rimantadine



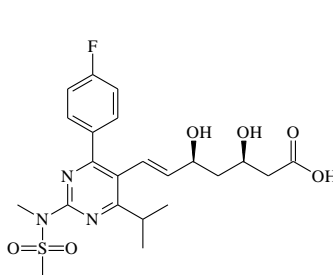
151. risperidone



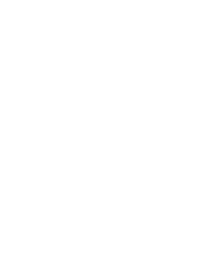
152. rizatriptan



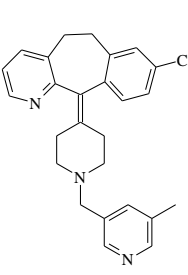
153. rosuvastatin



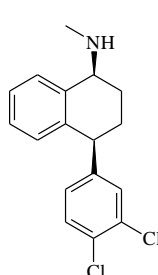
154. roxitromicin

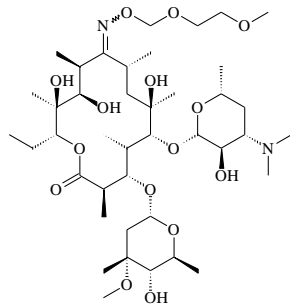


155. rupatadine

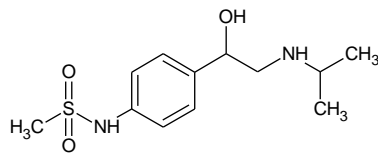


156. sertraline

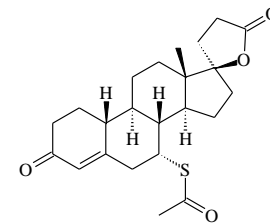




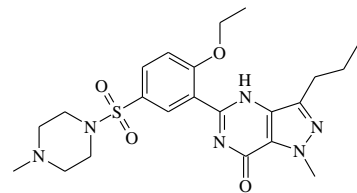
158. simvastatin



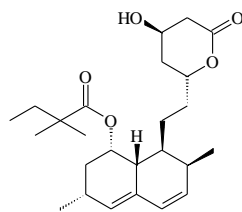
159. sotalol



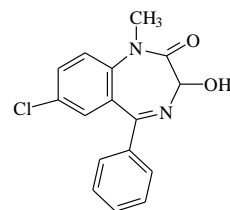
160. spironolactone



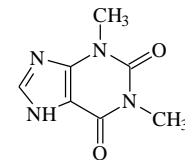
161. sulpiride



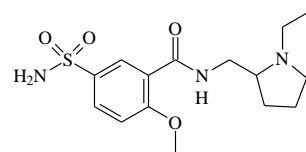
162. telmisartan



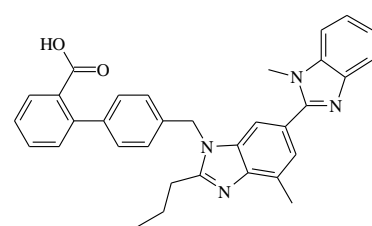
163. temazepam



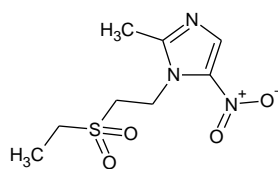
164. theophylline



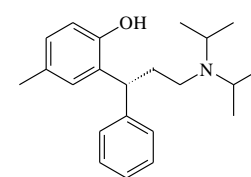
165. thioridazine



166. timolol

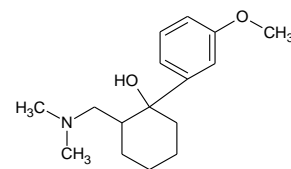


167. tinidazole

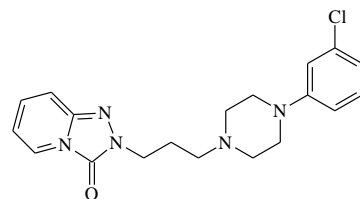


168. tolterodine

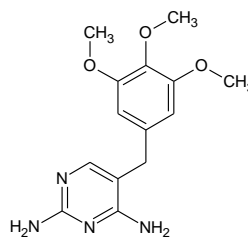
169. tramadol



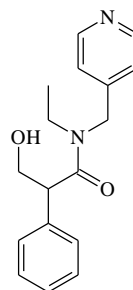
170. trazodone



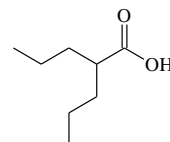
171. trimethoprim



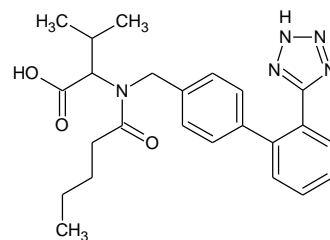
172. tropicamid



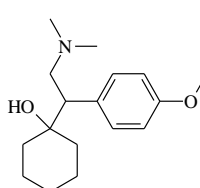
173. valproic acid



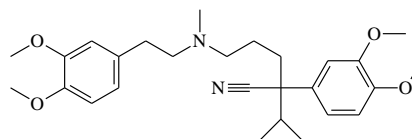
174. valsartan



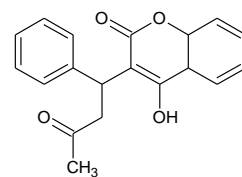
175. venlafaxine



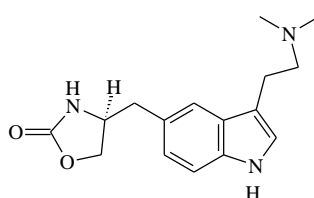
176. verapamil



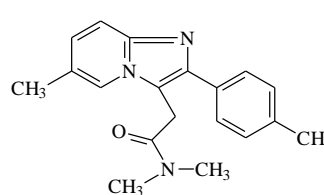
177. warfarin



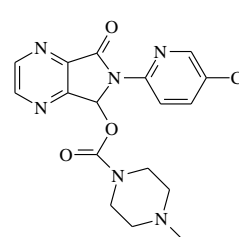
178. zolmitriptane



179. zolpidem



180. zopiclone



181. zuclopenthixol

