

**The eMolecules Project:  
PHARMACEUTICALS TEMPLATE INFORMATION**

Be sure that the information you provide in the template follows the format listed in the table below.

<b>Property</b>	<b>Data Format/Explanation</b>
<b>generic name and IUPAC name</b>	Name for the active ingredient in a medication; name is independent of the manufacturer; IUPAC name based on structure
<b>brand name or tradename</b>	proprietary name given by the manufacturer; may also include name(s) of formulations that contain the active ingredient
<b>molecular formula</b>	simplified chemical formula ( ex. C <sub>9</sub> H <sub>8</sub> O <sub>4</sub> )
<b>structural formula</b>	drawing of pharmaceutical structure
<b>structure (ball and stick)</b>	image of substance that can be displayed using Chime; files with extensions including .pdb, .mol, .xyz
<b>structure (space filling)</b>	image of substance that can be displayed using Chime; files with extensions including .pdb, .mol, .xyz
<b>classification (based on mode of action)</b>	general group to which this pharmaceutical belongs based on its physiological action (i.e. analgesic, beta-blocker, serotonin re-uptake inhibitor)
<b>mode of action</b>	pharmacodynamics; action of the drug in the human system
<b>indications/usage</b>	physiological or mental conditions for which this drug is used
<b>therapeutic dose</b>	dosage administered to obtain desired physiological effect mg or mcg drug/kg body mass
<b>therapeutic index</b>	ratio of toxic dose to therapeutic dose
<b>most frequent adverse reactions</b>	undesirable physiological or mental responses
<b>contraindications</b>	existing conditions that make use inadvisable or dangerous
<b>toxicity</b>	indications of overdose (and amount if available)
<b>special notes</b>	additional important or interesting information about the pharmaceutical
<b>citations</b>	bibliographic information for all material

	contained on this page using APA format; all Internet citations must include a hyperlinked URL
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