

# Supplementary Materials: Chemical Structure-Related Drug-Like Criteria of Global Approved Drugs

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**Table S1.** Common names, indications, CAS Registry Numbers and molecular formulas of 6891 approved drugs.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Abacavir	Antiviral	136470-78-5	Y	C <sub>14</sub> H <sub>18</sub> N <sub>6</sub> O
Abafungin	Antifungal	129639-79-8		C <sub>21</sub> H <sub>22</sub> N <sub>4</sub> OS
Abamectin Component B1a	Anthelmintic	65195-55-3		C <sub>48</sub> H <sub>72</sub> O <sub>14</sub>
Abamectin Component B1b	Anthelmintic	65195-56-4		C <sub>47</sub> H <sub>70</sub> O <sub>14</sub>
Abanoquil	Adrenergic	90402-40-7		C <sub>22</sub> H <sub>25</sub> N <sub>3</sub> O <sub>4</sub>
Abaperidone	Antipsychotic	183849-43-6		C <sub>25</sub> H <sub>25</sub> FN <sub>2</sub> O <sub>5</sub>
Abecarnil	Anxiolytic	111841-85-1	Y	C <sub>24</sub> H <sub>24</sub> N <sub>2</sub> O <sub>4</sub>
Abiraterone	Antineoplastic	154229-19-3	Y	C <sub>24</sub> H <sub>31</sub> NO
Abitesartan	Antihypertensive	137882-98-5		C <sub>26</sub> H <sub>31</sub> N <sub>5</sub> O <sub>3</sub>
Ablukast	Bronchodilator	96566-25-5		C <sub>28</sub> H <sub>34</sub> O <sub>8</sub>
Abunidazole	Antifungal	91017-58-2		C <sub>15</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub>
Acadesine	Cardiotonic	2627-69-2	Y	C <sub>9</sub> H <sub>14</sub> N <sub>4</sub> O <sub>5</sub>
Acamprostate	Alcohol Deterrant	77337-76-9	Y	C <sub>5</sub> H <sub>11</sub> NO <sub>4</sub> S
Acaprazine	Nootropic	55485-20-6	Y	C <sub>15</sub> H <sub>21</sub> Cl <sub>2</sub> N <sub>3</sub> O
Acarbose	Antidiabetic	56180-94-0	Y	C <sub>25</sub> H <sub>43</sub> NO <sub>18</sub>
Acebrochol	Steroid	514-50-1		C <sub>29</sub> H <sub>48</sub> Br <sub>2</sub> O <sub>2</sub>
Acebutolol	Antihypertensive	37517-30-9	Y	C <sub>18</sub> H <sub>28</sub> N <sub>2</sub> O <sub>4</sub>
Acecaidine	Antiarrhythmic	32795-44-1	Y	C <sub>15</sub> H <sub>23</sub> N <sub>3</sub> O <sub>2</sub>
Acecarbromal	Sedative	77-66-7	Y	C <sub>9</sub> H <sub>15</sub> BrN <sub>2</sub> O <sub>3</sub>
Aceclidine	Cholinergic	827-61-2		C <sub>9</sub> H <sub>15</sub> NO <sub>2</sub>
Aceclofenac	Antiinflammatory	89796-99-6	Y	C <sub>16</sub> H <sub>13</sub> Cl <sub>2</sub> NO <sub>4</sub>
Acedapsone	Antibiotic	77-46-3		C <sub>16</sub> H <sub>16</sub> N <sub>2</sub> O <sub>4</sub> S
Acediasulfone Sodium	Antibiotic	80-03-5		C <sub>14</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub> S
Acedoben	Nootropic	556-08-1		C <sub>9</sub> H <sub>9</sub> NO <sub>3</sub>
Acefluranol	Steroid	83282-71-7		C <sub>25</sub> H <sub>26</sub> F <sub>2</sub> O <sub>8</sub>
Acefylline Clobifrol	Bronchodilator	70788-27-1		C <sub>19</sub> H <sub>21</sub> ClN <sub>4</sub> O <sub>5</sub>
Acefylline Piperazine	Bronchodilator	652-37-9		C <sub>9</sub> H <sub>10</sub> N <sub>4</sub> O <sub>4</sub>
Aceglatone	Antineoplastic	642-83-1		C <sub>10</sub> H <sub>10</sub> O <sub>8</sub>
Aceglutamide	Antitumor	2490-97-3		C <sub>7</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub>
Acemetacin	Antiinflammatory	53164-05-9	Y	C <sub>21</sub> H <sub>18</sub> ClNO <sub>6</sub>
Acenocoumarol	Anticoagulant	152-72-7	Y	C <sub>19</sub> H <sub>15</sub> NO <sub>6</sub>
Aceperone	Adrenergic	807-31-8		C <sub>24</sub> H <sub>29</sub> FN <sub>2</sub> O <sub>2</sub>
Acepromazine	Sedative	61-00-7	Y	C <sub>19</sub> H <sub>22</sub> N <sub>2</sub> OS
Aceprometazine	Antidepressant	13461-01-3	Y	C <sub>19</sub> H <sub>22</sub> N <sub>2</sub> OS
Acetaminophen	Analgesic	103-90-2	Y	C <sub>8</sub> H <sub>9</sub> NO <sub>2</sub>
Acetaminosalol	Analgesic	118-57-0		C <sub>15</sub> H <sub>13</sub> NO <sub>4</sub>
Acetanilide	Analgesic	103-84-4		C <sub>8</sub> H <sub>9</sub> NO
Acetarsonic	Antiprotozoal	97-44-9		C <sub>8</sub> H <sub>10</sub> AsNO <sub>5</sub>
Acetazolamide	Antiglaucoma	59-66-5	Y	C <sub>4</sub> H <sub>6</sub> N <sub>4</sub> O <sub>3</sub> S <sub>2</sub>
Acetergamine	Nootropic	3031-48-9		C <sub>18</sub> H <sub>23</sub> N <sub>3</sub> O
Acetiromate	Antihyperlipidemic	2260-08-4		C <sub>15</sub> H <sub>19</sub> I <sub>3</sub> O <sub>5</sub>
Acetohexamide	Antidiabetic	968-81-0	Y	C <sub>15</sub> H <sub>20</sub> N <sub>2</sub> O <sub>4</sub> S
Acetohydroxamic Acid	Antiurolithic	546-88-3	Y	C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub>
Acetophenazine	Antipsychotic	2751-68-0	Y	C <sub>23</sub> H <sub>29</sub> N <sub>3</sub> O <sub>2</sub> S
Acetorphine	Sedative	25333-77-1		C <sub>27</sub> H <sub>35</sub> NO <sub>5</sub>
Acetosulfone Sodium	Antibacterial	80-80-8		C <sub>14</sub> H <sub>15</sub> N <sub>3</sub> O <sub>5</sub> S <sub>2</sub>
21-Acetoxyprogesterone	Antiinflammatory	566-78-9		C <sub>23</sub> H <sub>34</sub> O <sub>4</sub>
Acetryptine	Antihypertensive	3551-18-6		C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> O
Acetyl Strophanthidin	Cardiotonic	60-38-8		C <sub>25</sub> H <sub>34</sub> O <sub>7</sub>
Acetylcholine	Cholinergic	51-84-3		C <sub>7</sub> H <sub>16</sub> NO <sub>2</sub> <sup>+</sup>
Acetylcysteine	Expectorant	616-91-1	Y	C <sub>3</sub> H <sub>9</sub> NO <sub>3</sub> S
Acetyldigitoxin	Cardiotonic	1111-39-3	Y	C <sub>43</sub> H <sub>66</sub> O <sub>14</sub>
Acetyl-L-Leucine	Antiemetic	1188-21-2		C <sub>8</sub> H <sub>15</sub> NO <sub>3</sub>
Acexamic Acid	Antiinflammatory	57-08-9		C <sub>8</sub> H <sub>15</sub> NO <sub>3</sub>
Acifran	Antihyperlipidemic	72420-38-3		C <sub>12</sub> H <sub>10</sub> O <sub>4</sub>
Acipimox	Antihyperlipidemic	51037-30-0	Y	C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Acitazanostat	Bronchodilator	114607-46-4		C <sub>9</sub> H <sub>7</sub> N <sub>5</sub> O <sub>3</sub>
Acitemate	Antineoplastic	101197-99-3		C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O <sub>5</sub>
Acitretin	Dermatologic	55079-83-9	Y	C <sub>21</sub> H <sub>26</sub> O <sub>3</sub>
Acivicin	Antineoplastic	42228-92-2		C <sub>5</sub> H <sub>7</sub> ClN <sub>2</sub> O <sub>3</sub>
Aclantate	Antiinflammatory	39633-62-0		C <sub>15</sub> H <sub>14</sub> ClNO <sub>4</sub> S
Aclarubicin	Antineoplastic	57576-44-0		C <sub>42</sub> H <sub>53</sub> NO <sub>15</sub>
Aclatonium Napadisilate	Cholinergic	55077-30-0		C <sub>10</sub> H <sub>20</sub> NO <sub>4</sub> .1/2C <sub>10</sub> H <sub>6</sub> O <sub>6</sub> S <sub>2</sub>
Acodazole	Antineoplastic	79152-85-5		C <sub>20</sub> H <sub>19</sub> N <sub>5</sub> O
Acolbifene	Antineoplastic	182167-02-8		C <sub>29</sub> H <sub>31</sub> NO <sub>4</sub>
Aconiazide	Antibiotic	13410-86-1		C <sub>15</sub> H <sub>13</sub> N <sub>3</sub> O <sub>4</sub>
Aconitine	Analgesic	302-27-2		C <sub>34</sub> H <sub>47</sub> NO <sub>11</sub>
Acotiamide	Gastroprokinetic	185106-16-5	Y	C <sub>21</sub> H <sub>30</sub> N <sub>4</sub> O <sub>5</sub> S
Acoxatrine	Vasodilator	748-44-7		C <sub>23</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub>
Acreozast	Bronchodilator	123548-56-1		C <sub>15</sub> H <sub>14</sub> ClN <sub>3</sub> O <sub>6</sub>
Acridorex	Gastroprokinetic	47487-22-9		C <sub>24</sub> H <sub>24</sub> N <sub>2</sub>
Acrihellin	Cardiotonic	67696-82-6		C <sub>29</sub> H <sub>38</sub> O <sub>7</sub>
Acrisorcin	Antifungal	90-45-9		C <sub>13</sub> H <sub>10</sub> N <sub>2</sub>
Acrivastine	Antihistaminic	87848-99-5	Y	C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub>
Acrocinnonide	Steroid	28971-58-6		C <sub>24</sub> H <sub>29</sub> FO <sub>6</sub>
Acronine	Antineoplastic	7008-42-6		C <sub>20</sub> H <sub>19</sub> NO <sub>3</sub>
Actarit	Antirheumatic	18699-02-0	Y	C <sub>10</sub> H <sub>11</sub> NO <sub>3</sub>
Actinoquinol Sodium	Dermatologic	15301-40-3		C <sub>11</sub> H <sub>11</sub> NO <sub>4</sub> S
Actisomide	Antiarrhythmic	96914-39-5		C <sub>23</sub> H <sub>35</sub> N <sub>5</sub> O
Actodigin	Cardiotonic	36983-69-4		C <sub>29</sub> H <sub>44</sub> O <sub>9</sub>
Acyclovir	Antiviral	59277-89-3	Y	C <sub>8</sub> H <sub>11</sub> N <sub>5</sub> O <sub>3</sub>
Adafenoxate	Antidepressant	82168-26-1		C <sub>20</sub> H <sub>26</sub> ClNO <sub>3</sub>
Adamexine	Mucolytic	54785-02-3		C <sub>20</sub> H <sub>26</sub> Br <sub>2</sub> N <sub>2</sub> O
Adapalene	Dermatologic	106685-40-9		C <sub>28</sub> H <sub>28</sub> O <sub>3</sub>
Adaprolol Maleate	Antihypertensive	101479-70-3		C <sub>26</sub> H <sub>39</sub> NO <sub>4</sub>
Adatanserin	Antidepressant	127266-56-2		C <sub>21</sub> H <sub>31</sub> N <sub>5</sub> O
Adefovir	Antiviral	106941-25-7		C <sub>8</sub> H <sub>12</sub> N <sub>5</sub> O <sub>4</sub> P
Adefovir Dipivoxil	Antiviral	142340-99-6	Y	C <sub>20</sub> H <sub>32</sub> N <sub>5</sub> O <sub>8</sub> P
Adekalant	Cardiotonic	227940-00-3		C <sub>22</sub> H <sub>31</sub> N <sub>3</sub> O <sub>4</sub>
Adelmidrol	Oxytocic	1675-66-7		C <sub>13</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub>
Ademetionine	Hepatic Protectant	29908-03-0	Y	C <sub>15</sub> H <sub>22</sub> N <sub>6</sub> O <sub>5</sub> S
Adenine	Antineoplastic	73-24-5		C <sub>5</sub> H <sub>5</sub> N <sub>5</sub>
Adenosine	Antiarrhythmic	58-61-7		C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>4</sub>
Adibendan	Cardiotonic	100510-33-6		C <sub>16</sub> H <sub>14</sub> N <sub>4</sub> O
Adicillin	Antibiotic	525-94-0		C <sub>14</sub> H <sub>21</sub> N <sub>3</sub> O <sub>6</sub> S
Adimolol	Antihypertensive	78459-19-5		C <sub>25</sub> H <sub>29</sub> N <sub>3</sub> O <sub>3</sub>
Adinazolam	Antidepressant	37115-32-5		C <sub>19</sub> H <sub>18</sub> ClN <sub>5</sub>
Adiphenine	Antispasmodic	64-95-9		C <sub>20</sub> H <sub>25</sub> NO <sub>2</sub>
Adosopine	Urologic	88124-26-9		C <sub>17</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>
Adozelesin	Antineoplastic	110314-48-2		C <sub>30</sub> H <sub>22</sub> N <sub>4</sub> O <sub>4</sub>
Adrafinil	Antidepressant	63547-13-7	Y	C <sub>15</sub> H <sub>15</sub> NO <sub>3</sub> S
Adrenalone	Hemostatic	99-45-6		C <sub>9</sub> H <sub>11</sub> NO <sub>3</sub>
Adrenochrome	Hemostatic	1214-74-0		C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>2</sub>
Monoaminoguanidine Mesilate				
Adrogolide	Antiparkinsonian	171752-56-0		C <sub>22</sub> H <sub>25</sub> NO <sub>4</sub> S
Afeletecan	Antineoplastic	215604-75-4		C <sub>45</sub> H <sub>49</sub> N <sub>7</sub> O <sub>11</sub> S
Afloqualone	Muscle Relaxant	56287-74-2		C <sub>16</sub> H <sub>14</sub> FN <sub>3</sub> O
Afurolol	Antihypertensive	65776-67-2		C <sub>15</sub> H <sub>21</sub> NO <sub>4</sub>
Aganodine	Cardiotonic	86696-87-9		C <sub>9</sub> H <sub>10</sub> Cl <sub>2</sub> N <sub>4</sub>
Aglepristone	Progestogen	124478-60-0		C <sub>29</sub> H <sub>37</sub> NO <sub>2</sub>
Agomelatine	Antidepressant	138112-76-2	Y	C <sub>15</sub> H <sub>17</sub> NO <sub>2</sub>
Ajmaline	Antihypertensive	4360-12-7		C <sub>20</sub> H <sub>26</sub> N <sub>2</sub> O <sub>2</sub>
Aklomide	Antibacterial	3011-89-0		C <sub>7</sub> H <sub>5</sub> ClN <sub>2</sub> O <sub>3</sub>
Alacepril	Antihypertensive	74258-86-9	Y	C <sub>20</sub> H <sub>26</sub> N <sub>2</sub> O <sub>5</sub> S
Alafosfalin	Bone Resorption Inhibitor	60668-24-8		C <sub>5</sub> H <sub>13</sub> N <sub>2</sub> O <sub>4</sub> P
Alagebrium Chloride	Antidiabetic	341028-37-3		C <sub>13</sub> H <sub>14</sub> ClNOS
Alamifovir	Antiviral	193681-12-8		C <sub>19</sub> H <sub>20</sub> F <sub>6</sub> N <sub>5</sub> O <sub>5</sub> PS
Alaproclate	Antidepressant	60719-82-6		C <sub>13</sub> H <sub>18</sub> ClNO <sub>2</sub>
Alatrofloxacin	Antibacterial	146961-76-4		C <sub>26</sub> H <sub>25</sub> F <sub>3</sub> N <sub>6</sub> O <sub>5</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Alazanine Triclofenate	Antiinflammatory	7775-97-5		C <sub>21</sub> H <sub>21</sub> N <sub>2</sub> S <sub>2</sub> .C <sub>6</sub> H <sub>2</sub> Cl <sub>3</sub> O
Albaconazole	Antifungal	187949-02-6		C <sub>20</sub> H <sub>16</sub> ClF <sub>2</sub> N <sub>5</sub> O <sub>2</sub>
Albendazole	Anthelmintic	54965-21-8	Y	C <sub>12</sub> H <sub>15</sub> N <sub>3</sub> O <sub>2</sub> S
Albendazole Oxide	Anthelmintic	54029-12-8		C <sub>12</sub> H <sub>15</sub> N <sub>3</sub> O <sub>3</sub> S
Albuterol	Bronchodilator	18559-94-9		C <sub>13</sub> H <sub>21</sub> NO <sub>3</sub>
Albutoin	Anticonvulsant	830-89-7		C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> OS
Alclofenac	Analgesic	22131-79-9		C <sub>11</sub> H <sub>11</sub> ClO <sub>3</sub>
Alclometasone Dipropionate	Antiinflammatory	66734-13-2		C <sub>28</sub> H <sub>37</sub> ClO <sub>7</sub>
Alcohol	Antidote	64-17-5		C <sub>2</sub> H <sub>6</sub> O
Alcuronium Chloride	Neuromuscular Blocking Agent	15180-03-7		C <sub>44</sub> H <sub>50</sub> N <sub>4</sub> O <sub>2</sub> .2Cl
Aldioxa	Antiulcerative	5579-81-7		C <sub>4</sub> H <sub>7</sub> AlN <sub>4</sub> O <sub>5</sub>
Alemcinal	Gastroprokinetic	150785-53-8		C <sub>38</sub> H <sub>67</sub> NO <sub>10</sub>
Alendronic Acid	Bone Resorption Inhibitor	66376-36-1	Y	C <sub>4</sub> H <sub>13</sub> NO <sub>7</sub> P <sub>2</sub>
Alentemol Hydrobromide	Antipsychotic	112891-97-1		C <sub>19</sub> H <sub>25</sub> NO
Alepride	Gastroprokinetic	66564-15-6		C <sub>22</sub> H <sub>30</sub> ClN <sub>3</sub> O <sub>2</sub>
Alestramustine	Antineoplastic	139402-18-9		C <sub>26</sub> H <sub>36</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>4</sub>
Aletamine	Antidepressant	4255-23-6		C <sub>11</sub> H <sub>15</sub> N
Alexidine	Antibacterial	22573-93-9		C <sub>26</sub> H <sub>56</sub> N <sub>10</sub>
Alfadex	Erectile Dysfunction	10016-20-3	Y	C <sub>36</sub> H <sub>60</sub> O <sub>30</sub>
Alfadolone	Anesthetic	14107-37-0		C <sub>21</sub> H <sub>32</sub> O <sub>4</sub>
Alfaprostol	Prostaglandin	74176-31-1		C <sub>24</sub> H <sub>38</sub> O <sub>5</sub>
Alfatradiol	Estrogen	57-91-0		C <sub>18</sub> H <sub>24</sub> O <sub>2</sub>
Alfaxalone	Anesthetic	23930-19-0		C <sub>21</sub> H <sub>32</sub> O <sub>3</sub>
Alfentanil	Analgesic	71195-58-9		C <sub>21</sub> H <sub>32</sub> N <sub>6</sub> O <sub>3</sub>
Alfuzosin	Antihypertensive	81403-80-7		C <sub>19</sub> H <sub>27</sub> N <sub>5</sub> O <sub>4</sub>
Algestone Acetonide	Antiinflammatory	4968-09-6		C <sub>24</sub> H <sub>34</sub> O <sub>4</sub>
Algestone Acetophenide	Dermatologic	24356-94-3		C <sub>29</sub> H <sub>36</sub> O <sub>4</sub>
Alibendol	Choleretic	26750-81-2		C <sub>13</sub> H <sub>17</sub> NO <sub>4</sub>
Aliconazole	Antifungal	63824-12-4		C <sub>18</sub> H <sub>13</sub> Cl <sub>3</sub> N <sub>2</sub>
Alifedrine	Cardiotonic	78756-61-3		C <sub>18</sub> H <sub>27</sub> NO <sub>2</sub>
Aliflurane	Anesthetic	56689-41-9		C <sub>4</sub> H <sub>5</sub> ClF <sub>4</sub> O
Alimadol	Nootropic	52742-40-2		C <sub>19</sub> H <sub>23</sub> NO
Alinastine	Antihistaminic	154541-72-7	Y	C <sub>28</sub> H <sub>39</sub> N <sub>3</sub> O
Alinidine	Antiarrhythmic	33178-86-8		C <sub>12</sub> H <sub>13</sub> Cl <sub>2</sub> N <sub>3</sub>
Alipamide	Diuretic	3184-59-6		C <sub>9</sub> H <sub>12</sub> ClN <sub>3</sub> O <sub>3</sub> S
Aliskiren	Antihypertensive	173334-57-1	Y	C <sub>30</sub> H <sub>53</sub> N <sub>3</sub> O <sub>6</sub>
Alitretinoin	Antineoplastic	5300-03-8		C <sub>20</sub> H <sub>28</sub> O <sub>2</sub>
Alizapride	Antiemetic	59338-93-1	Y	C <sub>16</sub> H <sub>21</sub> N <sub>5</sub> O <sub>2</sub>
Alkofanone	Antidiarrheal	7527-94-8		C <sub>21</sub> H <sub>19</sub> NO <sub>3</sub> S
Allantoin	Dermatologic	97-59-6		C <sub>4</sub> H <sub>6</sub> N <sub>4</sub> O <sub>3</sub>
Alletorphine	Analgesic	23758-80-7		C <sub>27</sub> H <sub>35</sub> NO <sub>4</sub>
Allobarbitol	Sedative	52-43-7		C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>
Alloclamide	Antitussive	5486-77-1		C <sub>16</sub> H <sub>23</sub> ClN <sub>2</sub> O <sub>2</sub>
Allocupreide Sodium	Antirheumatic	500-48-1		C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> S
Allomethadione	Anticonvulsant	526-35-2		C <sub>7</sub> H <sub>9</sub> NO <sub>3</sub>
Allopurinol	Antiurolithic	315-30-0	Y	C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O
Allyl Isothiocyanate	Dermatologic	57-06-7		C <sub>4</sub> H <sub>5</sub> NS
Allylestrenol	Progestogen	432-60-0		C <sub>21</sub> H <sub>32</sub> O
Allylprodine	Analgesic	25384-17-2		C <sub>18</sub> H <sub>25</sub> NO <sub>2</sub>
Almecillin	Antibiotic	87-09-2		C <sub>13</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub> S <sub>2</sub>
Almestrone	Steroid	10448-96-1		C <sub>19</sub> H <sub>24</sub> O <sub>2</sub>
Alminoprofen	Antiinflammatory	39718-89-3		C <sub>13</sub> H <sub>17</sub> NO <sub>2</sub>
Almitrine	Respiratory Stimulant	27469-53-0		C <sub>26</sub> H <sub>29</sub> F <sub>2</sub> N <sub>7</sub>
Almokalant	Antiarrhythmic	123955-10-2		C <sub>18</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub> S
Almotriptan	Antimigraine	154323-57-6	Y	C <sub>17</sub> H <sub>25</sub> N <sub>3</sub> O <sub>2</sub> S
Almoxatone	Antidepressant	84145-89-1		C <sub>18</sub> H <sub>19</sub> ClN <sub>2</sub> O <sub>3</sub>
Almurtide	Immunomodulator	61136-12-7		C <sub>18</sub> H <sub>30</sub> N <sub>4</sub> O <sub>11</sub>
Alnespirone	Antidepressant	138298-79-0		C <sub>26</sub> H <sub>38</sub> N <sub>2</sub> O <sub>4</sub>
Alniditan Di	Antimigraine	152317-89-0		C <sub>17</sub> H <sub>26</sub> N <sub>4</sub> O
Alonacic	Ophthalmic	105292-70-4		C <sub>9</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub> S
Alonimid	Sedative	2897-83-8		C <sub>14</sub> H <sub>13</sub> NO <sub>3</sub>
Aloracetam	Nootropic	119610-26-3		C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Alosetron	Antidiarrheal	122852-42-0	Y	C <sub>17</sub> H <sub>18</sub> N <sub>4</sub> O
Alovudine	Antiviral	25526-93-6		C <sub>10</sub> H <sub>13</sub> F <sub>2</sub> N <sub>2</sub> O <sub>4</sub>
Aloxistatin	Immunomodulator	88321-09-9		C <sub>17</sub> H <sub>30</sub> N <sub>2</sub> O <sub>5</sub>
Alozafone	Anticonvulsant	65899-72-1		C <sub>21</sub> H <sub>21</sub> ClFN <sub>3</sub> O <sub>2</sub>
Alpertine	Antipsychotic	27076-46-6		C <sub>25</sub> H <sub>31</sub> N <sub>3</sub> O <sub>4</sub>
Alphacetylmethadol	Analgesic	17199-58-5		C <sub>23</sub> H <sub>31</sub> NO <sub>2</sub>
Alpha Cypermethrin	Ectoparasiticide	67375-30-8		C <sub>22</sub> H <sub>19</sub> Cl <sub>2</sub> NO <sub>3</sub>
Alphameprodine	Analgesic	468-51-9		C <sub>17</sub> H <sub>25</sub> NO <sub>2</sub>
Alphamethadol	Analgesic	17199-54-1		C <sub>21</sub> H <sub>29</sub> NO
Alphaprodine	Analgesic	77-20-3		C <sub>16</sub> H <sub>23</sub> NO <sub>2</sub>
Alpidem	Anxiolytic	82626-01-5		C <sub>21</sub> H <sub>23</sub> Cl <sub>2</sub> N <sub>3</sub> O
Alpiropride	Antimigraine	81982-32-3		C <sub>17</sub> H <sub>26</sub> N <sub>4</sub> O <sub>4</sub> S
Alprafenone	Antiarrhythmic	124316-02-5		C <sub>25</sub> H <sub>35</sub> NO <sub>4</sub>
Alprazolam	Anxiolytic	28981-97-7	Y	C <sub>17</sub> H <sub>13</sub> ClN <sub>4</sub>
Alprenolol	Antihypertensive	13655-52-2	Y	C <sub>15</sub> H <sub>23</sub> NO <sub>2</sub>
Alprenoxime	Antiglaucoma	118552-63-9		C <sub>15</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>
Alprostadiol	Vasodilator	745-65-3		C <sub>20</sub> H <sub>34</sub> O <sub>5</sub>
Alrestatin	Antidiabetic	51411-04-2		C <sub>14</sub> H <sub>9</sub> NO <sub>4</sub>
Altanserin Tartrate	Antidepressant	76330-71-7		C <sub>22</sub> H <sub>22</sub> FN <sub>3</sub> O <sub>2</sub> S
Altapizone	Vasodilator	93277-96-4		C <sub>24</sub> H <sub>28</sub> N <sub>4</sub> O <sub>2</sub>
Alteconazole	Antifungal	93479-96-0		C <sub>17</sub> H <sub>12</sub> Cl <sub>3</sub> N <sub>3</sub> O
Althiazide	Diuretic	5588-16-9		C <sub>11</sub> H <sub>14</sub> ClN <sub>3</sub> O <sub>4</sub> S <sub>3</sub>
Altinicline	Nootropic	179120-92-4		C <sub>12</sub> H <sub>14</sub> N <sub>2</sub>
Altoqualine	Antibiotic	121029-11-6		C <sub>27</sub> H <sub>36</sub> N <sub>2</sub> O <sub>8</sub>
Altrenogest	Progestogen	850-52-2		C <sub>21</sub> H <sub>26</sub> O <sub>2</sub>
Altretamine	Antineoplastic	645-05-6		C <sub>9</sub> H <sub>18</sub> N <sub>6</sub>
Alvameline Maleate	Antipsychotic	120241-31-8		C <sub>9</sub> H <sub>15</sub> N <sub>5</sub>
Alverine	Antispasmodic	150-59-4		C <sub>20</sub> H <sub>27</sub> N
Alvimopan	Antiemetic	156053-89-3	Y	C <sub>25</sub> H <sub>32</sub> N <sub>2</sub> O <sub>4</sub>
Alvocidib	Antineoplastic	146426-40-6		C <sub>21</sub> H <sub>20</sub> ClNO <sub>5</sub>
Amadinone Acetate	Progestogen	22304-34-3		C <sub>22</sub> H <sub>27</sub> ClO <sub>4</sub>
Amafolone	Steroid	50588-47-1		C <sub>19</sub> H <sub>31</sub> NO <sub>2</sub>
Amanozine	Diuretic	537-17-7		C <sub>9</sub> H <sub>9</sub> N <sub>5</sub>
Amantadine	Antiviral	768-94-5	Y	C <sub>10</sub> H <sub>17</sub> N
Amantocillin	Antibiotic	10004-67-8		C <sub>19</sub> H <sub>27</sub> N <sub>3</sub> O <sub>4</sub> S
Ambamustine	Antineoplastic	85754-59-2		C <sub>29</sub> H <sub>39</sub> Cl <sub>2</sub> FN <sub>4</sub> O <sub>4</sub> S
Ambasilide	Antiarrhythmic	83991-25-7		C <sub>21</sub> H <sub>25</sub> N <sub>3</sub> O
Ambazone	Antibacterial	539-21-9		C <sub>8</sub> H <sub>11</sub> N <sub>7</sub> S
Ambenonium	Neuromuscular Blocking Agent	7648-98-8	Y	C <sub>28</sub> H <sub>42</sub> Cl <sub>2</sub> N <sub>4</sub> O <sub>2</sub>
Ambenoxan	Anxiolytic	2455-84-7		C <sub>14</sub> H <sub>21</sub> NO <sub>4</sub>
Ambrisentan	Anticoagulant	177036-94-1	Y	C <sub>22</sub> H <sub>22</sub> N <sub>2</sub> O <sub>4</sub>
Ambroxol	Expectorant	18683-91-5	Y	C <sub>13</sub> H <sub>18</sub> Br <sub>2</sub> N <sub>2</sub> O
Ambruticin	Antifungal	58857-02-6		C <sub>28</sub> H <sub>42</sub> O <sub>6</sub>
Ambucaine	Anesthetic	119-29-9		C <sub>17</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub>
Ambucetamide	Antispasmodic	519-88-0		C <sub>17</sub> H <sub>28</sub> N <sub>2</sub> O <sub>2</sub>
Ambuphylline	Bronchodilator	124-68-5		C <sub>4</sub> H <sub>11</sub> NO
Ambuside	Diuretic	3754-19-6		C <sub>13</sub> H <sub>16</sub> ClN <sub>3</sub> O <sub>5</sub> S <sub>2</sub>
Ambuton Bromide	Antispasmodic	115-51-5		C <sub>20</sub> H <sub>27</sub> BrN <sub>2</sub> O
Amcinafal	Antiinflammatory	3924-70-7		C <sub>26</sub> H <sub>35</sub> FO <sub>6</sub>
Amcinafide	Antiinflammatory	7332-27-6		C <sub>29</sub> H <sub>33</sub> FO <sub>6</sub>
Amcinonide	Glucocorticoid	51022-69-6		C <sub>28</sub> H <sub>35</sub> FO <sub>7</sub>
Amdinocillin	Antibiotic	32887-01-7		C <sub>15</sub> H <sub>23</sub> N <sub>3</sub> O <sub>5</sub> S
Amdoxovir	Antiviral	145514-04-1		C <sub>9</sub> H <sub>12</sub> N <sub>6</sub> O <sub>3</sub>
Amebucort	Glucocorticoid	83625-35-8		C <sub>28</sub> H <sub>40</sub> O <sub>7</sub>
Amedalin	Antidepressant	22136-26-1		C <sub>19</sub> H <sub>22</sub> N <sub>2</sub> O
Amelometasone	Steroid	123013-22-9		C <sub>26</sub> H <sub>35</sub> FO <sub>6</sub>
Ameltolide	Anticonvulsant	787-93-9		C <sub>15</sub> H <sub>16</sub> N <sub>2</sub> O
Amelubant	Antirheumatic	346735-24-8		C <sub>33</sub> H <sub>34</sub> N <sub>2</sub> O <sub>5</sub>
Amesergide	Antidepressant	121588-75-8		C <sub>25</sub> H <sub>35</sub> N <sub>3</sub> O
Ametantrone Acetate	Antineoplastic	64862-96-0		C <sub>22</sub> H <sub>28</sub> N <sub>4</sub> O <sub>4</sub>
Amezepine	Analgesic	60575-32-8		C <sub>18</sub> H <sub>20</sub> N <sub>2</sub>
Amezinium Metilsulfate	Antihypertensive	41658-78-0		C <sub>11</sub> H <sub>12</sub> N <sub>3</sub> O

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Amfenac	Antiinflammatory	51579-82-9		C <sub>15</sub> H <sub>13</sub> NO <sub>3</sub>
Amfepentorex	Anorexic	15686-27-8		C <sub>15</sub> H <sub>25</sub> N
Amfetaminil	Nootropic	17590-01-1		C <sub>17</sub> H <sub>18</sub> N <sub>2</sub>
Amflutizole	Antiuro lithic	82114-19-0		C <sub>11</sub> H <sub>7</sub> F <sub>3</sub> N <sub>2</sub> O <sub>2</sub> S
Amfonelic Acid	Nootropic	15180-02-6		C <sub>18</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>
Amicarbalide	Antiprotozoal	3459-96-9		C <sub>15</sub> H <sub>16</sub> N <sub>6</sub> O
Amicibone	Antitussive	23271-63-8		C <sub>22</sub> H <sub>31</sub> NO <sub>3</sub>
Amicycline	Antibiotic	5874-95-3		C <sub>21</sub> H <sub>23</sub> N <sub>3</sub> O <sub>7</sub>
Amidantel	Anthelminthic	49745-00-8		C <sub>13</sub> H <sub>19</sub> N <sub>3</sub> O <sub>2</sub>
Amidapsone	Antiviral	3569-77-5		C <sub>13</sub> H <sub>13</sub> N <sub>3</sub> O <sub>3</sub> S
Amidephrine Mesylate	Decongestant	37571-84-9		C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub> S
Amiflamine	Antidepressant	77518-07-1		C <sub>12</sub> H <sub>20</sub> N <sub>2</sub>
Amifloverine	Antispasmodic	54063-24-0		C <sub>16</sub> H <sub>27</sub> NO <sub>3</sub>
Amifloxacin	Antibiotic	86393-37-5		C <sub>16</sub> H <sub>19</sub> FN <sub>4</sub> O <sub>3</sub>
Amifostine	Antineoplastic	20537-88-6		C <sub>5</sub> H <sub>15</sub> N <sub>2</sub> O <sub>3</sub> PS
Amiglumide	Gastroprokinetic	119363-62-1		C <sub>26</sub> H <sub>36</sub> N <sub>2</sub> O <sub>4</sub>
Amikacin	Antibiotic	37517-28-5		C <sub>22</sub> H <sub>43</sub> N <sub>5</sub> O <sub>13</sub>
Amikhelline	Antispasmodic	4439-67-2		C <sub>18</sub> H <sub>21</sub> NO <sub>5</sub>
Amiloride	Diuretic	2609-46-3	Y	C <sub>6</sub> H <sub>8</sub> ClN <sub>7</sub> O
Amiloxate	Dermatologic	71617-10-2		C <sub>15</sub> H <sub>20</sub> O <sub>3</sub>
Amindocate	Estrogen	31386-24-0		C <sub>19</sub> H <sub>29</sub> N <sub>3</sub> O <sub>2</sub>
Amineptine	Nootropic	57574-09-1	Y	C <sub>22</sub> H <sub>27</sub> NO <sub>2</sub>
Aminobenzoic Acid	Dermatologic	1321-11-5		C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub>
Aminocaproic Acid	Hemostatic	1319-82-0	Y	C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub>
Aminoethyl Nitrate	Unclassified	646-02-6		C <sub>2</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub>
Aminoglutethimide	Antineoplastic	125-84-8	Y	C <sub>13</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>
Aminolevulinic Acid	Antineoplastic	106-60-5	Y	C <sub>5</sub> H <sub>9</sub> NO <sub>3</sub>
Aminometradine	Diuretic	642-44-4		C <sub>9</sub> H <sub>13</sub> N <sub>3</sub> O <sub>2</sub>
Aminopentamide Sulfate	Antispasmodic	60-46-8		C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> O
Aminophenazone Cyclamate	Analgesic	100-88-9		C <sub>6</sub> H <sub>13</sub> NO <sub>3</sub> S
Aminopromazine	Antispasmodic	58-37-7		C <sub>19</sub> H <sub>25</sub> N <sub>3</sub> S
Aminopterin	Antibacterial	54-62-6		C <sub>19</sub> H <sub>20</sub> N <sub>8</sub> O <sub>5</sub>
Aminopyrine	Antiinflammatory	58-15-1		C <sub>13</sub> H <sub>17</sub> N <sub>3</sub> O
Aminorex	Anorexic	2207-50-3		C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> O
Aminosalicilic Acid	Antibacterial	28088-64-4	Y	C <sub>7</sub> H <sub>7</sub> NO <sub>3</sub>
Amiodarone	Antiarrhythmic	1951-25-3	Y	C <sub>25</sub> H <sub>29</sub> I <sub>2</sub> NO <sub>3</sub>
Amiperone	Sedative	1580-71-8		C <sub>24</sub> H <sub>28</sub> ClFN <sub>2</sub> O <sub>2</sub>
Amiphenazole	Nootropic	490-55-1		C <sub>9</sub> H <sub>9</sub> N <sub>3</sub> S
Amipizone	Bronchodilator	69635-63-8		C <sub>14</sub> H <sub>16</sub> ClN <sub>3</sub> O <sub>2</sub>
Amiprilose	Immunosuppressant	56824-20-5		C <sub>14</sub> H <sub>27</sub> NO <sub>6</sub>
Amiquinsin	Antihypertensive	13425-92-8		C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>
Amisometradine	Diuretic	550-28-7		C <sub>9</sub> H <sub>13</sub> N <sub>3</sub> O <sub>2</sub>
Amisulpride	Antipsychotic	71675-85-9	Y	C <sub>17</sub> H <sub>27</sub> N <sub>3</sub> O <sub>4</sub> S
Amiterol	Bronchodilator	54063-25-1		C <sub>12</sub> H <sub>20</sub> N <sub>2</sub> O
Amithiozone	Antibacterial	104-06-3		C <sub>10</sub> H <sub>12</sub> N <sub>4</sub> OS
Amitivir	Antiviral	111393-84-1		C <sub>3</sub> H <sub>2</sub> N <sub>4</sub> S
Amitraz	Ectoparasiticide	33089-61-1		C <sub>19</sub> H <sub>23</sub> N <sub>3</sub>
Amitriptyline	Antidepressant	50-48-6	Y	C <sub>20</sub> H <sub>23</sub> N
Amitriptylinoxide	Antidepressant	4317-14-0		C <sub>20</sub> H <sub>23</sub> NO
Amixetrine	Antiinflammatory	24622-72-8		C <sub>17</sub> H <sub>27</sub> NO
Amlexanox	Antihistaminic	68302-57-8		C <sub>16</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub>
Amlodipine	Antianginal	88150-42-9	Y	C <sub>20</sub> H <sub>25</sub> ClN <sub>2</sub> O <sub>5</sub>
Ammonium Valerate	Sedative	109-52-4		C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>
Amobarbital	Sedative	57-43-2		C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>
Amocarzine	Anthelminthic	36590-19-9		C <sub>18</sub> H <sub>21</sub> N <sub>5</sub> O <sub>2</sub> S
Amodiaquine	Antimalarial	86-42-0	Y	C <sub>20</sub> H <sub>22</sub> ClN <sub>3</sub> O
Amogastrin	Antispasmodic	16870-37-4		C <sub>35</sub> H <sub>46</sub> N <sub>6</sub> O <sub>8</sub> S
Amolanone	Anesthetic	76-65-3		C <sub>20</sub> H <sub>23</sub> NO <sub>2</sub>
Amonafide	Antineoplastic	69408-81-7		C <sub>16</sub> H <sub>17</sub> N <sub>3</sub> O <sub>2</sub>
Amoproxan	Antiarrhythmic	22661-76-3		C <sub>22</sub> H <sub>35</sub> NO <sub>7</sub>
Amopyroquine	Antimalarial	550-81-2		C <sub>20</sub> H <sub>20</sub> ClN <sub>3</sub> O
Amorolfine	Antibacterial	78613-35-1		C <sub>21</sub> H <sub>35</sub> NO
Amoscanate	Anthelminthic	26328-53-0		C <sub>13</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub> S

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Amosulalol	Antihypertensive	85320-68-9	Y	C <sub>18</sub> H <sub>24</sub> N <sub>2</sub> O <sub>5</sub> S
Amotosalen	Dermatologic	161262-29-9		C <sub>17</sub> H <sub>19</sub> NO <sub>4</sub>
Amotriphene	Vasodilator	5585-64-8		C <sub>26</sub> H <sub>29</sub> NO <sub>3</sub>
Amoxapine	Antidepressant	14028-44-5	Y	C <sub>17</sub> H <sub>16</sub> ClN <sub>3</sub> O
Amoxecaine	Anesthetic	553-65-1		C <sub>17</sub> H <sub>29</sub> N <sub>3</sub> O <sub>2</sub>
Amoxicillin	Antibiotic	26787-78-0	Y	C <sub>16</sub> H <sub>19</sub> N <sub>3</sub> O <sub>5</sub> S
Amoxydramine Camsilate	Antihypertensive	3922-74-5		C <sub>17</sub> H <sub>21</sub> NO <sub>2</sub>
Amoxydramine Camsilate	Antihypertensive	3144-16-9		C <sub>10</sub> H <sub>16</sub> O <sub>4</sub> S
Amperozide	Sedative	75558-90-6		C <sub>23</sub> H <sub>29</sub> F <sub>2</sub> N <sub>3</sub> O
Amphecloral	Anorexic	5581-35-1		C <sub>11</sub> H <sub>12</sub> Cl <sub>3</sub> N
Amphenidone	Sedative	134-37-2		C <sub>11</sub> H <sub>10</sub> N <sub>2</sub> O
Amphetamine	Nootropic	300-62-9	Y	C <sub>9</sub> H <sub>13</sub> N
Amphotilide	Antithrombotic	1673-06-9		C <sub>19</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub>
Ampicillin	Antibiotic	69-53-4	Y	C <sub>16</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub> S
Ampiroxicam	Antiinflammatory	99464-64-9		C <sub>20</sub> H <sub>21</sub> N <sub>3</sub> O <sub>7</sub> S
Ampronavir	Antiviral	161814-49-9	Y	C <sub>25</sub> H <sub>35</sub> N <sub>3</sub> O <sub>6</sub> S
Amprolium	Antibacterial	121-25-5		C <sub>14</sub> H <sub>19</sub> N <sub>4</sub> Cl
Amprotropine Phosphate	Antihypertensive	148-32-3		C <sub>18</sub> H <sub>29</sub> NO <sub>3</sub>
Ampyrimine	Antineoplastic	5587-93-9		C <sub>12</sub> H <sub>11</sub> N <sub>7</sub>
Ampyzine Sulfate	Nootropic	5214-29-9		C <sub>6</sub> H <sub>9</sub> N <sub>3</sub>
Amquinat	Antimalarial	17230-85-2		C <sub>18</sub> H <sub>24</sub> N <sub>2</sub> O <sub>3</sub>
Amrinone	Cardiotonic	60719-84-8		C <sub>10</sub> H <sub>9</sub> N <sub>3</sub> O
Amrubicin	Antineoplastic	110267-81-7		C <sub>25</sub> H <sub>25</sub> NO <sub>9</sub>
Amsacrine	Antineoplastic	51264-14-3		C <sub>21</sub> H <sub>19</sub> N <sub>3</sub> O <sub>3</sub> S
Amtolmetin Guacil	Analgesic	87344-06-7	Y	C <sub>24</sub> H <sub>24</sub> N <sub>2</sub> O <sub>5</sub>
Amustaline Dihydrochloride	Antibacterial	878189-87-8		C <sub>22</sub> H <sub>25</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>2</sub>
Amylene Hydrate	Sedative	75-85-4		C <sub>5</sub> H <sub>12</sub> O
Amylocaine	Anesthetic	644-26-8		C <sub>14</sub> H <sub>21</sub> NO <sub>2</sub>
Anagestone Acetate	Progestogen	3137-73-3		C <sub>24</sub> H <sub>36</sub> O <sub>3</sub>
Anagrelide	Antithrombotic	68475-42-3	Y	C <sub>10</sub> H <sub>7</sub> Cl <sub>2</sub> N <sub>3</sub> O
Anastrozole	Antineoplastic	120511-73-1	Y	C <sub>17</sub> H <sub>19</sub> N <sub>5</sub>
Anatibant	Antirheumatic	209733-45-9		C <sub>34</sub> H <sub>36</sub> Cl <sub>2</sub> N <sub>6</sub> O <sub>5</sub> S
Anaxirone	Antineoplastic	99212-42-7		C <sub>11</sub> H <sub>15</sub> N <sub>3</sub> O <sub>5</sub>
Anazocine	Analgesic	15378-99-1		C <sub>16</sub> H <sub>23</sub> NO
Ancarolol	Antihypertensive	75748-50-4		C <sub>18</sub> H <sub>24</sub> N <sub>2</sub> O <sub>4</sub>
Ancitabine	Antineoplastic	31698-14-3		C <sub>9</sub> H <sub>11</sub> N <sub>3</sub> O <sub>4</sub>
Ancriviroc	Antiviral	370893-06-4		C <sub>28</sub> H <sub>37</sub> BrN <sub>4</sub> O <sub>3</sub>
Andolast	Bronchodilator	132640-22-3		C <sub>15</sub> H <sub>11</sub> N <sub>9</sub> O
Androstenediol	Steroid	521-17-5		C <sub>19</sub> H <sub>30</sub> O <sub>2</sub>
Androstenedione	Steroid	63-05-8		C <sub>19</sub> H <sub>26</sub> O <sub>2</sub>
Anecortave Acetate	Ophthalmic	7753-60-8		C <sub>23</sub> H <sub>30</sub> O <sub>5</sub>
Anethole	Antitussive	104-46-1		C <sub>10</sub> H <sub>12</sub> O
Anidoxime	Analgesic	34297-34-2		C <sub>21</sub> H <sub>27</sub> N <sub>3</sub> O <sub>3</sub>
Anilamate	Anticonvulsant	5591-49-1		C <sub>15</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>
Anileridine	Analgesic	144-14-9		C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> O <sub>2</sub>
Anilopam	Analgesic	53716-46-4		C <sub>20</sub> H <sub>26</sub> N <sub>2</sub> O
Anipamil	Antianginal	83200-10-6		C <sub>34</sub> H <sub>52</sub> N <sub>2</sub> O <sub>2</sub>
Aniracetam	Nootropic	72432-10-1	Y	C <sub>12</sub> H <sub>13</sub> NO <sub>3</sub>
Anirolac	Antiinflammatory	66635-85-6		C <sub>16</sub> H <sub>15</sub> NO <sub>4</sub>
Anisacril	Unclassified	5129-14-6		C <sub>22</sub> H <sub>18</sub> O <sub>3</sub>
Anisindione	Anticoagulant	117-37-3	Y	C <sub>16</sub> H <sub>12</sub> O <sub>3</sub>
Anisomycin	Antibiotic	22862-76-6		C <sub>14</sub> H <sub>19</sub> NO <sub>4</sub>
Anisopirol	Unclassified	857-62-5		C <sub>21</sub> H <sub>27</sub> FN <sub>2</sub> O <sub>2</sub>
Anisotropine	Antispasmodic	25333-49-7	Y	C <sub>16</sub> H <sub>29</sub> NO <sub>2</sub>
Anisperimus	Immunosuppressant	170368-04-4		C <sub>18</sub> H <sub>39</sub> N <sub>7</sub> O <sub>3</sub>
Anitrazafen	Antiinflammatory	63119-27-7		C <sub>18</sub> H <sub>17</sub> N <sub>3</sub> O <sub>2</sub>
Anpirtoline	Analgesic	98330-05-3		C <sub>10</sub> H <sub>13</sub> ClN <sub>2</sub> S
Ansoxetine	Antidepressant	79130-64-6		C <sub>26</sub> H <sub>25</sub> NO <sub>3</sub>
Antafenite	Antiprotozoal	6649-73-6		C <sub>11</sub> H <sub>10</sub> N <sub>2</sub> S
Antazoline	Antihistaminic	91-75-8		C <sub>17</sub> H <sub>19</sub> N <sub>3</sub>
Antazonite	Antihistaminic	5028-87-5		C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> S <sub>2</sub>
Anthralin	Dermatologic	1143-38-0		C <sub>14</sub> H <sub>10</sub> O <sub>3</sub>
Anthelmycin	Anthelminthic	12706-94-4		C <sub>21</sub> H <sub>37</sub> N <sub>5</sub> O <sub>14</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Anthiolimine	Diuretic	70-49-5		C <sub>4</sub> H <sub>6</sub> O <sub>4</sub> S
Anthracene	Antineoplastic	120-12-7		C <sub>14</sub> H <sub>10</sub>
Anthramycin	Antineoplastic	4803-27-4		C <sub>16</sub> H <sub>17</sub> N <sub>3</sub> O <sub>4</sub>
Antienite	Unclassified	5719-88-0		C <sub>9</sub> H <sub>8</sub> N <sub>2</sub> S <sub>2</sub>
Antimony Sodium Thioglycollate	Anthelminthic	1843-43-2		C <sub>4</sub> H <sub>5</sub> O <sub>4</sub> S <sub>2</sub> Sb
Antipyrine	Antiinflammatory	60-80-0		C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O
Antrafenine	Analgesic	55300-29-3		C <sub>30</sub> H <sub>26</sub> F <sub>6</sub> N <sub>4</sub> O <sub>2</sub>
Apadoline	Analgesic	135003-30-4		C <sub>23</sub> H <sub>29</sub> N <sub>3</sub> OS
Apafant	Antithrombotic	105219-56-5		C <sub>22</sub> H <sub>22</sub> ClN <sub>5</sub> O <sub>2</sub> S
Apalcillin	Antibacterial	63469-19-2		C <sub>25</sub> H <sub>23</sub> N <sub>5</sub> O <sub>6</sub> S
Apaxifylline	Bronchodilator	151581-23-6		C <sub>16</sub> H <sub>22</sub> N <sub>4</sub> O <sub>3</sub>
Apaziqune	Antineoplastic	114560-48-4		C <sub>15</sub> H <sub>16</sub> N <sub>2</sub> O <sub>4</sub>
Apazone	Antiinflammatory	13539-59-8	Y	C <sub>16</sub> H <sub>20</sub> N <sub>4</sub> O <sub>2</sub>
Apicycline	Antibiotic	15599-51-6		C <sub>30</sub> H <sub>38</sub> N <sub>4</sub> O <sub>11</sub>
Apixaban	Anticoagulant	503612-47-3	Y	C <sub>25</sub> H <sub>25</sub> N <sub>5</sub> O <sub>4</sub>
Aplindore Fumarate	Antipsychotic	189681-70-7		C <sub>18</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>
Apomorphine	Antiparkinsonian	58-00-4		C <sub>17</sub> H <sub>17</sub> NO <sub>2</sub>
Apovincamine	Cardiotonic	4880-92-6		C <sub>21</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub>
Apraclonidine	Ophthalmic	66711-21-5		C <sub>9</sub> H <sub>10</sub> Cl <sub>2</sub> N <sub>4</sub>
Apramycin	Antibiotic	37321-09-8		C <sub>21</sub> H <sub>41</sub> N <sub>5</sub> O <sub>11</sub>
Aprastat	Antihyperlipidemic	287405-51-0		C <sub>17</sub> H <sub>22</sub> N <sub>2</sub> O <sub>6</sub> S <sub>2</sub>
Aprepitant	Antiemetic	170729-80-3	Y	C <sub>23</sub> H <sub>21</sub> F <sub>7</sub> N <sub>4</sub> O <sub>3</sub>
Aprikalim	Cardiotonic	132562-26-6		C <sub>12</sub> H <sub>16</sub> N <sub>2</sub> OS <sub>2</sub>
Aprindine	Antiarrhythmic	37640-71-4	Y	C <sub>22</sub> H <sub>30</sub> N <sub>2</sub>
Aprobarbital	Sedative	77-02-1		C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>
Aprofene	Antihypertensive	3563-01-7		C <sub>21</sub> H <sub>27</sub> NO <sub>2</sub>
Aptazapine Maleate	Antidepressant	71576-40-4		C <sub>16</sub> H <sub>19</sub> N <sub>3</sub>
Aptiganel	Nootropic	137159-92-3		C <sub>20</sub> H <sub>21</sub> N <sub>3</sub>
Aptocaine	Anesthetic	19281-29-9		C <sub>14</sub> H <sub>20</sub> N <sub>2</sub> O
Aranidipine	Antihypertensive	86780-90-7		C <sub>19</sub> H <sub>20</sub> N <sub>2</sub> O <sub>7</sub>
Aranotin	Antiviral	19885-51-9		C <sub>20</sub> H <sub>18</sub> N <sub>2</sub> O <sub>7</sub> S <sub>2</sub>
Araprofen	Antiinflammatory	15250-13-2		C <sub>16</sub> H <sub>15</sub> NO <sub>4</sub>
Arasertaconazole	Antifungal	583057-48-1		C <sub>20</sub> H <sub>15</sub> Cl <sub>3</sub> N <sub>2</sub> OS
Arbaprostil	Antilucerative	55028-70-1		C <sub>21</sub> H <sub>34</sub> O <sub>5</sub>
Arbekacin	Antibiotic	51025-85-5		C <sub>22</sub> H <sub>44</sub> N <sub>6</sub> O <sub>10</sub>
Arbutamine	Antihypotensive	128470-16-6		C <sub>18</sub> H <sub>23</sub> NO <sub>4</sub>
Arbutin	Dermatologic	497-76-7		C <sub>12</sub> H <sub>16</sub> O <sub>7</sub>
Arecoline	Anthelminthic	63-75-2		C <sub>8</sub> H <sub>13</sub> NO <sub>2</sub>
Arfendazam	Anxiolytic	37669-57-1		C <sub>18</sub> H <sub>17</sub> ClN <sub>2</sub> O <sub>3</sub>
Arformoterol Tartrate	Bronchodilator	67346-49-0		C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> O <sub>4</sub>
Argatroban	Anticoagulant	74863-84-6		C <sub>23</sub> H <sub>36</sub> N <sub>6</sub> O <sub>5</sub> S
Argimesna	Antineoplastic	74-79-3		C <sub>6</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub>
Arildone	Antiviral	56219-57-9		C <sub>20</sub> H <sub>29</sub> ClO <sub>4</sub>
Arimoclomol	Capillary Protectant	289893-25-0	Y	C <sub>14</sub> H <sub>20</sub> ClN <sub>3</sub> O <sub>3</sub>
Aripiprazole	Antipsychotic	129722-12-9	Y	C <sub>23</sub> H <sub>27</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>2</sub>
Armodafinil	Nootropic	112111-43-0	Y	C <sub>15</sub> H <sub>15</sub> NO <sub>2</sub> S
Arnolol	Antihypertensive	87129-71-3		C <sub>14</sub> H <sub>23</sub> NO <sub>3</sub>
Arofylline	Bronchodilator	136145-07-8		C <sub>14</sub> H <sub>13</sub> ClN <sub>4</sub> O <sub>2</sub>
Aronixil	Antihypertensive	86627-15-8		C <sub>14</sub> H <sub>15</sub> ClN <sub>4</sub> O <sub>2</sub>
Arotinolol	Antianginal	68377-92-4	Y	C <sub>15</sub> H <sub>21</sub> N <sub>3</sub> O <sub>2</sub> S <sub>3</sub>
Arprinocid	Antibacterial	55779-18-5		C <sub>12</sub> H <sub>9</sub> ClFN <sub>5</sub>
Arpromidine	Analgesic	106669-71-0		C <sub>21</sub> H <sub>25</sub> FN <sub>6</sub>
Arsanilic Acid	Antibacterial	98-50-0		C <sub>6</sub> H <sub>8</sub> AsNO <sub>3</sub>
Arsphenamine	Antibiotic	150-44-7		C <sub>12</sub> H <sub>12</sub> As <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Arsthinol	Antiamoebic	119-96-0		C <sub>11</sub> H <sub>14</sub> AsNO <sub>3</sub> S <sub>2</sub>
Arteflene	Antimalarial	123407-36-3		C <sub>19</sub> H <sub>18</sub> F <sub>6</sub> O <sub>3</sub>
Artemether	Antimalarial	71963-77-4	Y	C <sub>16</sub> H <sub>26</sub> O <sub>5</sub>
Artemifone	Antimalarial	255730-18-8		C <sub>19</sub> H <sub>31</sub> NO <sub>6</sub> S
Artemisinin	Antimalarial	63968-64-9		C <sub>15</sub> H <sub>22</sub> O <sub>5</sub>
Artemotil	Antimalarial	75887-54-6		C <sub>17</sub> H <sub>28</sub> O <sub>5</sub>
Artenimol	Antimalarial	71939-50-9	Y	C <sub>15</sub> H <sub>24</sub> O <sub>5</sub>
Artesunate	Antimalarial	88495-63-0	Y	C <sub>19</sub> H <sub>28</sub> O <sub>8</sub>
Articaine	Anesthetic	23964-58-1		C <sub>13</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> S

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Artilide Fumarate	Antiarrhythmic	133267-19-3		C <sub>19</sub> H <sub>34</sub> N <sub>2</sub> O <sub>3</sub> S
Arundic Acid	Nootropic	185517-21-9		C <sub>11</sub> H <sub>22</sub> O <sub>2</sub>
Arzoxifene	Progestogen	182133-25-1		C <sub>28</sub> H <sub>29</sub> NO <sub>4</sub> S
Asenapine Maleate	Antipsychotic	65576-45-6		C <sub>17</sub> H <sub>16</sub> CINO
Aseripide	Antispasmodic	153242-02-5		C <sub>26</sub> H <sub>30</sub> FN <sub>3</sub> O <sub>6</sub> S
Asimadoline	Analgesic	153205-46-0	Y	C <sub>27</sub> H <sub>30</sub> N <sub>2</sub> O <sub>2</sub>
Asobamast	Antihistaminic	104777-03-9		C <sub>13</sub> H <sub>15</sub> N <sub>3</sub> O <sub>5</sub> S
Asocainol	Antiarrhythmic	77400-65-8		C <sub>27</sub> H <sub>31</sub> NO <sub>3</sub>
Asoprisnil	Progestogen	199396-76-4		C <sub>28</sub> H <sub>35</sub> NO <sub>4</sub>
Asoprisnil Ecamate	Progestogen	222732-94-7		C <sub>31</sub> H <sub>40</sub> N <sub>2</sub> O <sub>5</sub>
Aspartocin	Antibacterial	4117-65-1		C <sub>42</sub> H <sub>64</sub> N <sub>12</sub> O <sub>12</sub> S <sub>2</sub>
Asperlin	Antibacterial	30387-51-0		C <sub>10</sub> H <sub>12</sub> O <sub>5</sub>
Aspirin	Antiinflammatory	50-78-2	Y	C <sub>9</sub> H <sub>8</sub> O <sub>4</sub>
Aspoxicillin	Antibiotic	63358-49-6		C <sub>21</sub> H <sub>27</sub> N <sub>5</sub> O <sub>7</sub> S
Astemizole	Antihistaminic	68844-77-9		C <sub>28</sub> H <sub>31</sub> FN <sub>4</sub> O
Astromicin Sulfate	Antibacterial	55779-06-1		C <sub>17</sub> H <sub>35</sub> N <sub>5</sub> O <sub>6</sub>
Asulacrine	Antineoplastic	80841-47-0		C <sub>24</sub> H <sub>24</sub> N <sub>4</sub> O <sub>4</sub> S
Ataciguat	Vasodilator	254877-67-3		C <sub>21</sub> H <sub>19</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>6</sub> S <sub>3</sub>
Atamestane	Antineoplastic	96301-34-7		C <sub>20</sub> H <sub>26</sub> O <sub>2</sub>
Ataprost	Prostaglandin	83997-19-7		C <sub>21</sub> H <sub>32</sub> O <sub>4</sub>
Ataquimast	Antihistaminic	586348-21-2		C <sub>11</sub> H <sub>13</sub> N <sub>3</sub> O
Atazanavir	Antiviral	198904-31-3	Y	C <sub>38</sub> H <sub>52</sub> N <sub>6</sub> O <sub>7</sub>
Atenolol	Antihypertensive	29122-68-7	Y	C <sub>14</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub>
Ateviridine Mesylate	Antiviral	136816-75-6		C <sub>21</sub> H <sub>25</sub> N <sub>5</sub> O <sub>2</sub>
Atibeprone	Anticonvulsant	153420-96-3		C <sub>17</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub> S
Atipamezole	Antihypertensive	104054-27-5		C <sub>14</sub> H <sub>16</sub> N <sub>2</sub>
Atiprimod Dihydrochloride	Antiarrhythmic	123018-47-3		C <sub>22</sub> H <sub>44</sub> N <sub>2</sub>
Atiprosin Maleate	Antihypertensive	89303-63-9		C <sub>20</sub> H <sub>29</sub> N <sub>3</sub>
Atizoram	Dermatologic	135637-46-6		C <sub>18</sub> H <sub>24</sub> N <sub>2</sub> O <sub>3</sub>
Atliprofen	Antiinflammatory	108912-14-7		C <sub>13</sub> H <sub>12</sub> O <sub>2</sub> S
Atolide	Anticonvulsant	16231-75-7		C <sub>18</sub> H <sub>23</sub> N <sub>3</sub> O
Atomoxetine	Nootropic	83015-26-3	Y	C <sub>17</sub> H <sub>21</sub> NO
Atorvastatin	Antihyperlipidemic	134523-00-5	Y	C <sub>33</sub> H <sub>35</sub> FN <sub>2</sub> O <sub>5</sub>
Atosiban	Tocolytic	90779-69-4		C <sub>43</sub> H <sub>67</sub> N <sub>11</sub> O <sub>12</sub> S <sub>2</sub>
Atovaquone	Antimalarial	95233-18-4	Y	C <sub>22</sub> H <sub>19</sub> ClO <sub>3</sub>
Atracurium	Anticonvulsant	64228-79-1		C <sub>53</sub> H <sub>72</sub> N <sub>2</sub> O <sub>122+</sub>
Atrasentan	Anesthetic	173937-91-2	Y	C <sub>29</sub> H <sub>38</sub> N <sub>2</sub> O <sub>6</sub>
Atreleuton	Bronchodilator	154355-76-7		C <sub>16</sub> H <sub>15</sub> FN <sub>2</sub> O <sub>2</sub> S
Atrimustine	Antineoplastic	75219-46-4		C <sub>41</sub> H <sub>47</sub> Cl <sub>2</sub> NO <sub>6</sub>
Atrinositol	Vasodilator	28841-62-5		C <sub>6</sub> H <sub>15</sub> O <sub>15</sub> P <sub>3</sub>
Atromepine	Antispasmodic	428-07-9		C <sub>18</sub> H <sub>25</sub> NO <sub>3</sub>
Atropine	Mydriatic	51-55-8		C <sub>17</sub> H <sub>23</sub> NO <sub>3</sub>
Atropine Methylbromide	Antihypotensive	80-49-9	Y	C <sub>17</sub> H <sub>13</sub> BrNO <sub>3</sub>
Atropine Oxide	Antihypotensive	4438-22-6		C <sub>17</sub> H <sub>23</sub> NO <sub>4</sub>
Auranofin	Antirheumatic	34031-32-8	Y	C <sub>20</sub> H <sub>34</sub> AuO <sub>9</sub> PS
Aurothiogluucose	Antirheumatic	12192-57-3		C <sub>6</sub> H <sub>11</sub> AuO <sub>5</sub> S
Aurothioglycanide	Antirheumatic	16925-51-2		C <sub>8</sub> H <sub>8</sub> AuNOS
Avanafil	Erectile Dysfunction	330784-47-9	Y	C <sub>23</sub> H <sub>26</sub> ClN <sub>7</sub> O <sub>3</sub>
Avasimibe	Antihyperlipidemic	166518-60-1		C <sub>29</sub> H <sub>43</sub> NO <sub>4</sub> S
Avitriptan Fumarate	Antimigraine	151140-96-4		C <sub>22</sub> H <sub>30</sub> N <sub>6</sub> O <sub>3</sub> S
Avizafone	Anticonvulsant	65617-86-9		C <sub>22</sub> H <sub>27</sub> ClN <sub>4</sub> O <sub>3</sub>
Avobenzone	Dermatologic	70356-09-1		C <sub>20</sub> H <sub>22</sub> O <sub>3</sub>
Avosentan	Anesthetic	290815-26-8		C <sub>23</sub> H <sub>21</sub> N <sub>5</sub> O <sub>5</sub> S
Avridine	Antiviral	35607-20-6		C <sub>43</sub> H <sub>50</sub> N <sub>2</sub> O <sub>2</sub>
Axamozide	Antipsychotic	85076-06-8		C <sub>21</sub> H <sub>22</sub> ClN <sub>3</sub> O <sub>3</sub>
Axitinib	Antineoplastic	319460-85-0	Y	C <sub>22</sub> H <sub>18</sub> N <sub>4</sub> OS
Axitirome	Antihyperlipidemic	156740-57-7		C <sub>25</sub> H <sub>24</sub> FN <sub>6</sub> O <sub>6</sub>
Axomadol	Analgesic	187219-99-4		C <sub>16</sub> H <sub>25</sub> NO <sub>3</sub>
Azabon	Nootropic	1150-20-5		C <sub>14</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub> S
Azabuperone	Antipsychotic	2856-81-7		C <sub>17</sub> H <sub>23</sub> FN <sub>2</sub> O
Azacididine	Antineoplastic	320-67-2		C <sub>8</sub> H <sub>12</sub> N <sub>4</sub> O <sub>5</sub>
Azaclorzine	Vasodilator	49864-70-2		C <sub>22</sub> H <sub>24</sub> ClN <sub>3</sub> OS
Azaconazole	Antifungal	60207-31-0		C <sub>12</sub> H <sub>11</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>2</sub>



Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Azasterol	Antibacterial	313-05-3		C <sub>25</sub> H <sub>44</sub> N <sub>2</sub> O
Azacyclonol	Anxiolytic	115-46-8		C <sub>18</sub> H <sub>21</sub> NO
Azaftozine	Anxiolytic	54063-26-2		C <sub>23</sub> H <sub>24</sub> F <sub>3</sub> N <sub>3</sub> OS
Azalanstat Dihydrochloride	Antihyperlipidemic	143393-27-5		C <sub>22</sub> H <sub>24</sub> ClN <sub>3</sub> O <sub>2</sub> S
Azaloxan Fumarate	Antidepressant	72822-56-1		C <sub>18</sub> H <sub>25</sub> N <sub>3</sub> O <sub>3</sub>
Azamethiphos	Antineoplastic	35575-96-3		C <sub>9</sub> H <sub>10</sub> ClN <sub>2</sub> O <sub>5</sub> PS
Azamethonium Bromide	Antihypertensive	306-53-6		C <sub>13</sub> H <sub>33</sub> Br <sub>2</sub> N <sub>3</sub>
Azamulin	Antibacterial	76530-44-4		C <sub>24</sub> H <sub>38</sub> N <sub>4</sub> O <sub>4</sub> S
Azinator Maleate	Bronchodilator	37855-92-8		C <sub>18</sub> H <sub>18</sub> N <sub>2</sub> O
Azanidazole	Antiprotozoal	62973-76-6		C <sub>10</sub> H <sub>10</sub> N <sub>6</sub> O <sub>2</sub>
Azaperone	Sedative	1649-18-9		C <sub>19</sub> H <sub>22</sub> FN <sub>3</sub> O
Azapetine Phosphate	Anxiolytic	146-36-1		C <sub>17</sub> H <sub>17</sub> N
Azaprocin	Antibiotic	448-34-0		C <sub>18</sub> H <sub>24</sub> N <sub>2</sub> O
Azaquinzole	Unclassified	5234-86-6		C <sub>12</sub> H <sub>16</sub> N <sub>2</sub>
Azaribine	Dermatologic	2169-64-4		C <sub>14</sub> H <sub>17</sub> N <sub>3</sub> O <sub>9</sub>
Azarole	Immunomodulator	55872-82-7		C <sub>14</sub> H <sub>12</sub> N <sub>4</sub>
Azaserine	Antifungal	115-02-6		C <sub>5</sub> H <sub>7</sub> N <sub>3</sub> O <sub>4</sub>
Azasetron	Antiemetic	123040-69-7		C <sub>17</sub> H <sub>20</sub> ClN <sub>3</sub> O <sub>3</sub>
Azaspirium Chloride	Unclassified	34959-30-3		C <sub>22</sub> H <sub>24</sub> ClNO <sub>5</sub>
Azastene	Immunomodulator	13074-00-5		C <sub>23</sub> H <sub>33</sub> NO <sub>2</sub>
Azatadine	Antihistaminic	3964-81-6	Y	C <sub>20</sub> H <sub>22</sub> N <sub>2</sub>
Azathioprine	Immunosuppressant	446-86-6	Y	C <sub>9</sub> H <sub>7</sub> N <sub>7</sub> O <sub>2</sub> S
Azelaic Acid	Dermatologic	123-99-9		C <sub>9</sub> H <sub>16</sub> O <sub>4</sub>
Azelastine	Antihistaminic	58581-89-8		C <sub>22</sub> H <sub>24</sub> ClN <sub>3</sub> O
Azelmidipine	Antihypertensive	123524-52-7	Y	C <sub>33</sub> H <sub>34</sub> N <sub>4</sub> O <sub>6</sub>
Azepexole	Antihypertensive	36067-73-9		C <sub>9</sub> H <sub>15</sub> N <sub>3</sub> O
Azepindole	Antidepressant	26304-61-0		C <sub>12</sub> H <sub>14</sub> N <sub>2</sub>
Azetepa	Antineoplastic	125-45-1		C <sub>8</sub> H <sub>14</sub> N <sub>5</sub> OPS
Azetirelin	Thyroid	95729-65-0		C <sub>15</sub> H <sub>20</sub> N <sub>6</sub> O <sub>4</sub>
Azidamfenicol	Antibiotic	13838-08-9		C <sub>11</sub> H <sub>13</sub> N <sub>5</sub> O <sub>5</sub>
Azidocillin	Antibacterial	17243-38-8		C <sub>16</sub> H <sub>17</sub> N <sub>5</sub> O <sub>4</sub> S
Azimexon	Immunomodulator	64118-86-1		C <sub>9</sub> H <sub>14</sub> N <sub>4</sub> O
Azimilide Dihydrochloride	Antiarrhythmic	149908-53-2	Y	C <sub>23</sub> H <sub>28</sub> ClN <sub>5</sub> O <sub>3</sub>
Azintamide	Choleretic	1830-32-6		C <sub>10</sub> H <sub>14</sub> ClN <sub>3</sub> OS
Azipramine	Antidepressant	58503-82-5		C <sub>26</sub> H <sub>26</sub> N <sub>2</sub>
Azithromycin	Antibiotic	83905-01-5	Y	C <sub>38</sub> H <sub>72</sub> N <sub>2</sub> O <sub>12</sub>
Azlocillin	Antibiotic	37091-66-0		C <sub>20</sub> H <sub>23</sub> N <sub>5</sub> O <sub>6</sub> S
Azolimine	Diuretic	40828-45-3		C <sub>10</sub> H <sub>11</sub> N <sub>3</sub> O
Azosemide	Diuretic	27589-33-9	Y	C <sub>12</sub> H <sub>11</sub> ClN <sub>6</sub> O <sub>2</sub> S <sub>2</sub>
Azosulfamide	Diuretic	132-38-7		C <sub>18</sub> H <sub>16</sub> N <sub>4</sub> O <sub>10</sub> S <sub>3</sub>
Azotomycin	Antineoplastic	7644-67-9		C <sub>17</sub> H <sub>23</sub> N <sub>7</sub> O <sub>8</sub>
Aztreonam	Antibiotic	78110-38-0		C <sub>13</sub> H <sub>17</sub> N <sub>5</sub> O <sub>8</sub> S <sub>2</sub>
Azumolene Sodium	Muscle Relaxant	64748-79-4		C <sub>13</sub> H <sub>9</sub> BrN <sub>4</sub> O <sub>3</sub>
Bacampicillin	Antibiotic	50972-17-3	Y	C <sub>21</sub> H <sub>27</sub> N <sub>3</sub> O <sub>7</sub> S
Baclofen	Muscle Relaxant	1134-47-0	Y	C <sub>10</sub> H <sub>12</sub> ClNO <sub>2</sub>
Bacmecillinam	Antibacterial	50846-45-2		C <sub>20</sub> H <sub>31</sub> N <sub>3</sub> O <sub>6</sub> S
Bakeprofen	Antiinflammatory	74168-02-8		C <sub>16</sub> H <sub>14</sub> O <sub>4</sub>
Balaglitazone	Antidiabetic	199113-98-9		C <sub>20</sub> H <sub>17</sub> N <sub>3</sub> O <sub>4</sub> S
Balazipone	Antiinflammatory	137109-71-8		C <sub>13</sub> H <sub>11</sub> NO <sub>2</sub>
Balicatib	Unclassified	354813-19-7		C <sub>23</sub> H <sub>33</sub> N <sub>5</sub> O <sub>2</sub>
Balofloxacin	Antibacterial	127294-70-6		C <sub>20</sub> H <sub>24</sub> FN <sub>3</sub> O <sub>4</sub>
Balsalazide	Antiinflammatory	80573-04-2	Y	C <sub>17</sub> H <sub>15</sub> N <sub>3</sub> O <sub>6</sub>
Bamaluzole	Nootropic	87034-87-5		C <sub>14</sub> H <sub>12</sub> ClN <sub>3</sub> O
Bamaquimast	Antihistaminic	135779-82-7		C <sub>16</sub> H <sub>21</sub> N <sub>3</sub> O <sub>3</sub>
Bambuterol	Bronchodilator	81732-65-2	Y	C <sub>18</sub> H <sub>29</sub> N <sub>3</sub> O <sub>5</sub>
Bamethan	Vasodilator	3703-79-5		C <sub>12</sub> H <sub>19</sub> NO <sub>2</sub>
Bamifylline	Bronchodilator	2016-63-9		C <sub>20</sub> H <sub>27</sub> N <sub>5</sub> O <sub>3</sub>
Bamipine	Antihistaminic	4945-47-5		C <sub>19</sub> H <sub>24</sub> N <sub>2</sub>
Bamirastine	Antitussive	215529-47-8		C <sub>31</sub> H <sub>37</sub> N <sub>5</sub> O <sub>3</sub>
Bamnidazole	Antiprotozoal	31478-45-2		C <sub>7</sub> H <sub>10</sub> N <sub>4</sub> O <sub>4</sub>
Baquiloprim	Antibacterial	102280-35-3		C <sub>17</sub> H <sub>20</sub> N <sub>6</sub>
Barbital	Sedative	57-44-3	Y	C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>
Barixibat	Unclassified	263562-28-3		C <sub>42</sub> H <sub>55</sub> N <sub>5</sub> O <sub>8</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Barmastine	Antihistaminic	99156-66-8		C <sub>27</sub> H <sub>29</sub> N <sub>7</sub> O <sub>2</sub>
Barnidipine	Antihypertensive	104713-75-9	Y	C <sub>27</sub> H <sub>29</sub> N <sub>3</sub> O <sub>6</sub>
Barucainide	Antiarrhythmic	79784-22-8		C <sub>22</sub> H <sub>30</sub> N <sub>2</sub> O <sub>2</sub>
Barusiban	Tocolytic	285571-64-4		C <sub>40</sub> H <sub>63</sub> N <sub>9</sub> O <sub>8</sub> S
Batabulin Sodium	Antineoplastic	195533-53-0		C <sub>13</sub> H <sub>7</sub> F <sub>6</sub> NO <sub>3</sub> S
Batanopride	Antiemetic	102670-46-2		C <sub>17</sub> H <sub>26</sub> ClN <sub>3</sub> O <sub>3</sub>
Batebulast	Anticoagulant	81907-78-0		C <sub>19</sub> H <sub>29</sub> N <sub>3</sub> O <sub>2</sub>
Batelapine Maleate	Antipsychotic	95634-82-5		C <sub>16</sub> H <sub>20</sub> N <sub>6</sub>
Batimastat	Antineoplastic	130370-60-4		C <sub>23</sub> H <sub>31</sub> N <sub>3</sub> O <sub>4</sub> S <sub>2</sub>
Batoprazine	Antipsychotic	105685-11-8		C <sub>13</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Baxitazine	Anxiolytic	84386-11-8		C <sub>13</sub> H <sub>14</sub> O <sub>6</sub>
Bazedoxifene Acetate	Bone Resorption Inhibitor	198481-32-2	Y	C <sub>30</sub> H <sub>34</sub> N <sub>2</sub> O <sub>3</sub>
Bazinaprine	Antidepressant	94011-82-2		C <sub>17</sub> H <sub>19</sub> N <sub>5</sub> O
Becampanel	Antiseizure	188696-80-2		C <sub>10</sub> H <sub>11</sub> N <sub>4</sub> O <sub>7</sub> P
Becanthone	Anthelminthic	15351-04-9		C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> O <sub>2</sub> S
Becatecarin	Antineoplastic	119673-08-4		C <sub>33</sub> H <sub>34</sub> Cl <sub>2</sub> N <sub>4</sub> O <sub>7</sub>
Beciparcil	Antithrombotic	130782-54-6		C <sub>12</sub> H <sub>13</sub> NO <sub>3</sub> S <sub>2</sub>
Beclamide	Anticonvulsant	501-68-8		C <sub>10</sub> H <sub>12</sub> ClNO
Becliconazole	Antifungal	112893-26-2		C <sub>18</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>2</sub> O
Beclobrate	Antihyperlipidemic	55937-99-0		C <sub>20</sub> H <sub>23</sub> ClO <sub>3</sub>
Beclomethasone Dipropionate	Glucocorticoid	5534-09-8		C <sub>28</sub> H <sub>37</sub> ClO <sub>7</sub>
Befetupitant	Antidepressant	290296-68-3		C <sub>29</sub> H <sub>29</sub> F <sub>6</sub> N <sub>3</sub> O <sub>2</sub>
Befiperide	Antispasmodic	100927-14-8		C <sub>25</sub> H <sub>31</sub> N <sub>3</sub> O <sub>2</sub>
Befloxatone	Antidepressant	134564-82-2		C <sub>15</sub> H <sub>18</sub> F <sub>3</sub> NO <sub>5</sub>
Befunolol	Antiglaucoma	39552-01-7		C <sub>16</sub> H <sub>21</sub> NO <sub>4</sub>
Befuraline	Antidepressant	41717-30-0		C <sub>20</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>
Bekanamycin	Antibiotic	4696-76-8		C <sub>18</sub> H <sub>37</sub> N <sub>5</sub> O <sub>10</sub>
Belaperidone	Antipsychotic	208661-17-0		C <sub>22</sub> H <sub>22</sub> FN <sub>3</sub> O <sub>2</sub>
Belarizine	Antihistaminic	52395-99-0		C <sub>24</sub> H <sub>26</sub> N <sub>2</sub> O
Belfosdil	Antihypertensive	103486-79-9		C <sub>27</sub> H <sub>50</sub> O <sub>7</sub> P <sub>2</sub>
Belotecan	Antineoplastic	256411-32-2		C <sub>25</sub> H <sub>27</sub> N <sub>3</sub> O <sub>4</sub>
Beloxamide	Antihyperlipidemic	15256-58-3		C <sub>18</sub> H <sub>21</sub> NO <sub>2</sub>
Beloxepin	Antidepressant	135928-30-2		C <sub>19</sub> H <sub>21</sub> NO <sub>2</sub>
Bemarinone	Cardiotonic	92210-43-0		C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>
Bemegrade	Nootropic	64-65-3		C <sub>8</sub> H <sub>13</sub> NO <sub>2</sub>
Bemesetron	Antiemetic	40796-97-2		C <sub>15</sub> H <sub>17</sub> Cl <sub>2</sub> NO <sub>2</sub>
Bemetizide	Antidiabetic	1824-52-8		C <sub>15</sub> H <sub>16</sub> ClN <sub>3</sub> O <sub>4</sub> S <sub>2</sub>
Beminafil	Antihypertensive	566906-50-1		C <sub>25</sub> H <sub>24</sub> ClN <sub>3</sub> O <sub>3</sub> S
Bemitradine	Antihypertensive	88133-11-3		C <sub>15</sub> H <sub>17</sub> N <sub>5</sub> O
Bemoradan	Cardiotonic	112018-01-6		C <sub>13</sub> H <sub>13</sub> N <sub>3</sub> O <sub>3</sub>
Bemotrizinol	Dermatologic	187393-00-6		C <sub>38</sub> H <sub>49</sub> N <sub>3</sub> O <sub>5</sub>
Benactyzine	Antispasmodic	302-40-9		C <sub>20</sub> H <sub>25</sub> NO <sub>3</sub>
Benafentrine	Cardiotonic	35135-01-4		C <sub>23</sub> H <sub>27</sub> N <sub>3</sub> O <sub>3</sub>
Benapryzine	Antihypertensive	22487-42-9		C <sub>21</sub> H <sub>27</sub> NO <sub>3</sub>
Benaxibine	Antineoplastic	27661-27-4		C <sub>12</sub> H <sub>15</sub> NO <sub>6</sub>
Benazepril	Antihypertensive	86541-75-5	Y	C <sub>24</sub> H <sub>28</sub> N <sub>2</sub> O <sub>5</sub>
Benazeprilat	Antihypertensive	86541-78-8		C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>5</sub>
Bencianol	Antispasmodic	85443-48-7		C <sub>28</sub> H <sub>22</sub> O <sub>6</sub>
Bencisteine	Unclassified	42293-72-1		C <sub>15</sub> H <sub>19</sub> NO <sub>4</sub> S
Benclonidine	Antihypertensive	57647-79-7		C <sub>16</sub> H <sub>13</sub> Cl <sub>2</sub> N <sub>3</sub> O
Bencyclane	Vasodilator	2179-37-5		C <sub>19</sub> H <sub>31</sub> NO
Bendacalol Mesylate	Antihypertensive	81703-42-6		C <sub>20</sub> H <sub>23</sub> NO <sub>6</sub>
Bendamustine	Antineoplastic	16506-27-7		C <sub>16</sub> H <sub>21</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>2</sub>
Bendazac	Antiinflammatory	20187-55-7		C <sub>16</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>
Bendazol	Vasodilator	621-72-7	Y	C <sub>14</sub> H <sub>12</sub> N <sub>2</sub>
Benderizine	Vasodilator	59752-23-7		C <sub>28</sub> H <sub>34</sub> N <sub>2</sub> O <sub>2</sub>
Bendroflumethiazide	Diuretic	73-48-3	Y	C <sub>15</sub> H <sub>14</sub> F <sub>3</sub> N <sub>3</sub> O <sub>4</sub> S <sub>2</sub>
Benethamine Penicillin	Antibacterial	3647-71-0		C <sub>15</sub> H <sub>17</sub> N
Benexate	Ant ulcerative	78718-52-2		C <sub>23</sub> H <sub>27</sub> N <sub>3</sub> O <sub>4</sub>
Benfluorex	Antihyperlipidemic	23602-78-0		C <sub>19</sub> H <sub>20</sub> F <sub>3</sub> NO <sub>2</sub>
Benfosformin	Antidiabetic	738523-03-0		C <sub>9</sub> H <sub>14</sub> N <sub>5</sub> O <sub>3</sub> P
Benfurodil Hemisuccinate	Cardiotonic	3447-95-8		C <sub>19</sub> H <sub>18</sub> O <sub>7</sub>
Benhepazone	Unclassified	363-13-3		C <sub>15</sub> H <sub>12</sub> N <sub>2</sub> O

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Benidipine	Antihypertensive	105979-17-7	Y	C <sub>28</sub> H <sub>31</sub> N <sub>3</sub> O <sub>6</sub>
Benmoxin	Antidepressant	7654-03-7		C <sub>15</sub> H <sub>16</sub> N <sub>2</sub> O
Benolizime	Antibiotic	61864-30-0		C <sub>19</sub> H <sub>26</sub> N <sub>2</sub> O <sub>3</sub>
Benorilate	Analgesic	5003-48-5		C <sub>17</sub> H <sub>15</sub> NO <sub>5</sub>
Benorterone	Steroid	3570-10-3		C <sub>19</sub> H <sub>28</sub> O <sub>2</sub>
Benoxafos	Antineoplastic	16759-59-4		C <sub>12</sub> H <sub>14</sub> Cl <sub>2</sub> NO <sub>3</sub> PS <sub>2</sub>
Benoxaprofen	Antiinflammatory	51234-28-7		C <sub>16</sub> H <sub>12</sub> ClNO <sub>3</sub>
Benoxinate	Anesthetic	99-43-4		C <sub>17</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub>
Benperidol	Antipsychotic	2062-84-2		C <sub>22</sub> H <sub>24</sub> FN <sub>3</sub> O <sub>2</sub>
Benproperine	Antitussive	2156-27-6		C <sub>21</sub> H <sub>27</sub> NO
Benrixate	Unclassified	24671-26-9		C <sub>19</sub> H <sub>30</sub> N <sub>2</sub> O <sub>2</sub>
Benserazide	Antiparkinsonian	322-35-0		C <sub>10</sub> H <sub>15</sub> N <sub>3</sub> O <sub>5</sub>
Bensulide	Antiinflammatory	741-58-2		C <sub>14</sub> H <sub>24</sub> NO <sub>4</sub> PS <sub>3</sub>
Bentazepam	Sedative	29462-18-8		C <sub>17</sub> H <sub>16</sub> N <sub>2</sub> OS
Bentemazole	Antifungal	63927-95-7		C <sub>11</sub> H <sub>10</sub> N <sub>6</sub>
Bentipimine	Analgesic	17692-23-8		C <sub>27</sub> H <sub>31</sub> ClN <sub>2</sub> S
Benurestat	Antibacterial	38274-54-3		C <sub>9</sub> H <sub>9</sub> ClN <sub>2</sub> O <sub>3</sub>
Benzaprinoxide	Antidepressant	52758-02-8		C <sub>20</sub> H <sub>20</sub> ClNO
Benzarone	Capillary Protectant	1477-19-6		C <sub>17</sub> H <sub>14</sub> O <sub>3</sub>
Benzbromarone	Uricosuric	3562-84-3	Y	C <sub>17</sub> H <sub>12</sub> Br <sub>2</sub> O <sub>3</sub>
Benzestrol	Estrogen	85-95-0		C <sub>20</sub> H <sub>26</sub> O <sub>2</sub>
Benzethidine	Antihypertensive	3691-78-9		C <sub>23</sub> H <sub>29</sub> NO <sub>3</sub>
Benzetimide	Antihypertensive	14051-33-3		C <sub>23</sub> H <sub>26</sub> N <sub>2</sub> O <sub>2</sub>
Benzilonium Bromide	Antihypertensive	1050-48-2		C <sub>22</sub> H <sub>28</sub> NO <sub>3</sub> .Br
Benzindopyrine	Antipsychotic	16571-59-8		C <sub>22</sub> H <sub>20</sub> N <sub>2</sub>
Benziodarone	Vasodilator	68-90-6		C <sub>17</sub> H <sub>12</sub> I <sub>2</sub> O <sub>3</sub>
Benzmalecene	Antihyperlipidemic	148-07-2		C <sub>20</sub> H <sub>19</sub> Cl <sub>2</sub> NO <sub>3</sub>
Benznidazole	Antiprotozoal	22994-85-0	Y	C <sub>12</sub> H <sub>12</sub> N <sub>4</sub> O <sub>3</sub>
Benzobarbital	Sedative	744-80-9		C <sub>19</sub> H <sub>16</sub> N <sub>2</sub> O <sub>4</sub>
Benzocaine	Anesthetic	94-09-7		C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>
Benzoclidine	Antihypertensive	16852-81-6		C <sub>14</sub> H <sub>17</sub> NO <sub>2</sub>
Benzoctamine	Muscle Relaxant	17243-39-9		C <sub>18</sub> H <sub>19</sub> N
Benzodepa	Antineoplastic	1980-45-6		C <sub>12</sub> H <sub>16</sub> N <sub>3</sub> O <sub>3</sub> P
Benzomethamine Chloride	Antihypotensive	510-08-7		C <sub>22</sub> H <sub>31</sub> ClN <sub>2</sub> O <sub>2</sub>
Benzonate	Antitussive	104-31-4	Y	C <sub>30</sub> H <sub>53</sub> NO <sub>11</sub>
Benzotript	Gastroprokinetic	39544-74-6		C <sub>18</sub> H <sub>15</sub> ClN <sub>2</sub> O <sub>3</sub>
Benzoyl Peroxide	Dermatologic	94-36-0		C <sub>14</sub> H <sub>10</sub> O <sub>4</sub>
Benzoylpas Calcium	Antibacterial	13898-58-3		C <sub>14</sub> H <sub>11</sub> NO <sub>4</sub>
Benzphetamine	Anorexic	156-08-1	Y	C <sub>17</sub> H <sub>21</sub> N
Benzpiperylon	Antiinflammatory	53-89-4		C <sub>22</sub> H <sub>25</sub> N <sub>3</sub> O
Benzpyrinium Bromide	Cholinergic	587-46-2		C <sub>15</sub> H <sub>17</sub> BrN <sub>2</sub> O <sub>2</sub>
Benzquercin	Capillary Protectant	13157-90-9		C <sub>50</sub> H <sub>40</sub> O <sub>7</sub>
Benzquinamide	Antipsychotic	63-12-7		C <sub>22</sub> H <sub>32</sub> N <sub>2</sub> O <sub>5</sub>
Benzthiazide	Diuretic	91-33-8	Y	C <sub>15</sub> H <sub>14</sub> ClN <sub>3</sub> O <sub>4</sub> S <sub>3</sub>
Benztropine	Antiparkinsonian	86-13-5	Y	C <sub>21</sub> H <sub>25</sub> NO
Benzydamine	Analgesic	642-72-8		C <sub>19</sub> H <sub>23</sub> N <sub>3</sub> O
Benzyl Benzoate	Dermatologic	120-51-4		C <sub>14</sub> H <sub>12</sub> O <sub>2</sub>
Benzyl Nicotinate	Dermatologic	94-44-0		C <sub>13</sub> H <sub>11</sub> NO <sub>2</sub>
Benzyl Salicylate	Ant ulcerative	118-58-1		C <sub>14</sub> H <sub>12</sub> O <sub>3</sub>
Benzylhydrochlorothiazide	Diuretic	1824-50-6		C <sub>14</sub> H <sub>14</sub> ClN <sub>3</sub> O <sub>4</sub> S <sub>2</sub>
Benzylpenicillin	Antibiotic	61-33-6		C <sub>16</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub> S
Bepafant	Antithrombotic	114776-28-2		C <sub>23</sub> H <sub>22</sub> ClN <sub>3</sub> O <sub>2</sub> S
Beperidium Iodide	Antibiotic	86434-57-3		C <sub>23</sub> H <sub>34</sub> IN <sub>3</sub> O <sub>3</sub>
Bephenium Hydroxynaphthoate	Anthelminthic	3818-50-6		C <sub>28</sub> H <sub>29</sub> NO <sub>4</sub>
Bepiastine	Antihistaminic	10189-94-3		C <sub>16</sub> H <sub>17</sub> N <sub>3</sub> OS
Bepotastine	Antihistaminic	125602-71-3		C <sub>21</sub> H <sub>25</sub> ClN <sub>2</sub> O <sub>3</sub>
Bepridil	Antianginal	64706-54-3	Y	C <sub>24</sub> H <sub>34</sub> N <sub>2</sub> O
Beraprost Sodium	Prostaglandin	88430-50-6	Y	C <sub>24</sub> H <sub>30</sub> O <sub>5</sub>
Berberine	Antiprotozoal	2086-83-1		C <sub>20</sub> H <sub>18</sub> N <sub>3</sub> O <sub>4</sub> +
Berefrine	Mydriatic	105567-83-7		C <sub>14</sub> H <sub>21</sub> NO <sub>2</sub>
Bergenin	Ant ulcerative	477-90-7		C <sub>14</sub> H <sub>16</sub> O <sub>9</sub>
Berlafenone	Antiarrhythmic	18965-97-4		C <sub>19</sub> H <sub>25</sub> NO <sub>2</sub>
Bermopfen	Antiinflammatory	78499-27-1		C <sub>18</sub> H <sub>16</sub> O <sub>4</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Bertosamil	Antiarrhythmic	126825-36-3		C <sub>19</sub> H <sub>36</sub> N <sub>2</sub>
Berupipam	Antipsychotic	150490-85-0		C <sub>19</sub> H <sub>19</sub> BrClNO <sub>2</sub>
Bervastatin	Antihyperlipidemic	132017-01-7		C <sub>28</sub> H <sub>31</sub> FO <sub>5</sub>
Berythromycin	Antiamebic	527-75-3		C <sub>37</sub> H <sub>67</sub> NO <sub>12</sub>
Besipirdine	Nootropic	119257-34-0		C <sub>16</sub> H <sub>17</sub> N <sub>3</sub>
Besonprodil	Antiparkinsonian	253450-09-8		C <sub>21</sub> H <sub>23</sub> FN <sub>2</sub> O <sub>3</sub> S
Besulpamide	Diuretic	90992-25-9		C <sub>15</sub> H <sub>16</sub> ClN <sub>3</sub> O <sub>3</sub> S
Besunide	Glucocorticoid	36148-38-6		C <sub>18</sub> H <sub>22</sub> N <sub>2</sub> O <sub>4</sub> S
Betacetylmethadol	Analgesic	17199-59-6		C <sub>23</sub> H <sub>31</sub> NO <sub>2</sub>
Betahistine	Vasodilator	5638-76-6		C <sub>8</sub> H <sub>12</sub> N <sub>2</sub>
Betaine	Antidote	107-43-7	Y	C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub>
Betameprodine	Analgesic	468-50-8		C <sub>17</sub> H <sub>25</sub> NO <sub>2</sub>
Betamethadol	Glucocorticoid	17199-55-2		C <sub>21</sub> H <sub>29</sub> NO
Betamethasone	Glucocorticoid	378-44-9		C <sub>22</sub> H <sub>29</sub> FO <sub>5</sub>
Betamethasone Acetate	Glucocorticoid	987-24-6		C <sub>24</sub> H <sub>31</sub> FO <sub>6</sub>
Betamethasone Acibutate	Glucocorticoid	5534-05-4		C <sub>28</sub> H <sub>37</sub> FO <sub>7</sub>
Betamethasone Benzoate	Glucocorticoid	22298-29-9		C <sub>29</sub> H <sub>33</sub> FO <sub>6</sub>
Betamethasone Butyrate Propionate	Glucocorticoid	5534-02-1		C <sub>29</sub> H <sub>39</sub> FO <sub>7</sub>
Betamethasone Dipropionate	Glucocorticoid	5593-20-4		C <sub>28</sub> H <sub>37</sub> FO <sub>7</sub>
Betamethasone Sodium Phosphate	Glucocorticoid	360-63-4		C <sub>22</sub> H <sub>30</sub> FO <sub>8</sub> P
Betamethasone Valerate	Glucocorticoid	2152-44-5		C <sub>27</sub> H <sub>37</sub> FO <sub>6</sub>
Betamicin Sulfate	Antibacterial	36889-15-3		C <sub>19</sub> H <sub>38</sub> N <sub>4</sub> O <sub>10</sub>
Betamipron	Antibacterial	3440-28-6		C <sub>10</sub> H <sub>11</sub> NO <sub>3</sub>
Betaprodine	Analgesic	468-59-7		C <sub>16</sub> H <sub>23</sub> NO <sub>2</sub>
Betaxolol	Antianginal	63659-18-7	Y	C <sub>18</sub> H <sub>29</sub> NO <sub>3</sub>
Bethanechol	Cholinergic	674-38-4	Y	C <sub>7</sub> H <sub>17</sub> N <sub>2</sub> O <sub>2</sub>
Bethanidine	Antihypertensive	55-73-2	Y	C <sub>10</sub> H <sub>15</sub> N <sub>3</sub>
Betoxycaine	Anesthetic	3818-62-0		C <sub>19</sub> H <sub>32</sub> N <sub>2</sub> O <sub>4</sub>
Bevantolol	Antianginal	59170-23-9		C <sub>20</sub> H <sub>27</sub> NO <sub>4</sub>
Bevonium Metilsulfate	Antihypotensive	5205-82-3		C <sub>22</sub> H <sub>28</sub> NO <sub>3</sub> .CH <sub>3</sub> O <sub>4</sub> S
Bexarotene	Antineoplastic	153559-49-0	Y	C <sub>24</sub> H <sub>28</sub> O <sub>2</sub>
Bexlosteride	Antineoplastic	148905-78-6	Y	C <sub>14</sub> H <sub>16</sub> ClNO
Bezafibrate	Antihyperlipidemic	41859-67-0	Y	C <sub>19</sub> H <sub>20</sub> ClNO <sub>4</sub>
Beziramide	Analgesic	15301-48-1		C <sub>31</sub> H <sub>32</sub> N <sub>4</sub> O <sub>2</sub>
Bialamicol	Antiamebic	493-75-4	Y	C <sub>28</sub> H <sub>40</sub> N <sub>2</sub> O <sub>2</sub>
Biapenem	Antibacterial	120410-24-4		C <sub>15</sub> H <sub>18</sub> N <sub>4</sub> O <sub>4</sub> S
Bibenzonium Bromide	Antitussive	15585-70-3	Y	C <sub>19</sub> H <sub>26</sub> BrNO
Bibrocathol	Unclassified	6915-57-7		C <sub>6</sub> HBiBr <sub>4</sub> O <sub>3</sub>
Bicalutamide	Antineoplastic	90357-06-5	Y	C <sub>18</sub> H <sub>14</sub> F <sub>4</sub> N <sub>2</sub> O <sub>4</sub> S
Bicifadine	Analgesic	71195-57-8	Y	C <sub>12</sub> H <sub>15</sub> N
Biclodil	Antihypertensive	85125-49-1		C <sub>8</sub> H <sub>8</sub> Cl <sub>2</sub> N <sub>4</sub> O
Biclofibrate	Antihyperlipidemic	54063-27-3		C <sub>20</sub> H <sub>21</sub> Cl <sub>2</sub> NO <sub>4</sub>
Bicozamycin	Antibiotic	38129-37-2		C <sub>12</sub> H <sub>18</sub> N <sub>2</sub> O <sub>7</sub>
Bidimazium Iodide	Unclassified	21817-73-2		C <sub>26</sub> H <sub>25</sub> N <sub>2</sub> S.I
Bidisomide	Antiarrhythmic	116078-65-0		C <sub>22</sub> H <sub>34</sub> ClN <sub>3</sub> O <sub>2</sub>
Bietamiverine	Antispasmodic	479-81-2		C <sub>19</sub> H <sub>30</sub> N <sub>2</sub> O <sub>2</sub>
Bietaserpine	Antihypertensive	53-18-9		C <sub>39</sub> H <sub>53</sub> N <sub>3</sub> O <sub>9</sub>
Bifemelane	Nootropic	90293-01-9		C <sub>18</sub> H <sub>23</sub> NO
Bifepramide	Analgesic	70976-76-0		C <sub>21</sub> H <sub>28</sub> N <sub>2</sub> O
Bifeprufen	Antiinflammatory	108210-73-7		C <sub>22</sub> H <sub>25</sub> ClN <sub>2</sub> O <sub>3</sub>
Bifeprunox	Antipsychotic	350992-10-8		C <sub>24</sub> H <sub>23</sub> N <sub>3</sub> O <sub>2</sub>
Bifluranol	Steroid	34633-34-6		C <sub>17</sub> H <sub>18</sub> F <sub>2</sub> O <sub>2</sub>
Bifonazole	Antifungal	60628-96-8		C <sub>22</sub> H <sub>18</sub> N <sub>2</sub>
Bilastine	Antihistaminic	202189-78-4	Y	C <sub>28</sub> H <sub>37</sub> N <sub>3</sub> O <sub>3</sub>
Bimakalim	Antihypertensive	117545-11-6		C <sub>17</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Bimatoprost	Antiglaucoma	155206-00-1		C <sub>25</sub> H <sub>37</sub> NO <sub>4</sub>
Bimethoxycaïne Lactate	Analgesic	47302-54-5		C <sub>20</sub> H <sub>27</sub> NO <sub>2</sub>
Bimoclolmol	Capillary Protectant	130493-03-7		C <sub>14</sub> H <sub>20</sub> ClN <sub>3</sub> O <sub>2</sub>
Bimosiamose	Antiinflammatory	187269-40-5		C <sub>46</sub> H <sub>54</sub> O <sub>16</sub>
Bindarit	Antirheumatic	130641-38-2		C <sub>19</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub>
Binedaline	Antidepressant	60662-16-0		C <sub>19</sub> H <sub>23</sub> N <sub>3</sub>
Binfloxacin	Antibacterial	108437-28-1		C <sub>19</sub> H <sub>22</sub> FN <sub>3</sub> O <sub>3</sub>
Binifibrate	Antihyperlipidemic	69047-39-8	Y	C <sub>25</sub> H <sub>23</sub> ClN <sub>2</sub> O <sub>7</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Binizolast	Bronchodilator	86662-54-6		C <sub>18</sub> H <sub>23</sub> N <sub>5</sub> O
Binodenoson	Vasodilator	144348-08-3		C <sub>17</sub> H <sub>25</sub> N <sub>7</sub> O <sub>4</sub>
Binospirone Mesylate	Anxiolytic	102908-59-8		C <sub>20</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub>
Bioresmethrin	Dermatologic	28434-01-7		C <sub>22</sub> H <sub>26</sub> O <sub>3</sub>
Bipenamol	Antidepressant	79467-22-4		C <sub>14</sub> H <sub>15</sub> NOS
Biperiden	Antiparkinsonian	514-65-8	Y	C <sub>21</sub> H <sub>29</sub> NO
Biphenamine	Anesthetic	3572-52-9		C <sub>19</sub> H <sub>23</sub> NO <sub>3</sub>
Biricodar	Antineoplastic	159997-94-1		C <sub>34</sub> H <sub>41</sub> N <sub>3</sub> O <sub>7</sub>
Biriperone	Antipsychotic	42021-34-1		C <sub>24</sub> H <sub>26</sub> FN <sub>3</sub> O
Bisacodyl	Laxative	603-50-9	Y	C <sub>22</sub> H <sub>19</sub> NO <sub>4</sub>
Bisantrene	Antineoplastic	78186-34-2		C <sub>22</sub> H <sub>22</sub> N <sub>8</sub>
Bisaramil	Antiarrhythmic	89194-77-4		C <sub>17</sub> H <sub>23</sub> ClN <sub>2</sub> O <sub>2</sub>
Bisbendazole	Antifungal	32195-33-8		C <sub>28</sub> H <sub>28</sub> N <sub>6</sub> S <sub>4</sub>
Bisdequalinium Diacetate	Antibacterial	3785-44-2		C <sub>44</sub> H <sub>64</sub> N <sub>4</sub> O <sub>4</sub>
Bisfenazone	Antiinflammatory	55837-24-6		C <sub>25</sub> H <sub>29</sub> N <sub>5</sub> O <sub>2</sub>
Bisfentidine	Antihistaminic	96153-56-9		C <sub>14</sub> H <sub>18</sub> N <sub>4</sub>
Bismuth Sodium Triglycollamate	Immunomodulator	738525-05-8		C <sub>6</sub> H <sub>8</sub> BiNO <sub>7</sub>
Bismuth Sodium Triglycollamate	Immunomodulator	139-13-9		C <sub>6</sub> H <sub>9</sub> NO <sub>6</sub>
Bismuth Subsalicylate	Antidiarrheal	14882-18-9		C <sub>7</sub> H <sub>5</sub> BiO <sub>4</sub>
Bisnafide Dimesylate	Antineoplastic	144849-63-8		C <sub>32</sub> H <sub>28</sub> N <sub>6</sub> O <sub>8</sub>
Bisobrin Lactate	Anticoagulant	22407-74-5		C <sub>26</sub> H <sub>36</sub> N <sub>2</sub> O <sub>4</sub>
Bisoctrazole	Dermatologic	103597-45-1		C <sub>41</sub> H <sub>50</sub> N <sub>6</sub> O <sub>2</sub>
Bisoprolol	Antihypertensive	66722-44-9	Y	C <sub>18</sub> H <sub>31</sub> NO <sub>4</sub>
Bisoxatin Acetate	Laxative	14008-48-1		C <sub>24</sub> H <sub>19</sub> NO <sub>6</sub>
Bithionolate Sodium	Antibacterial	97-18-7		C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub> O <sub>2</sub> S
Bithionoloxide	Anthelmintic	844-26-8		C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub> O <sub>3</sub> S
Bitipazone	Antiinflammatory	13456-08-1		C <sub>20</sub> H <sub>38</sub> N <sub>8</sub> S <sub>2</sub>
Bitolterol	Bronchodilator	30392-40-6		C <sub>28</sub> H <sub>31</sub> NO <sub>5</sub>
Bitoscanate	Anthelmintic	4044-65-9		C <sub>8</sub> H <sub>4</sub> N <sub>2</sub> S <sub>2</sub>
Bizelesin	Antineoplastic	129655-21-6		C <sub>43</sub> H <sub>36</sub> Cl <sub>2</sub> N <sub>8</sub> O <sub>5</sub>
Blastomycin	Antifungal	522-70-3		C <sub>26</sub> H <sub>36</sub> N <sub>2</sub> O <sub>9</sub>
Blonanserin	Antipsychotic	132810-10-7	Y	C <sub>23</sub> H <sub>30</sub> FN <sub>3</sub>
Bluensomycin	Antineoplastic	11011-72-6		C <sub>21</sub> H <sub>39</sub> N <sub>5</sub> O <sub>14</sub>
Bofumustine	Antineoplastic	55102-44-8		C <sub>18</sub> H <sub>21</sub> ClN <sub>4</sub> O <sub>9</sub>
Bolandiol Dipropionate	Steroid	1986-53-4		C <sub>24</sub> H <sub>36</sub> O <sub>4</sub>
Bolasterone	Steroid	1605-89-6		C <sub>21</sub> H <sub>32</sub> O <sub>2</sub>
Bolazine	Antiinflammatory	4267-81-6		C <sub>40</sub> H <sub>64</sub> N <sub>2</sub> O <sub>2</sub>
Boldenone Undecylenate	Steroid	13103-34-9		C <sub>30</sub> H <sub>44</sub> O <sub>3</sub>
Bolenol	Steroid	16915-78-9		C <sub>20</sub> H <sub>32</sub> O
Bolmantalate	Steroid	1491-81-2		C <sub>29</sub> H <sub>40</sub> O <sub>3</sub>
Bometolol	Antiarrhythmic	65008-93-7		C <sub>25</sub> H <sub>32</sub> N <sub>2</sub> O <sub>7</sub>
Bopindolol	Antihypertensive	62658-63-3	Y	C <sub>23</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub>
Bornaprine	Antihypertensive	20448-86-6		C <sub>21</sub> H <sub>31</sub> NO <sub>2</sub>
Bornaprolol	Antihypertensive	66451-06-7		C <sub>19</sub> H <sub>29</sub> NO <sub>2</sub>
Bortezomib	Antineoplastic	179324-69-7		C <sub>19</sub> H <sub>25</sub> N <sub>4</sub> O <sub>4</sub>
Bosentan	Anticoagulant	147536-97-8	Y	C <sub>27</sub> H <sub>29</sub> N <sub>5</sub> O <sub>6</sub> S
Bosutinib	Antineoplastic	380843-75-4	Y	C <sub>26</sub> H <sub>29</sub> Cl <sub>2</sub> N <sub>5</sub> O <sub>3</sub>
Botiacrine	Nootropic	4774-53-2		C <sub>20</sub> H <sub>24</sub> N <sub>2</sub> OS
Boxidine	Antihyperlipidemic	10355-14-3		C <sub>19</sub> H <sub>20</sub> F <sub>3</sub> NO
Brallobarbital	Sedative	561-86-4		C <sub>10</sub> H <sub>11</sub> BrN <sub>2</sub> O <sub>3</sub>
Brasofensine	Antiparkinsonian	171655-91-7		C <sub>16</sub> H <sub>20</sub> Cl <sub>2</sub> N <sub>2</sub> O
Brazergoline	Antiparkinsonian	60019-20-7		C <sub>23</sub> H <sub>30</sub> BrN <sub>3</sub> O <sub>2</sub>
Brecanavir	Antiviral	313682-08-5		C <sub>33</sub> H <sub>41</sub> N <sub>3</sub> O <sub>10</sub> S <sub>2</sub>
Brefonalol	Antiarrhythmic	103880-26-8		C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> O <sub>2</sub>
Bremazocine	Analgesic	75684-07-0		C <sub>20</sub> H <sub>29</sub> NO <sub>2</sub>
Brequinar Sodium	Antineoplastic	96187-53-0		C <sub>23</sub> H <sub>15</sub> F <sub>2</sub> NO <sub>2</sub>
Bretazenil	Anxiolytic	84379-13-5		C <sub>19</sub> H <sub>20</sub> BrN <sub>3</sub> O <sub>3</sub>
Bretylum	Antiarrhythmic	59-41-6		C <sub>11</sub> H <sub>17</sub> BrN
Brimonidine	Antiglaucoma	59803-98-4		C <sub>11</sub> H <sub>10</sub> BrN <sub>5</sub>
Brinazarone	Antiarrhythmic	89622-90-2		C <sub>25</sub> H <sub>32</sub> N <sub>2</sub> O <sub>2</sub>
Brindoxime	Analgesic	55837-17-7		C <sub>18</sub> H <sub>19</sub> Br <sub>2</sub> N <sub>5</sub> O <sub>2</sub>
Brinzolamide	Antiglaucoma	138890-62-7		C <sub>12</sub> H <sub>21</sub> N <sub>3</sub> O <sub>5</sub> S <sub>3</sub>
Brivaracetam	Nootropic	357336-20-0	Y	C <sub>11</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Brivudine	Antiviral	69304-47-8		C <sub>11</sub> H <sub>13</sub> BrN <sub>2</sub> O <sub>5</sub>
Brobactam	Antibiotic	26631-90-3		C <sub>8</sub> H <sub>10</sub> BrNO <sub>3</sub> S
Broclepride	Gastroprokinetic	71195-56-7		C <sub>20</sub> H <sub>23</sub> BrClN <sub>3</sub> O <sub>2</sub>
Brocresine	Antiparkinsonian	555-65-7		C <sub>7</sub> H <sub>8</sub> BrNO <sub>2</sub>
Brocrinat	Diuretic	72481-99-3		C <sub>15</sub> H <sub>9</sub> BrFNO <sub>4</sub>
Brodimoprim	Antineoplastic	56518-41-3		C <sub>13</sub> H <sub>15</sub> BrN <sub>4</sub> O <sub>2</sub>
Brofaromine	Antidepressant	63638-91-5		C <sub>14</sub> H <sub>16</sub> BrNO <sub>2</sub>
Profezil	Nootropic	17969-45-8		C <sub>12</sub> H <sub>10</sub> BrNO <sub>2</sub> S
Brofoxine	Antipsychotic	21440-97-1		C <sub>10</sub> H <sub>10</sub> BrNO <sub>2</sub>
Brolaconazole	Antifungal	118528-04-4		C <sub>17</sub> H <sub>15</sub> BrN <sub>2</sub>
Brolamfetamine	Nootropic	64638-07-9		C <sub>11</sub> H <sub>16</sub> BrNO <sub>2</sub>
Bromacrylide	Antineoplastic	4213-51-8		C <sub>7</sub> H <sub>11</sub> BrN <sub>2</sub> O <sub>2</sub>
Bromadoline Maleate	Analgesic	67579-24-2		C <sub>15</sub> H <sub>21</sub> BrN <sub>2</sub> O
Bromamid	Unclassified	332-69-4		C <sub>11</sub> H <sub>15</sub> BrN <sub>2</sub> O
Bromazepam	Anxiolytic	1812-30-2	Y	C <sub>14</sub> H <sub>10</sub> BrN <sub>3</sub> O
Bromebric Acid	Antineoplastic	5711-40-0		C <sub>11</sub> H <sub>9</sub> BrO <sub>4</sub>
Bromerguride	Antipsychotic	83455-48-5		C <sub>20</sub> H <sub>25</sub> BrN <sub>4</sub> O
Bromfenac	Antiinflammatory	91714-94-2		C <sub>15</sub> H <sub>12</sub> BrNO <sub>3</sub>
Bromhexine	Expectorant	3572-43-8	Y	C <sub>14</sub> H <sub>20</sub> Br <sub>2</sub> N <sub>2</sub>
Bromindione	Anticoagulant	1146-98-1		C <sub>15</sub> H <sub>9</sub> BrO <sub>2</sub>
Bromisovalum	Sedative	496-67-3		C <sub>6</sub> H <sub>11</sub> BrN <sub>2</sub> O <sub>2</sub>
Bromociclen	Unclassified	1715-40-8		C <sub>8</sub> H <sub>5</sub> BrCl <sub>6</sub>
Bromocriptine	Pituitary	25614-03-3	Y	C <sub>32</sub> H <sub>40</sub> BrN <sub>5</sub> O <sub>5</sub>
Bromodiphenhydramine	Antihistaminic	118-23-0		C <sub>17</sub> H <sub>20</sub> BrNO
Bromofenofos	Antineoplastic	21466-07-9		C <sub>12</sub> H <sub>7</sub> Br <sub>4</sub> O <sub>5</sub> P
Bromoform	Sedative	75-25-2		CHBr <sub>3</sub>
Bromofos	Antineoplastic	2104-96-3		C <sub>8</sub> H <sub>8</sub> BrCl <sub>2</sub> O <sub>3</sub> PS
Bromopride	Antiemetic	4093-35-0		C <sub>14</sub> H <sub>22</sub> BrN <sub>3</sub> O <sub>2</sub>
Bromoxanide	Anthelminthic	41113-86-4		C <sub>19</sub> H <sub>18</sub> Br <sub>3</sub> N <sub>2</sub> O <sub>4</sub>
Bromperidol	Antipsychotic	10457-90-6		C <sub>21</sub> H <sub>23</sub> BrFNO <sub>2</sub>
Bromperidol Decanoate	Antipsychotic	75067-66-2		C <sub>31</sub> H <sub>41</sub> BrFNO <sub>3</sub>
Brompheniramine	Antihistaminic	86-22-6	Y	C <sub>16</sub> H <sub>19</sub> BrN <sub>2</sub>
Broparestrol	Estrogen	479-68-5		C <sub>22</sub> H <sub>19</sub> Br
Properamole	Antiinflammatory	33144-79-5		C <sub>15</sub> H <sub>18</sub> Br <sub>4</sub> N <sub>5</sub> O
Bropirimine	Antineoplastic	56741-95-8		C <sub>10</sub> H <sub>8</sub> BrN <sub>3</sub> O
Brosotamide	Nootropic	40912-73-0		C <sub>8</sub> H <sub>8</sub> BrNO <sub>2</sub>
Brostallicin	Antibiotic	203258-60-0		C <sub>30</sub> H <sub>35</sub> BrN <sub>12</sub> O <sub>5</sub>
Brosuximide	Antineoplastic	22855-57-8		C <sub>10</sub> H <sub>8</sub> BrNO <sub>2</sub>
Brotianide	Antiarrhythmic	23233-88-7		C <sub>15</sub> H <sub>10</sub> Br <sub>2</sub> ClNO <sub>2</sub> S
Brotizolam	Sedative	57801-81-7	Y	C <sub>15</sub> H <sub>10</sub> BrClN <sub>4</sub> S
Brovanexine	Expectorant	54340-61-3		C <sub>24</sub> H <sub>28</sub> Br <sub>2</sub> N <sub>2</sub> O <sub>4</sub>
Brovincamine	Vasodilator	57475-17-9	Y	C <sub>21</sub> H <sub>25</sub> Br <sub>2</sub> N <sub>2</sub> O <sub>3</sub>
Broxaldine	Antibacterial	3684-46-6		C <sub>17</sub> H <sub>11</sub> Br <sub>2</sub> NO <sub>2</sub>
Broxaterol	Bronchodilator	76596-57-1		C <sub>9</sub> H <sub>15</sub> BrN <sub>2</sub> O <sub>2</sub>
Broxitalamic Acid	Unclassified	86216-41-3		C <sub>12</sub> H <sub>11</sub> Br <sub>3</sub> N <sub>2</sub> O <sub>5</sub>
Broxuridine	Antineoplastic	59-14-3		C <sub>9</sub> H <sub>11</sub> BrN <sub>2</sub> O <sub>5</sub>
Brucine	Nootropic	357-57-3		C <sub>23</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub>
Bucainide Maleate	Antiarrhythmic	51481-62-0		C <sub>21</sub> H <sub>35</sub> N <sub>3</sub>
Bucetin	Analgesic	1083-57-4		C <sub>12</sub> H <sub>17</sub> NO <sub>3</sub>
Buciclovir	Antiviral	86304-28-1		C <sub>9</sub> H <sub>13</sub> N <sub>5</sub> O <sub>3</sub>
Bucillamine	Antirheumatic	65002-17-7	Y	C <sub>7</sub> H <sub>13</sub> NO <sub>3</sub> S <sub>2</sub>
Bucindolol	Antihypertensive	71119-11-4	Y	C <sub>22</sub> H <sub>25</sub> N <sub>3</sub> O <sub>2</sub>
Bucladesine	Cardiotonic	362-74-3		C <sub>18</sub> H <sub>24</sub> N <sub>5</sub> O <sub>8</sub> P
Buclizine	Antiemetic	82-95-1		C <sub>28</sub> H <sub>33</sub> ClN <sub>2</sub>
Buclosamide	Antifungal	575-74-6		C <sub>11</sub> H <sub>14</sub> ClNO <sub>2</sub>
Bucloxic Acid	Antiinflammatory	32808-51-8		C <sub>16</sub> H <sub>19</sub> ClO <sub>3</sub>
Bucolome	Antiinflammatory	841-73-6		C <sub>14</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub>
Bucricaine	Analgesic	316-15-4		C <sub>17</sub> H <sub>22</sub> N <sub>2</sub>
Bucromarone	Antiarrhythmic	78371-66-1		C <sub>29</sub> H <sub>37</sub> NO <sub>4</sub>
Bucumolol	Antianginal	58409-59-9		C <sub>17</sub> H <sub>23</sub> NO <sub>4</sub>
Budesonide	Glucocorticoid	51333-22-3	Y	C <sub>25</sub> H <sub>34</sub> O <sub>6</sub>
Budipine	Antiparkinsonian	57982-78-2	Y	C <sub>21</sub> H <sub>27</sub> N
Budralazine	Antihypertensive	36798-79-5		C <sub>14</sub> H <sub>16</sub> N <sub>4</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Bufenadrine	Antihistaminic	604-74-0		C <sub>21</sub> H <sub>29</sub> NO
Bufeniode	Antihypertensive	22103-14-6		C <sub>19</sub> H <sub>23</sub> I <sub>2</sub> NO <sub>2</sub>
Bufetolol	Antiarrhythmic	53684-49-4		C <sub>18</sub> H <sub>29</sub> NO <sub>4</sub>
Bufexamac	Antiinflammatory	2438-72-4		C <sub>12</sub> H <sub>17</sub> NO <sub>3</sub>
Bufezolac	Antiinflammatory	50270-32-1		C <sub>21</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>
Buflomedil	Vasodilator	55837-25-7	Y	C <sub>17</sub> H <sub>25</sub> NO <sub>4</sub>
Bufogenin	Cardiotonic	465-39-4		C <sub>24</sub> H <sub>32</sub> O <sub>4</sub>
Buformin	Antidiabetic	692-13-7		C <sub>6</sub> H <sub>15</sub> N <sub>5</sub>
Bufrolin	Antihistaminic	54867-56-0		C <sub>18</sub> H <sub>16</sub> N <sub>2</sub> O <sub>6</sub>
Bufuralol	Antianginal	54340-62-4		C <sub>16</sub> H <sub>23</sub> NO <sub>2</sub>
Bulaquine	Antimalarial	79781-00-3	Y	C <sub>21</sub> H <sub>27</sub> N <sub>3</sub> O <sub>3</sub>
Bumadizone	Analgesic	3583-64-0		C <sub>19</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub>
Bumecaine	Anesthetic	30103-44-7		C <sub>18</sub> H <sub>28</sub> N <sub>2</sub> O
Bumepidil	Antihypertensive	62052-97-5		C <sub>12</sub> H <sub>17</sub> N <sub>5</sub>
Bumetanide	Diuretic	28395-03-1	Y	C <sub>17</sub> H <sub>20</sub> N <sub>2</sub> O <sub>5</sub> S
Bumetrizole	Dermatologic	3896-11-5		C <sub>17</sub> H <sub>18</sub> ClN <sub>3</sub> O
Bunaftine	Antiarrhythmic	32421-46-8		C <sub>21</sub> H <sub>30</sub> N <sub>2</sub> O
Bunamidine	Anthelminthic	3748-77-4		C <sub>25</sub> H <sub>38</sub> N <sub>2</sub> O
Bunamiodyl Sodium	Unclassified	1233-53-0		C <sub>15</sub> H <sub>16</sub> I <sub>3</sub> NO <sub>3</sub>
Bunaprolast	Bronchodilator	99107-52-5		C <sub>17</sub> H <sub>20</sub> O <sub>3</sub>
Bunazosin	Antihypertensive	80755-51-7	Y	C <sub>19</sub> H <sub>27</sub> N <sub>5</sub> O <sub>3</sub>
Bunitrolol	Antianginal	34915-68-9		C <sub>14</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>
Bunolol	Antihypertensive	27591-01-1		C <sub>17</sub> H <sub>25</sub> NO <sub>3</sub>
Buparvaquone	Antineoplastic	88426-33-9		C <sub>21</sub> H <sub>26</sub> O <sub>3</sub>
Bupicomide	Antihypertensive	22632-06-0		C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O
Bupivacaine	Anesthetic	38396-39-3		C <sub>18</sub> H <sub>28</sub> N <sub>2</sub> O
Bupranolol	Antianginal	14556-46-8		C <sub>14</sub> H <sub>22</sub> ClNO <sub>2</sub>
Buprenorphine	Analgesic	52485-79-7		C <sub>29</sub> H <sub>41</sub> NO <sub>4</sub>
Bupropion	Antidepressant	34911-55-2	Y	C <sub>13</sub> H <sub>18</sub> ClNO
Buquineran	Cardiotonic	59184-78-0		C <sub>20</sub> H <sub>29</sub> N <sub>5</sub> O <sub>3</sub>
Buquinolate	Antibacterial	5486/3/3		C <sub>20</sub> H <sub>27</sub> NO <sub>5</sub>
Buquiterine	Antispasmodic	76536-74-8		C <sub>18</sub> H <sub>23</sub> N <sub>3</sub> O <sub>3</sub>
Buramate	Anticonvulsant	4663-83-6		C <sub>10</sub> H <sub>13</sub> NO <sub>3</sub>
Burodiline	Vasodilator	36121-13-8		C <sub>19</sub> H <sub>29</sub> NO <sub>5</sub>
Buspirone	Anxiolytic	36505-84-7	Y	C <sub>21</sub> H <sub>31</sub> N <sub>5</sub> O <sub>2</sub>
Busulfan	Antineoplastic	55-98-1	Y	C <sub>6</sub> H <sub>14</sub> O <sub>6</sub> S <sub>2</sub>
Butabarbital	Sedative	125-40-6	Y	C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>
Butacaine	Anesthetic	149-16-6		C <sub>18</sub> H <sub>30</sub> N <sub>2</sub> O <sub>2</sub>
Butacetin	Analgesic	2109-73-1		C <sub>6</sub> H <sub>12</sub> O
Butaclamol	Antipsychotic	51152-91-1		C <sub>25</sub> H <sub>31</sub> NO
Butadiazamide	Analgesic	7007-88-7		C <sub>12</sub> H <sub>14</sub> ClN <sub>3</sub> O <sub>2</sub> S <sub>2</sub>
Butafosfan	Antineoplastic	17316-67-5		C <sub>7</sub> H <sub>18</sub> NO <sub>2</sub> P
Butalamine	Vasodilator	22131-35-7		C <sub>18</sub> H <sub>28</sub> N <sub>4</sub> O
Butalbital	Sedative	77-26-9		C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>
Butallylonal	Sedative	1142-70-7		C <sub>11</sub> H <sub>15</sub> BrN <sub>2</sub> O <sub>3</sub>
Butamben	Anesthetic	94-25-7		C <sub>11</sub> H <sub>15</sub> NO <sub>2</sub>
Butamin	Unclassified	891-33-8		C <sub>14</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>
Butamirate	Anesthetic	18109-80-3	Y	C <sub>18</sub> H <sub>29</sub> NO <sub>3</sub>
Butamisole	Anthelminthic	54400-59-8		C <sub>15</sub> H <sub>19</sub> N <sub>3</sub> OS
Butamoxane	Sedative	4442-60-8		C <sub>13</sub> H <sub>19</sub> NO <sub>2</sub>
Butanilicaine	Anesthetic	3785-21-5		C <sub>13</sub> H <sub>19</sub> ClN <sub>2</sub> O
Butanixin	Antiinflammatory	55285-35-3		C <sub>16</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>
Butanserlin	Antihypertensive	87051-46-5		C <sub>24</sub> H <sub>26</sub> FN <sub>3</sub> O <sub>3</sub>
Butantrone	Dermatologic	75464-11-8		C <sub>18</sub> H <sub>16</sub> O <sub>4</sub>
Butaperazine	Antipsychotic	653-03-2		C <sub>24</sub> H <sub>31</sub> N <sub>3</sub> OS
Butaprost	Bronchodilator	69648-38-0		C <sub>24</sub> H <sub>40</sub> O <sub>5</sub>
Butaverine	Antispasmodic	55837-14-4		C <sub>18</sub> H <sub>27</sub> NO <sub>2</sub>
Butedronic Acid	Bone Resorption Inhibitor	51395-42-7		C <sub>5</sub> H <sub>10</sub> O <sub>10</sub> P <sub>2</sub>
Butenafine	Antifungal	101828-21-1		C <sub>23</sub> H <sub>27</sub> N
Buterizine	Vasodilator	68741-18-4		C <sub>31</sub> H <sub>38</sub> N <sub>4</sub>
Butetamate	Antitussive	14007-64-8		C <sub>16</sub> H <sub>25</sub> NO <sub>2</sub>
Butethal	Sedative	77-28-1		C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>
Butethamine	Anesthetic	2090-89-3		C <sub>13</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Buthalital Sodium	Anesthetic	468-65-5		C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub> S
Buthiazide	Diuretic	2043-38-1		C <sub>11</sub> H <sub>16</sub> ClN <sub>3</sub> O <sub>4</sub> S <sub>2</sub>
Butibufen	Antiinflammatory	55837-18-8		C <sub>14</sub> H <sub>20</sub> O <sub>2</sub>
Butidrine	Antiarrhythmic	7433-10-5		C <sub>16</sub> H <sub>25</sub> NO
Butikacin	Antibacterial	59733-86-7		C <sub>22</sub> H <sub>45</sub> N <sub>5</sub> O <sub>12</sub>
Butinazocine	Analgesic	93821-75-1		C <sub>18</sub> H <sub>23</sub> NO <sub>2</sub>
Butixirate	Analgesic	5769-10-8		C <sub>12</sub> H <sub>17</sub> N
Butixocort	Bronchodilator	120815-74-9		C <sub>25</sub> H <sub>36</sub> O <sub>5</sub> S
Butobendine	Antiarrhythmic	55769-65-8		C <sub>32</sub> H <sub>48</sub> N <sub>2</sub> O <sub>10</sub>
Butoconazole	Antifungal	64872-76-0		C <sub>19</sub> H <sub>17</sub> Cl <sub>3</sub> N <sub>2</sub> S
Butocrolol	Unclassified	55165-22-5		C <sub>19</sub> H <sub>23</sub> NO <sub>6</sub>
Butoctamide	Sedative	32838-26-9		C <sub>12</sub> H <sub>25</sub> NO <sub>2</sub>
Butofilolol	Antihypertensive	58930-32-8		C <sub>17</sub> H <sub>26</sub> FNO <sub>3</sub>
Butonate	Anthelminthic	126-22-7		C <sub>8</sub> H <sub>14</sub> Cl <sub>3</sub> O <sub>5</sub> P
Butopamine	Cardiotonic	66734-12-1		C <sub>18</sub> H <sub>23</sub> NO <sub>3</sub>
Butopiprine	Unclassified	55837-15-5		C <sub>19</sub> H <sub>29</sub> NO <sub>3</sub>
Butoprozine	Antiarrhythmic	62228-20-0		C <sub>28</sub> H <sub>38</sub> N <sub>2</sub> O <sub>2</sub>
Butorphanol	Analgesic	42408-82-2		C <sub>21</sub> H <sub>29</sub> NO <sub>2</sub>
Butoxamine	Antidiabetic	1937-89-9		C <sub>15</sub> H <sub>25</sub> NO <sub>3</sub>
Butoxylate	Antihypertensive	15302-05-3		C <sub>32</sub> H <sub>36</sub> N <sub>2</sub> O <sub>2</sub>
Butriptyline	Antidepressant	35941-65-2	Y	C <sub>21</sub> H <sub>27</sub> N
Butropium Bromide	Antispasmodic	29025-14-7		C <sub>28</sub> H <sub>38</sub> NO <sub>4</sub> .Br
Butyl Chloride	Anthelminthic	109-69-3		C <sub>4</sub> H <sub>9</sub> Cl
Butylphenamide	Antiglaucoma	131-90-8		C <sub>17</sub> H <sub>19</sub> NO <sub>2</sub>
Butylscopolamine Bromide	Antispasmodic	149-64-4	Y	C <sub>21</sub> H <sub>30</sub> BrNO <sub>4</sub>
Butynamine	Antispasmodic	3735-65-7		C <sub>10</sub> H <sub>19</sub> N
Buzepide Metiodide	Antispasmodic	15351-05-0		C <sub>23</sub> H <sub>31</sub> N <sub>2</sub> O.I
Cabastine	Antineoplastic	79449-98-2		C <sub>26</sub> H <sub>29</sub> FN <sub>2</sub> O <sub>2</sub>
Cabergoline	Antiparkinsonian	81409-90-7	Y	C <sub>26</sub> H <sub>37</sub> N <sub>5</sub> O <sub>2</sub>
Cadralazine	Vasodilator	64241-34-5	Y	C <sub>12</sub> H <sub>21</sub> N <sub>5</sub> O <sub>3</sub>
Cadroxifloxacin	Antibiotic	153808-85-6		C <sub>19</sub> H <sub>20</sub> F <sub>3</sub> N <sub>3</sub> O <sub>4</sub>
Cafaminol	Decongestant	30924-31-3		C <sub>11</sub> H <sub>17</sub> N <sub>5</sub> O <sub>3</sub>
Cafedrine	Nootropic	58166-83-9		C <sub>18</sub> H <sub>23</sub> N <sub>5</sub> O <sub>3</sub>
Caffeine	Nootropic	58-08-2	Y	C <sub>8</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub>
Calcifediol	Bone Resorption Inhibitor	19356-17-3	Y	C <sub>27</sub> H <sub>44</sub> O <sub>2</sub>
Calcipotriene	Dermatologic	112965-21-6		C <sub>27</sub> H <sub>40</sub> O <sub>3</sub>
Calcium Carbimide	Alcohol Deterrant	420-04-2		CH <sub>2</sub> N <sub>2</sub>
Calcium Dobesilate	Capillary Protectant	88-46-0		C <sub>6</sub> H <sub>6</sub> O <sub>5</sub> S
Calcobutrol	Unclassified	138168-36-2		C <sub>18</sub> H <sub>34</sub> N <sub>4</sub> O <sub>9</sub>
Caldaret	Cardiotonic	133804-44-1		C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub> S
Calusterone	Antineoplastic	17021-26-0		C <sub>21</sub> H <sub>32</sub> O <sub>2</sub>
Camazepam	Anxiolytic	36104-80-0		C <sub>19</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>3</sub>
Cambendazole	Anthelminthic	26097-80-3		C <sub>14</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub> S
Camiglibose	Antidiabetic	127214-23-7		C <sub>13</sub> H <sub>25</sub> NO <sub>9</sub>
Camiverine	Antispasmodic	54063-28-4		C <sub>19</sub> H <sub>30</sub> N <sub>2</sub> O <sub>2</sub>
Camonagrel	Anticoagulant	105920-77-2		C <sub>15</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>
Camostat	Antiviral	59721-28-7	Y	C <sub>20</sub> H <sub>22</sub> N <sub>4</sub> O <sub>5</sub>
Camphor	Analgesic	76-22-2		C <sub>10</sub> H <sub>16</sub> O
Camphoric Acid	Analgesic	5394-83-2		C <sub>10</sub> H <sub>16</sub> O <sub>4</sub>
Camphotamide	Nootropic	4876-45-3		C <sub>21</sub> H <sub>32</sub> N <sub>2</sub> O <sub>5</sub> S
Camptothecin	Antineoplastic	7689-03-4		C <sub>20</sub> H <sub>16</sub> N <sub>2</sub> O <sub>4</sub>
Camyllofin	Antispasmodic	54-30-8		C <sub>19</sub> H <sub>32</sub> N <sub>2</sub> O <sub>2</sub>
Canbisol	Anxiolytic	56689-43-1		C <sub>24</sub> H <sub>38</sub> O <sub>3</sub>
Candesartan	Antihypertensive	139481-59-7	Y	C <sub>24</sub> H <sub>20</sub> N <sub>6</sub> O <sub>3</sub>
Candesartan Cilexetil	Antihypertensive	145040-37-5	Y	C <sub>33</sub> H <sub>34</sub> N <sub>6</sub> O <sub>6</sub>
Candocurionium Iodide	Muscle Relaxant	54278-85-2		C <sub>26</sub> H <sub>46</sub> I <sub>2</sub> N <sub>2</sub>
Candoxatril	Cardiotonic	123122-55-4		C <sub>29</sub> H <sub>41</sub> NO <sub>7</sub>
Candoxatrilat	Cardiotonic	123122-54-3		C <sub>20</sub> H <sub>33</sub> NO <sub>7</sub>
Canertinib Dihydrochloride	Antineoplastic	267243-28-7		C <sub>24</sub> H <sub>25</sub> ClFN <sub>5</sub> O <sub>3</sub>
Canfosamide	Antineoplastic	158382-37-7		C <sub>26</sub> H <sub>40</sub> Cl <sub>4</sub> N <sub>5</sub> O <sub>10</sub> PS
Cangrelor	Anticoagulant	163706-06-7		C <sub>17</sub> H <sub>25</sub> Cl <sub>2</sub> F <sub>3</sub> N <sub>5</sub> O <sub>12</sub> P <sub>3</sub> S <sub>2</sub>
Cannabinol	Antiemetic	521-35-7		C <sub>21</sub> H <sub>26</sub> O <sub>2</sub>
Canrenoate	Diuretic	4138-96-9		C <sub>22</sub> H <sub>30</sub> O <sub>4</sub>



Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Canrenone	Diuretic	976-71-6		C <sub>22</sub> H <sub>28</sub> O <sub>3</sub>
Cantharides	Dermatologic	56-25-7		C <sub>10</sub> H <sub>12</sub> O <sub>4</sub>
Capecitabine	Antineoplastic	154361-50-9	Y	C <sub>15</sub> H <sub>22</sub> FN <sub>3</sub> O <sub>6</sub>
Capobenic Acid	Antiarrhythmic	21434-91-3		C <sub>16</sub> H <sub>23</sub> NO <sub>6</sub>
Capravirine	Antiviral	178979-85-6		C <sub>20</sub> H <sub>20</sub> Cl <sub>2</sub> N <sub>4</sub> O <sub>2</sub> S
Capromorelin Tartrate	Cardiotonic	193273-66-4		C <sub>28</sub> H <sub>35</sub> N <sub>5</sub> O <sub>4</sub>
Caproxamine	Antidepressant	53078-44-7		C <sub>15</sub> H <sub>25</sub> N <sub>3</sub> O
Caprylate	Antifungal	74-81-7		C <sub>8</sub> H <sub>15</sub> O <sub>2</sub>
Capsaicin	Analgesic	404-86-4		C <sub>18</sub> H <sub>27</sub> NO <sub>3</sub>
Captamine	Dermatologic	108-02-1		C <sub>4</sub> H <sub>11</sub> NS
Captodiamine	Anxiolytic	486-17-9		C <sub>21</sub> H <sub>29</sub> NS <sub>2</sub>
Captopril	Antihypertensive	62571-86-2	Y	C <sub>9</sub> H <sub>15</sub> NO <sub>3</sub> S
Capuride	Sedative	5579-13-5		C <sub>9</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>
Carabersat	Antimigraine	184653-84-7		C <sub>20</sub> H <sub>20</sub> FNO <sub>4</sub>
Caracemide	Antineoplastic	81424-67-1		C <sub>6</sub> H <sub>11</sub> N <sub>3</sub> O <sub>4</sub>
Carafiban	Antithrombotic	177563-40-5		C <sub>24</sub> H <sub>27</sub> N <sub>5</sub> O <sub>5</sub>
Caramiphen	Antitussive	77-22-5		C <sub>18</sub> H <sub>27</sub> NO <sub>2</sub>
Carazolol	Antihypertensive	57775-29-8		C <sub>18</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>
Carbachol	Cholinergic	51-83-2		C <sub>6</sub> H <sub>15</sub> N <sub>2</sub> O <sub>2</sub> .Cl
Carbadox	Antibacterial	6804-07-5		C <sub>11</sub> H <sub>10</sub> N <sub>4</sub> O <sub>4</sub>
Carbamazepine	Anticonvulsant	298-46-4	Y	C <sub>15</sub> H <sub>12</sub> N <sub>2</sub> O
Carbanteil Lauryl Sulfate	Anthelmintic	22790-84-7		C <sub>12</sub> H <sub>16</sub> ClN <sub>3</sub> O
Carbanteil Lauryl Sulfate	Anthelmintic	151-41-7		C <sub>12</sub> H <sub>26</sub> O <sub>4</sub> S
Carbaril	Ectoparasiticide	63-25-2		C <sub>12</sub> H <sub>11</sub> NO <sub>2</sub>
Carbarosone	Antiamebic	121-59-5		C <sub>7</sub> H <sub>9</sub> AsN <sub>2</sub> O <sub>4</sub>
Carbazeran	Cardiotonic	70724-25-3		C <sub>18</sub> H <sub>24</sub> N <sub>4</sub> O <sub>4</sub>
Carbazochrome	Hemostatic	69-81-8	Y	C <sub>10</sub> H <sub>12</sub> N <sub>4</sub> O <sub>3</sub>
Carbazocine	Analgesic	15686-38-1		C <sub>22</sub> H <sub>28</sub> N <sub>2</sub>
Carbenicillin	Antibiotic	4697-36-3		C <sub>17</sub> H <sub>18</sub> N <sub>2</sub> O <sub>6</sub> S
Carbenicillin Indanyl Sodium	Antibiotic	35531-88-5		C <sub>26</sub> H <sub>26</sub> N <sub>2</sub> O <sub>6</sub> S
Carbenicillin Phenyl Sodium	Antibiotic	27025-49-6		C <sub>23</sub> H <sub>22</sub> N <sub>2</sub> O <sub>6</sub> S
Carbenoxolone	Antiulcerative	5697-56-3	Y	C <sub>34</sub> H <sub>50</sub> O <sub>7</sub>
Carbenzide	Antipsychotic	3240-20-8		C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>
Carbetapentane Citrate	Antitussive	77-23-6		C <sub>20</sub> H <sub>31</sub> NO <sub>3</sub>
Carbethyl Salicylate	Unclassified	118-27-4		C <sub>19</sub> H <sub>18</sub> O <sub>7</sub>
Carbetocin	Oxytocic	37025-55-1		C <sub>45</sub> H <sub>69</sub> N <sub>11</sub> O <sub>12</sub> S
Carbidopa	Antiparkinsonian	28860-95-9	Y	C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub>
Carbimazole	Thyroid	22232-54-8	Y	C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> S
Carbinoxamine	Antihistaminic	486-16-8	Y	C <sub>16</sub> H <sub>19</sub> ClN <sub>2</sub> O
Carbiphen	Analgesic	15687-16-8		C <sub>28</sub> H <sub>34</sub> N <sub>2</sub> O <sub>2</sub>
Carbocloral	Sedative	541-79-7		C <sub>5</sub> H <sub>8</sub> Cl <sub>3</sub> NO <sub>3</sub>
Carbocysteine	Mucolytic	638-23-3	Y	C <sub>5</sub> H <sub>9</sub> NO <sub>4</sub> S
Carbofenotion	Dermatologic	786-19-6		C <sub>11</sub> H <sub>16</sub> ClO <sub>2</sub> PS <sub>3</sub>
Carbol Fuchsin	Antifungal	682730-74-1		C <sub>21</sub> H <sub>21</sub> N <sub>3</sub>
Carbomycin	Antibiotic	4564-87-8		C <sub>42</sub> H <sub>67</sub> NO <sub>16</sub>
Carbon Tetrachloride	Anthelmintic	56-23-5		CCl <sub>4</sub>
Carboprost	Oxytocic	35700-23-3		C <sub>21</sub> H <sub>36</sub> O <sub>5</sub>
Carboprost Methyl	Oxytocic	35700-21-1		C <sub>22</sub> H <sub>38</sub> O <sub>5</sub>
Carboquone	Antineoplastic	24279-91-2		C <sub>15</sub> H <sub>19</sub> N <sub>3</sub> O <sub>5</sub>
Carbromal	Sedative	77-65-6		C <sub>7</sub> H <sub>13</sub> BrN <sub>2</sub> O <sub>2</sub>
Carbubarb	Sedative	960-05-4		C <sub>11</sub> H <sub>17</sub> N <sub>3</sub> O <sub>5</sub>
Carburazepam	Anxiolytic	59009-93-7		C <sub>17</sub> H <sub>16</sub> ClN <sub>3</sub> O <sub>2</sub>
Carbutamide	Antidiabetic	339-43-5		C <sub>11</sub> H <sub>17</sub> N <sub>3</sub> O <sub>3</sub> S
Carbuterol	Bronchodilator	34866-47-2		C <sub>13</sub> H <sub>21</sub> N <sub>3</sub> O <sub>3</sub>
Carcainium Chloride	Anesthetic	1042-42-8		C <sub>18</sub> H <sub>22</sub> ClN <sub>3</sub> O <sub>2</sub>
Carebastine	Antihistaminic	90729-42-3		C <sub>32</sub> H <sub>37</sub> NO <sub>4</sub>
Carfentanil Citrate	Analgesic	59708-52-0		C <sub>24</sub> H <sub>30</sub> N <sub>2</sub> O <sub>3</sub>
Carfimate	Sedative	3567-38-2		C <sub>10</sub> H <sub>9</sub> NO <sub>2</sub>
Cargutocin	Oxytocic	33605-67-3		C <sub>42</sub> H <sub>65</sub> N <sub>11</sub> O <sub>12</sub>
Caricotamide	Antithrombotic	64881-21-6		C <sub>8</sub> H <sub>11</sub> N <sub>3</sub> O <sub>2</sub>
Cariporide	Cardiotonic	159138-80-4		C <sub>12</sub> H <sub>17</sub> N <sub>3</sub> O <sub>3</sub> S
Carisoprodol	Muscle Relaxant	78-44-4	Y	C <sub>12</sub> H <sub>24</sub> N <sub>2</sub> O <sub>4</sub>
Carmantidine	Antiparkinsonian	38081-67-3		C <sub>14</sub> H <sub>21</sub> NO <sub>2</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Carmetizide	Antidiabetic	42583-55-1		C <sub>10</sub> H <sub>12</sub> ClN <sub>3</sub> O <sub>6</sub> S <sub>2</sub>
Carmofur	Antineoplastic	61422-45-5		C <sub>11</sub> H <sub>16</sub> FN <sub>3</sub> O <sub>3</sub>
Carmoterol	Bronchodilator	147568-66-9		C <sub>21</sub> H <sub>24</sub> N <sub>2</sub> O <sub>4</sub>
Carmoxirole	Antihypertensive	98323-83-2		C <sub>24</sub> H <sub>26</sub> N <sub>2</sub> O <sub>2</sub>
Carmustine	Antineoplastic	154-93-8		C <sub>5</sub> H <sub>9</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>2</sub>
Carnidazole	Antiprotozoal	42116-76-7		C <sub>8</sub> H <sub>12</sub> N <sub>4</sub> O <sub>3</sub> S
Carnitine	Antihyperlipidemic	541-15-1		C <sub>7</sub> H <sub>15</sub> NO <sub>3</sub>
Carocainide	Antiarrhythmic	66203-00-7		C <sub>18</sub> H <sub>25</sub> N <sub>3</sub> O <sub>5</sub>
Caroverine	Antispasmodic	23465-76-1		C <sub>22</sub> H <sub>27</sub> N <sub>3</sub> O <sub>2</sub>
Caroxazone	Antidepressant	18464-39-6		C <sub>10</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub>
Carperidine	Analgesic	7008-32-4		C <sub>17</sub> H <sub>24</sub> N <sub>2</sub> O <sub>3</sub>
Carperone	Antipsychotic	20977-50-8		C <sub>19</sub> H <sub>27</sub> FN <sub>2</sub> O <sub>3</sub>
Carphenazine	Antipsychotic	2622-30-2		C <sub>24</sub> H <sub>31</sub> N <sub>3</sub> O <sub>2</sub> S
Carpindolol	Antihypertensive	39731-05-0		C <sub>19</sub> H <sub>28</sub> N <sub>2</sub> O <sub>4</sub>
Carpipramine	Antipsychotic	5942-95-0	Y	C <sub>28</sub> H <sub>38</sub> N <sub>4</sub> O
Carprazidil	Antihypertensive	68020-77-9		C <sub>12</sub> H <sub>13</sub> N <sub>5</sub> O <sub>4</sub>
Carprofen	Antiinflammatory	53716-49-7	Y	C <sub>15</sub> H <sub>12</sub> ClNO <sub>2</sub>
Carpronium Chloride	Cholinergic	13254-33-6		C <sub>8</sub> H <sub>18</sub> ClNO <sub>2</sub>
Carsalam	Analgesic	2037-95-8		C <sub>8</sub> H <sub>5</sub> NO <sub>3</sub>
Carsatrin Succinate	Cardiotonic	125345-93-9		C <sub>25</sub> H <sub>26</sub> F <sub>2</sub> N <sub>6</sub> OS
Cartasteine	Mucolytic	149079-51-6		C <sub>9</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub> S <sub>2</sub>
Cartazolate	Antidepressant	34966-41-1		C <sub>15</sub> H <sub>22</sub> N <sub>4</sub> O <sub>2</sub>
Carteolol	Antihypertensive	51781-06-7		C <sub>16</sub> H <sub>24</sub> N <sub>2</sub> O <sub>3</sub>
Carubicin	Antineoplastic	50935-04-1		C <sub>26</sub> H <sub>27</sub> NO <sub>10</sub>
Carumonam Sodium	Antibacterial	87638-04-8		C <sub>12</sub> H <sub>14</sub> N <sub>6</sub> O <sub>10</sub> S <sub>2</sub>
Carvacrol	Anthelmintic	499-75-2		C <sub>10</sub> H <sub>14</sub> O
Carvedilol	Antihypertensive	72956-09-3	Y	C <sub>24</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub>
Carvotroline	Antipsychotic	107266-08-0		C <sub>18</sub> H <sub>18</sub> FN <sub>3</sub>
Carzelesin	Antineoplastic	119813-10-4		C <sub>41</sub> H <sub>37</sub> ClN <sub>6</sub> O <sub>5</sub>
Carzenide	Unclassified	138-41-0		C <sub>7</sub> H <sub>7</sub> NO <sub>4</sub> S
Casokefamide	Ant ulcerative	98815-38-4		C <sub>33</sub> H <sub>40</sub> N <sub>6</sub> O <sub>7</sub>
Cathine	Anorexic	492-39-7		C <sub>9</sub> H <sub>13</sub> NO
Cathinone	Nootropic	71031-15-7		C <sub>9</sub> H <sub>11</sub> NO
Cebaracetam	Nootropic	113957-09-8		C <sub>16</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>3</sub>
Cedefingol	Antineoplastic	35301-24-7		C <sub>20</sub> H <sub>41</sub> NO <sub>3</sub>
Cefaclor	Antibiotic	53994-73-3	Y	C <sub>15</sub> H <sub>14</sub> ClN <sub>3</sub> O <sub>4</sub> S
Cefadroxil	Antibiotic	50370-12-2	Y	C <sub>16</sub> H <sub>17</sub> N <sub>3</sub> O <sub>5</sub> S
Cefalonium	Antibiotic	5575-21-3		C <sub>20</sub> H <sub>18</sub> N <sub>4</sub> O <sub>5</sub> S <sub>2</sub>
Cefaloram	Antibiotic	859-07-4		C <sub>18</sub> H <sub>18</sub> N <sub>2</sub> O <sub>6</sub> S
Cefamandole	Antibiotic	34444-01-4		C <sub>18</sub> H <sub>18</sub> N <sub>6</sub> O <sub>5</sub> S <sub>2</sub>
Cefamandole Nafate	Antibiotic	57268-80-1		C <sub>19</sub> H <sub>18</sub> N <sub>6</sub> O <sub>6</sub> S <sub>2</sub>
Cefaparole	Antibiotic	51627-20-4		C <sub>19</sub> H <sub>19</sub> N <sub>5</sub> O <sub>5</sub> S <sub>3</sub>
Cefatrizine	Antibiotic	51627-14-6		C <sub>18</sub> H <sub>18</sub> N <sub>6</sub> O <sub>5</sub> S <sub>2</sub>
Cefazafur	Antibiotic	58665-96-6		C <sub>13</sub> H <sub>13</sub> F <sub>3</sub> N <sub>6</sub> O <sub>4</sub> S <sub>3</sub>
Cefazedone	Antibiotic	56187-47-4		C <sub>18</sub> H <sub>15</sub> Cl <sub>2</sub> N <sub>5</sub> O <sub>5</sub> S <sub>3</sub>
Cefazolin	Antibiotic	25953-19-9		C <sub>14</sub> H <sub>14</sub> N <sub>8</sub> O <sub>4</sub> S <sub>3</sub>
Cefbuperazone	Antibiotic	76610-84-9		C <sub>22</sub> H <sub>29</sub> N <sub>9</sub> O <sub>9</sub> S <sub>2</sub>
Cefcanel	Antibiotic	41952-52-7		C <sub>19</sub> H <sub>18</sub> N <sub>4</sub> O <sub>5</sub> S <sub>3</sub>
Cefcanel Daloxate	Antibiotic	97275-40-6		C <sub>27</sub> H <sub>27</sub> N <sub>5</sub> O <sub>9</sub> S <sub>3</sub>
Cefcapene	Antibiotic	135889-00-8	Y	C <sub>17</sub> H <sub>19</sub> N <sub>5</sub> O <sub>6</sub> S <sub>2</sub>
Cefclidin	Antibiotic	105239-91-6		C <sub>21</sub> H <sub>26</sub> N <sub>8</sub> O <sub>6</sub> S <sub>2</sub>
Cefdaloxime	Antibiotic	80195-36-4		C <sub>14</sub> H <sub>15</sub> N <sub>5</sub> O <sub>6</sub> S <sub>2</sub>
Cefdinir	Antibiotic	91832-40-5	Y	C <sub>14</sub> H <sub>13</sub> N <sub>5</sub> O <sub>5</sub> S <sub>2</sub>
Cefditoren	Antibiotic	104145-95-1	Y	C <sub>19</sub> H <sub>18</sub> N <sub>6</sub> O <sub>5</sub> S <sub>3</sub>
Cefditoren Pivoxil	Antibiotic	117467-28-4	Y	C <sub>25</sub> H <sub>28</sub> N <sub>6</sub> O <sub>7</sub> S <sub>3</sub>
Cefedrolor	Antibiotic	57847-69-5		C <sub>16</sub> H <sub>16</sub> ClN <sub>3</sub> O <sub>5</sub> S
Cefempidone	Antibiotic	103238-57-9		C <sub>22</sub> H <sub>21</sub> N <sub>7</sub> O <sub>6</sub> S <sub>2</sub>
Cefepime	Antibiotic	88040-23-7		C <sub>19</sub> H <sub>24</sub> N <sub>6</sub> O <sub>5</sub> S <sub>2</sub>
Cefetamet	Antibiotic	65052-63-3		C <sub>14</sub> H <sub>15</sub> N <sub>5</sub> O <sub>5</sub> S <sub>2</sub>
Cefetecol	Antibiotic	117211-03-7		C <sub>20</sub> H <sub>17</sub> N <sub>5</sub> O <sub>9</sub> S <sub>2</sub>
Cefetizole	Antibiotic	65307-12-2		C <sub>16</sub> H <sub>15</sub> N <sub>5</sub> O <sub>4</sub> S <sub>3</sub>
Cefivitril	Antibiotic	66474-36-0		C <sub>15</sub> H <sub>15</sub> N <sub>7</sub> O <sub>4</sub> S <sub>3</sub>
Cefixime	Antibiotic	79350-37-1		C <sub>16</sub> H <sub>15</sub> N <sub>5</sub> O <sub>7</sub> S <sub>2</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Cefluprenam	Antibiotic	116853-25-9		C <sub>20</sub> H <sub>25</sub> FN <sub>8</sub> O <sub>6</sub> S <sub>2</sub>
Cefmatilen	Antibiotic	140128-74-1		C <sub>15</sub> H <sub>14</sub> N <sub>8</sub> O <sub>5</sub> S <sub>4</sub>
Cefmenoxime	Antibiotic	65085-01-0		C <sub>16</sub> H <sub>17</sub> N <sub>9</sub> O <sub>5</sub> S <sub>3</sub>
Cefmepidium Chloride	Antibiotic	107452-79-9		C <sub>23</sub> H <sub>25</sub> N <sub>6</sub> O <sub>8</sub> S <sub>3</sub> .Cl
Cefmetazole	Antibiotic	56796-20-4		C <sub>15</sub> H <sub>17</sub> N <sub>7</sub> O <sub>5</sub> S <sub>3</sub>
Cefminox	Antibiotic	84305-41-9		C <sub>16</sub> H <sub>21</sub> N <sub>7</sub> O <sub>7</sub> S <sub>3</sub>
Cefodizime	Antibiotic	69739-16-8		C <sub>20</sub> H <sub>20</sub> N <sub>6</sub> O <sub>7</sub> S <sub>4</sub>
Cefonicid	Antibiotic	61270-58-4		C <sub>18</sub> H <sub>18</sub> N <sub>6</sub> O <sub>8</sub> S <sub>3</sub>
Cefoperazone	Antibiotic	62893-19-0		C <sub>25</sub> H <sub>27</sub> N <sub>9</sub> O <sub>8</sub> S <sub>2</sub>
Ceforanide	Antibiotic	60925-61-3		C <sub>20</sub> H <sub>21</sub> N <sub>7</sub> O <sub>6</sub> S <sub>2</sub>
Cefoselis	Antibiotic	122841-10-5		C <sub>19</sub> H <sub>22</sub> N <sub>8</sub> O <sub>6</sub> S <sub>2</sub>
Cefotaxime	Antibiotic	63527-52-6		C <sub>16</sub> H <sub>17</sub> N <sub>5</sub> O <sub>7</sub> S <sub>2</sub>
Cefotetan	Antibiotic	69712-56-7		C <sub>17</sub> H <sub>17</sub> N <sub>7</sub> O <sub>8</sub> S <sub>4</sub>
Cefotiam	Antibiotic	61622-34-2		C <sub>18</sub> H <sub>23</sub> N <sub>9</sub> O <sub>4</sub> S <sub>3</sub>
Cefovecin Sodium	Antibiotic	234096-34-5		C <sub>17</sub> H <sub>19</sub> N <sub>5</sub> O <sub>6</sub> S <sub>2</sub>
Cefoxazole	Antibiotic	36920-48-6		C <sub>21</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>7</sub> S
Cefoxitin	Antibiotic	35607-66-0		C <sub>16</sub> H <sub>17</sub> N <sub>3</sub> O <sub>7</sub> S <sub>2</sub>
Cefozopran	Antibiotic	113359-04-9		C <sub>19</sub> H <sub>17</sub> N <sub>9</sub> O <sub>5</sub> S <sub>2</sub>
Cefpimizole	Antibiotic	84880-03-5		C <sub>28</sub> H <sub>26</sub> N <sub>6</sub> O <sub>10</sub> S <sub>2</sub>
Cefpiramide	Antibiotic	70797-11-4		C <sub>25</sub> H <sub>24</sub> N <sub>8</sub> O <sub>7</sub> S <sub>2</sub>
Cefpodoxime Proxetil	Antibiotic	87239-81-4	Y	C <sub>21</sub> H <sub>27</sub> N <sub>5</sub> O <sub>9</sub> S <sub>2</sub>
Cefprozil	Antibiotic	92665-29-7	Y	C <sub>18</sub> H <sub>19</sub> N <sub>3</sub> O <sub>5</sub> S
Cefquinome Sulfate	Antibiotic	118443-88-2		C <sub>23</sub> H <sub>25</sub> N <sub>6</sub> O <sub>5</sub> S <sub>2</sub>
Cefrotil	Antibiotic	52231-20-6		C <sub>20</sub> H <sub>22</sub> N <sub>4</sub> O <sub>4</sub> S
Cefroxadine	Antibiotic	51762-05-1		C <sub>16</sub> H <sub>19</sub> N <sub>3</sub> O <sub>5</sub> S
Cefsulodin Sodium	Antibiotic	69705-63-1		C <sub>22</sub> H <sub>21</sub> N <sub>4</sub> O <sub>8</sub> S <sub>2</sub>
Cefsumide	Antibiotic	54818-11-0		C <sub>17</sub> H <sub>20</sub> N <sub>4</sub> O <sub>6</sub> S <sub>2</sub>
Ceftazidime	Antibiotic	72558-82-8		C <sub>22</sub> H <sub>22</sub> N <sub>6</sub> O <sub>7</sub> S <sub>2</sub>
Cefteram	Antibiotic	82547-58-8	Y	C <sub>16</sub> H <sub>17</sub> N <sub>9</sub> O <sub>5</sub> S <sub>2</sub>
Ceftazole	Antibiotic	26973-24-0		C <sub>13</sub> H <sub>12</sub> N <sub>8</sub> O <sub>4</sub> S <sub>3</sub>
Ceftibuten	Antibiotic	97519-39-6	Y	C <sub>15</sub> H <sub>14</sub> N <sub>4</sub> O <sub>6</sub> S <sub>2</sub>
Ceftiofur	Antibiotic	80370-57-6		C <sub>19</sub> H <sub>17</sub> N <sub>5</sub> O <sub>7</sub> S <sub>3</sub>
Ceftiolene	Antibiotic	77360-52-2		C <sub>20</sub> H <sub>18</sub> N <sub>8</sub> O <sub>8</sub> S <sub>3</sub>
Ceftioxide	Antibiotic	69132-42-9		C <sub>16</sub> H <sub>17</sub> N <sub>5</sub> O <sub>8</sub> S <sub>2</sub>
Ceftizoxime Alapivoxil	Antibiotic	135821-54-4		C <sub>22</sub> H <sub>28</sub> N <sub>6</sub> O <sub>8</sub> S <sub>2</sub>
Ceftizoxime	Antibiotic	68401-81-0		C <sub>13</sub> H <sub>13</sub> N <sub>5</sub> O <sub>5</sub> S <sub>2</sub>
Ceftobiprole	Antibiotic	209467-52-7		C <sub>20</sub> H <sub>22</sub> N <sub>8</sub> O <sub>6</sub> S <sub>2</sub>
Ceftobiprole Medocaril	Antibiotic	376653-43-9		C <sub>26</sub> H <sub>26</sub> N <sub>8</sub> O <sub>11</sub> S <sub>2</sub>
Ceftriaxone	Antibiotic	73384-59-5		C <sub>18</sub> H <sub>18</sub> N <sub>8</sub> O <sub>7</sub> S <sub>3</sub>
Cefuracetime	Antibiotic	39685-31-9		C <sub>17</sub> H <sub>17</sub> N <sub>3</sub> O <sub>8</sub> S
Cefuroxime	Antibiotic	55268-75-2	Y	C <sub>16</sub> H <sub>16</sub> N <sub>4</sub> O <sub>8</sub> S
Cefuroxime Axetil	Antibiotic	64544-07-6	Y	C <sub>20</sub> H <sub>22</sub> N <sub>4</sub> O <sub>10</sub> S
Cefuroxime Pivoxetil	Antibiotic	100680-33-9		C <sub>23</sub> H <sub>28</sub> N <sub>4</sub> O <sub>11</sub> S
Cefuzonam	Antibiotic	82219-78-1		C <sub>16</sub> H <sub>15</sub> N <sub>7</sub> O <sub>5</sub> S <sub>4</sub>
Celecoxib	Antiinflammatory	169590-42-5	Y	C <sub>17</sub> H <sub>14</sub> F <sub>3</sub> N <sub>3</sub> O <sub>2</sub> S
Celgosivir	Antiviral	121104-96-9	Y	C <sub>12</sub> H <sub>21</sub> NO <sub>5</sub>
Celiprolol	Antihypertensive	56980-93-9	Y	C <sub>20</sub> H <sub>33</sub> N <sub>3</sub> O <sub>4</sub>
Cemadotin	Antineoplastic	159776-69-9		C <sub>35</sub> H <sub>56</sub> N <sub>6</sub> O <sub>5</sub>
Cephacetrile Sodium	Antibiotic	10206-21-0		C <sub>13</sub> H <sub>13</sub> N <sub>3</sub> O <sub>6</sub> S
Cephalexin	Antibiotic	15686-71-2	Y	C <sub>16</sub> H <sub>17</sub> N <sub>3</sub> O <sub>4</sub> S
Cephaloglycin	Antibiotic	3577-01-3		C <sub>18</sub> H <sub>19</sub> N <sub>3</sub> O <sub>6</sub> S
Cephaloridine	Antibiotic	50-59-9		C <sub>19</sub> H <sub>17</sub> N <sub>3</sub> O <sub>4</sub> S <sub>2</sub>
Cephalosporin C	Antibiotic	61-24-5		C <sub>16</sub> H <sub>21</sub> N <sub>3</sub> O <sub>8</sub> S
Cephalothin	Antibiotic	153-61-7		C <sub>16</sub> H <sub>16</sub> N <sub>2</sub> O <sub>6</sub> S <sub>2</sub>
Cephapirin	Antibiotic	21593-23-7		C <sub>17</sub> H <sub>17</sub> N <sub>3</sub> O <sub>6</sub> S <sub>2</sub>
Cepharanthine	Antibiotic	481-49-2		C <sub>37</sub> H <sub>38</sub> N <sub>2</sub> O <sub>6</sub>
Cephradine	Antibiotic	38821-53-3	Y	C <sub>16</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub> S
Cericlamine	Antidepressant	112922-55-1		C <sub>12</sub> H <sub>17</sub> Cl <sub>2</sub> NO
Cerivastatin	Antihyperlipidemic	145599-86-6		C <sub>26</sub> H <sub>34</sub> FNO <sub>5</sub>
Ceronapril	Antihypertensive	111223-26-8		C <sub>21</sub> H <sub>33</sub> N <sub>2</sub> O <sub>6</sub> P
Cetaben Sodium	Antihyperlipidemic	55986-43-1		C <sub>23</sub> H <sub>39</sub> NO <sub>2</sub>
Cetalkonium Chloride	Antibacterial	122-18-9		C <sub>25</sub> H <sub>46</sub> ClN
Cetamolol	Antihypertensive	34919-98-7		C <sub>16</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Cetefloxacin	Antibiotic	141725-88-4		C <sub>20</sub> H <sub>16</sub> F <sub>3</sub> N <sub>3</sub> O <sub>3</sub>
Cethromycin	Antibacterial	205110-48-1	Y	C <sub>42</sub> H <sub>59</sub> N <sub>3</sub> O <sub>10</sub>
Cetiedil	Vasodilator	14176-10-4		C <sub>20</sub> H <sub>31</sub> NO <sub>2</sub> S
Cetilistat	Anticoagulant	282526-98-1	Y	C <sub>25</sub> H <sub>39</sub> NO <sub>3</sub>
Cetirizine	Antihistaminic	83881-51-0	Y	C <sub>21</sub> H <sub>25</sub> ClN <sub>2</sub> O <sub>3</sub>
Cetocycline	Antibacterial	29144-42-1		C <sub>22</sub> H <sub>21</sub> NO <sub>7</sub>
Cetohexazine	Unclassified	7007-92-3		C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O
Cetophenicol	Antibacterial	735-52-4		C <sub>13</sub> H <sub>15</sub> Cl <sub>2</sub> NO <sub>4</sub>
Cetoxime	Antihistaminic	25394-78-9		C <sub>15</sub> H <sub>17</sub> N <sub>3</sub> O
Cetraxate	Antiulcerative	34675-84-8	Y	C <sub>17</sub> H <sub>23</sub> NO <sub>4</sub>
Cevimeline	Gastroprokinetic	107233-08-9	Y	C <sub>10</sub> H <sub>17</sub> NOS
Chaulmoogric Acid	Antibacterial	29106-32-9		C <sub>18</sub> H <sub>32</sub> O <sub>2</sub>
Chaulmosulfone	Antibacterial	473-32-5		C <sub>48</sub> H <sub>76</sub> N <sub>2</sub> O <sub>4</sub> S
Chenodiol	Anticholelithogenic	474-25-9	Y	C <sub>24</sub> H <sub>40</sub> O <sub>4</sub>
Chiniofon	Antiamoebic	547-91-1		C <sub>9</sub> H <sub>6</sub> INO <sub>4</sub> S
Chlophedianol	Antitussive	791-35-5		C <sub>17</sub> H <sub>20</sub> ClNO
Chloracyzine	Vasodilator	800-22-6		C <sub>19</sub> H <sub>21</sub> ClN <sub>2</sub> O <sub>2</sub> S
Chloral Hydrate	Sedative	302-17-0		C <sub>2</sub> H <sub>3</sub> Cl <sub>3</sub> O <sub>2</sub>
Chloralformamide	Sedative	515-82-2		C <sub>3</sub> H <sub>4</sub> Cl <sub>3</sub> NO <sub>2</sub>
Chloralose	Sedative	15879-93-3		C <sub>8</sub> H <sub>11</sub> Cl <sub>3</sub> O <sub>6</sub>
Chlorambucil	Antineoplastic	305-03-3	Y	C <sub>14</sub> H <sub>19</sub> Cl <sub>2</sub> NO <sub>2</sub>
Chloramine-T	Antibacterial	144-86-5		C <sub>7</sub> H <sub>8</sub> ClNO <sub>2</sub> S
Chloramphenicol	Antibiotic	56-75-7		C <sub>11</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>5</sub>
Chloramphenicol Palmitate	Antibiotic	530-43-8		C <sub>27</sub> H <sub>42</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>6</sub>
Chloramphenicol Succinate	Antibiotic	3544-94-3		C <sub>15</sub> H <sub>16</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>8</sub>
Chloranil	Antifungal	118-75-2		C <sub>6</sub> Cl <sub>4</sub> O <sub>2</sub>
Chlorazaniol	Antifungal	500-42-5		C <sub>9</sub> H <sub>8</sub> ClN <sub>5</sub>
Chlorbenzoxamine	Antispasmodic	522-18-9		C <sub>27</sub> H <sub>31</sub> ClN <sub>2</sub> O
Chlorbetamide	Antiamoebic	97-27-8		C <sub>11</sub> H <sub>11</sub> Cl <sub>4</sub> NO <sub>2</sub>
Chlorcyclizine	Antihistaminic	82-93-9		C <sub>18</sub> H <sub>21</sub> ClN <sub>2</sub>
Chlordantoin	Antifungal	5588-20-5		C <sub>11</sub> H <sub>17</sub> Cl <sub>3</sub> N <sub>2</sub> O <sub>2</sub> S
Chlordiazepoxide	Anxiolytic	58-25-3	Y	C <sub>16</sub> H <sub>14</sub> ClN <sub>3</sub> O
Chlordimorine	Unclassified	494-14-4		C <sub>19</sub> H <sub>22</sub> ClNO <sub>2</sub>
Chlorhexadol	Sedative	3563-58-4		C <sub>8</sub> H <sub>15</sub> Cl <sub>3</sub> O <sub>3</sub>
Chlorindanol	Contraceptive	145-94-8		C <sub>9</sub> H <sub>9</sub> ClO
Chlorisondamine	Antihypertensive	69-27-2		C <sub>14</sub> H <sub>20</sub> Cl <sub>6</sub> N <sub>2</sub>
Chlormadinone Acetate	Progestogen	302-22-7	Y	C <sub>23</sub> H <sub>29</sub> ClO <sub>4</sub>
Chlormezanone	Anxiolytic	80-77-3		C <sub>11</sub> H <sub>12</sub> ClNO <sub>3</sub> S
Chlormidazole	Antifungal	3689-76-7		C <sub>15</sub> H <sub>13</sub> ClN <sub>2</sub>
Chlornaphazine	Antineoplastic	494-03-1		C <sub>14</sub> H <sub>15</sub> Cl <sub>2</sub> N
Chlorobutanol	Analgesic	57-15-8		C <sub>4</sub> H <sub>7</sub> Cl <sub>3</sub> O
Chloroform	Anesthetic	67-66-3		CHCl <sub>3</sub>
Chloroguanide	Antimalarial	500-92-5		C <sub>11</sub> H <sub>16</sub> ClN <sub>5</sub>
Chlorophenothane	Ectoparasiticide	50-29-3		C <sub>14</sub> H <sub>9</sub> Cl <sub>5</sub>
Chloroprednisone Acetate	Glucocorticoid	14066-79-6		C <sub>23</sub> H <sub>27</sub> ClO <sub>6</sub>
Chloroprocaine	Anesthetic	133-16-4		C <sub>13</sub> H <sub>19</sub> ClN <sub>2</sub> O <sub>2</sub>
Chloropyramine	Antihistaminic	59-32-5		C <sub>16</sub> H <sub>20</sub> ClN <sub>3</sub>
Chloroquine	Antimalarial	54-05-7	Y	C <sub>18</sub> H <sub>26</sub> ClN <sub>3</sub>
Chloroserpidine	Antihypertensive	7008-24-4		C <sub>32</sub> H <sub>37</sub> ClN <sub>2</sub> O <sub>8</sub>
Chlorothen Citrate	Antihistaminic	148-65-2		C <sub>14</sub> H <sub>18</sub> ClN <sub>3</sub> S
Chlorothiazide	Diuretic	58-94-6	Y	C <sub>7</sub> H <sub>6</sub> ClN <sub>3</sub> O <sub>4</sub> S <sub>2</sub>
Chlorotrianisene	Estrogen	569-57-3		C <sub>23</sub> H <sub>21</sub> ClO <sub>3</sub>
Chloroxine	Dermatologic	773-76-2		C <sub>9</sub> H <sub>5</sub> Cl <sub>2</sub> NO
Chlorphenesin Carbamate	Muscle Relaxant	886-74-8	Y	C <sub>10</sub> H <sub>12</sub> ClNO <sub>4</sub>
Chlorpheniramine	Antihistaminic	132-22-9	Y	C <sub>16</sub> H <sub>19</sub> ClN <sub>2</sub>
Chlorphenoctium Amsonate	Unclassified	7168-18-5		C <sub>31</sub> H <sub>41</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>7</sub> S <sub>2</sub>
Chlorphenoxamine	Antihistaminic	77-38-3		C <sub>18</sub> H <sub>22</sub> ClNO
Chlorphentermine	Anorexic	461-78-9		C <sub>10</sub> H <sub>14</sub> ClN
Chlorproethazine	Analgesic	84-01-5		C <sub>19</sub> H <sub>23</sub> ClN <sub>2</sub> S
Chlorproguanil	Antimalarial	537-21-3		C <sub>11</sub> H <sub>15</sub> Cl <sub>2</sub> N <sub>5</sub>
Chlorpromazine	Antiemetic	50-53-3	Y	C <sub>17</sub> H <sub>19</sub> ClN <sub>2</sub> S
Chlorpropamide	Antidiabetic	94-20-2	Y	C <sub>10</sub> H <sub>13</sub> ClN <sub>2</sub> O <sub>3</sub> S
Chlorprothixene	Antipsychotic	113-59-7		C <sub>18</sub> H <sub>18</sub> ClNS

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Chlorpyrifos	Ectoparasiticide	2921-88-2		C <sub>9</sub> H <sub>11</sub> Cl <sub>3</sub> NO <sub>3</sub> PS
Chlorquinaldol	Antibacterial	72-80-0		C <sub>10</sub> H <sub>7</sub> Cl <sub>2</sub> NO
Chlortetracycline	Antibiotic	57-62-5		C <sub>22</sub> H <sub>23</sub> ClN <sub>2</sub> O <sub>8</sub>
Chlorthalidone	Diuretic	77-36-1		C <sub>14</sub> H <sub>11</sub> ClN <sub>2</sub> O <sub>4</sub> S
Chlorthenoxazine	Analgesic	132-89-8		C <sub>10</sub> H <sub>10</sub> CINO <sub>2</sub>
Chlorzoxazone	Muscle Relaxant	95-25-0		C <sub>7</sub> H <sub>4</sub> CINO <sub>2</sub>
Cholic Acid	Choleretic	81-25-4	Y	C <sub>24</sub> H <sub>40</sub> O <sub>5</sub>
Choline Alfoscerate	Nootropic	28319-77-9	Y	C <sub>8</sub> H <sub>20</sub> NO <sub>6</sub> P
Choline	Cholinergic	62-49-7		C <sub>5</sub> H <sub>14</sub> NO+
Choline Iodide Sebacate	Dermatologic	17140-07-7		C <sub>20</sub> H <sub>42</sub> N <sub>2</sub> O <sub>4</sub> .2I
Chromocarb	Capillary Protectant	4940-39-0		C <sub>10</sub> H <sub>6</sub> O <sub>4</sub>
Chromonar	Vasodilator	804-10-4		C <sub>20</sub> H <sub>27</sub> NO <sub>5</sub>
Ciadox	Antibacterial	65884-46-0		C <sub>12</sub> H <sub>9</sub> N <sub>5</sub> O <sub>3</sub>
Ciamexon	Immunosuppressant	75985-31-8		C <sub>11</sub> H <sub>13</sub> N <sub>3</sub> O
Cianergoline	Antihypertensive	74627-35-3		C <sub>19</sub> H <sub>22</sub> N <sub>4</sub> O
Cianidanol	Antidiarrheal	154-23-4		C <sub>15</sub> H <sub>14</sub> O <sub>6</sub>
Cianopramine	Antidepressant	66834-24-0		C <sub>20</sub> H <sub>23</sub> N <sub>3</sub>
Ciapilome	Unclassified	53131-74-1		C <sub>7</sub> H <sub>6</sub> N <sub>4</sub> O <sub>2</sub>
Cicaprost	Oxytocic	94079-80-8		C <sub>22</sub> H <sub>30</sub> O <sub>5</sub>
Cicarperone	Antipsychotic	54063-29-5		C <sub>20</sub> H <sub>27</sub> FN <sub>2</sub> O <sub>3</sub>
Ciclactate	Unclassified	15145-14-9		C <sub>12</sub> H <sub>22</sub> O <sub>3</sub>
Ciclafrine	Antihypotensive	55694-98-9		C <sub>15</sub> H <sub>21</sub> NO <sub>2</sub>
Ciclazindol	Antidepressant	37751-39-6		C <sub>17</sub> H <sub>15</sub> ClN <sub>2</sub> O
Ciclesonide	Glucocorticoid	126544-47-6		C <sub>32</sub> H <sub>44</sub> O <sub>7</sub>
Cicletanine	Antihypertensive	89943-82-8	Y	C <sub>14</sub> H <sub>12</sub> ClNO <sub>2</sub>
Ciclonicate	Vasodilator	53449-58-4		C <sub>15</sub> H <sub>21</sub> NO <sub>2</sub>
Ciclonium Bromide	Antihypertensive	29546-59-6		C <sub>22</sub> H <sub>34</sub> BrNO
Ciclopirox	Antifungal	29342-05-0		C <sub>12</sub> H <sub>17</sub> NO <sub>2</sub>
Ciclopirox Olamine	Antifungal	41621-49-2		C <sub>14</sub> H <sub>24</sub> N <sub>2</sub> O <sub>3</sub>
Ciclopramine	Antidepressant	33545-56-1		C <sub>18</sub> H <sub>20</sub> N <sub>2</sub>
Cicloprofen	Antiinflammatory	36950-96-6		C <sub>16</sub> H <sub>14</sub> O <sub>2</sub>
Cicloprolol	Antihypertensive	94651-09-9		C <sub>18</sub> H <sub>29</sub> NO <sub>4</sub>
Ciclosidomine	Antihypertensive	66564-16-7		C <sub>13</sub> H <sub>20</sub> N <sub>4</sub> O <sub>3</sub>
Ciclotizolam	Anxiolytic	58765-21-2		C <sub>20</sub> H <sub>18</sub> BrClN <sub>4</sub> S
Ciclotropium Bromide	Antibacterial	85166-20-7		C <sub>24</sub> H <sub>36</sub> BrNO <sub>2</sub>
Cicloxilic Acid	Gastroprokinetic	57808-63-6		C <sub>13</sub> H <sub>16</sub> O <sub>3</sub>
Cicloxlone	Antiviral	52247-86-6		C <sub>38</sub> H <sub>56</sub> O <sub>7</sub>
Cicortonide	Glucocorticoid	19705-61-4		C <sub>29</sub> H <sub>37</sub> ClFNO <sub>7</sub>
Cicrotoic Acid	Choleretic	25229-42-9		C <sub>10</sub> H <sub>16</sub> O <sub>2</sub>
Cidofovir	Antiviral	113852-37-2		C <sub>8</sub> H <sub>14</sub> N <sub>3</sub> O <sub>6</sub> P
Cidoxepin	Antidepressant	3607-18-9		C <sub>19</sub> H <sub>21</sub> NO
Cifenline	Antiarrhythmic	53267-01-9	Y	C <sub>18</sub> H <sub>18</sub> N <sub>2</sub>
Cifostodine	Unclassified	633-90-9		C <sub>9</sub> H <sub>12</sub> N <sub>3</sub> O <sub>7</sub> P
Ciglitazone	Antidiabetic	74772-77-3		C <sub>18</sub> H <sub>23</sub> NO <sub>3</sub> S
Ciheptolane	Unclassified	34753-46-3		C <sub>20</sub> H <sub>23</sub> NO <sub>2</sub>
Ciladopa	Antiparkinsonian	80109-27-9		C <sub>21</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub>
Cilansetron	Antiemetic	120635-74-7		C <sub>20</sub> H <sub>21</sub> N <sub>3</sub> O
Cilastatin	Antibacterial	82009-34-5		C <sub>16</sub> H <sub>26</sub> N <sub>2</sub> O <sub>5</sub> S
Cilazapril	Antihypertensive	88768-40-5	Y	C <sub>22</sub> H <sub>31</sub> N <sub>3</sub> O <sub>5</sub>
Cilazaprilat	Antihypertensive	90139-06-3		C <sub>20</sub> H <sub>27</sub> N <sub>3</sub> O <sub>5</sub>
Cilengitide	Antineoplastic	188968-51-6		C <sub>27</sub> H <sub>40</sub> N <sub>8</sub> O <sub>7</sub>
Cilnidipine	Antihypertensive	132203-70-4	Y	C <sub>27</sub> H <sub>28</sub> N <sub>2</sub> O <sub>7</sub>
Cilobamine Mesylate	Antidepressant	69429-84-1		C <sub>17</sub> H <sub>23</sub> Cl <sub>2</sub> NO
Cilobradine	Antianginal	147541-45-5		C <sub>28</sub> H <sub>38</sub> N <sub>2</sub> O <sub>5</sub>
Cilomilast	Bronchodilator	153259-65-5		C <sub>20</sub> H <sub>25</sub> NO <sub>4</sub>
Cilostamide	Erectile Dysfunction	68550-75-4		C <sub>20</sub> H <sub>26</sub> N <sub>2</sub> O <sub>3</sub>
Cilostazol	Antithrombotic	73963-72-1	Y	C <sub>20</sub> H <sub>27</sub> N <sub>5</sub> O <sub>2</sub>
Ciltoprazine	Nootropic	54063-30-8		C <sub>23</sub> H <sub>29</sub> ClN <sub>4</sub> O <sub>3</sub>
Ciluprevir	Antiviral	300832-84-2		C <sub>40</sub> H <sub>50</sub> N <sub>6</sub> O <sub>8</sub> S
Cilutazoline	Antihypertensive	104902-08-1		C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O
Cimaterol	Bronchodilator	54239-37-1		C <sub>12</sub> H <sub>17</sub> N <sub>3</sub> O
Cimemoxin	Antipsychotic	3788-16-7		C <sub>7</sub> H <sub>16</sub> N <sub>2</sub>
Cimepanol	Antianginal	29474-12-2		C <sub>10</sub> H <sub>20</sub> O

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Cimetidine	Antilulcerative	51481-61-9	Y	C <sub>10</sub> H <sub>16</sub> N <sub>6</sub> S
Cimetropium Bromide	Antispasmodic	51598-60-8	Y	C <sub>21</sub> H <sub>28</sub> BrNO <sub>4</sub>
Cimicoxib	Antiinflammatory	265114-23-6		C <sub>16</sub> H <sub>13</sub> ClFN <sub>3</sub> O <sub>3</sub> S
Cimoxatone	Antidepressant	73815-11-9		C <sub>19</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub>
Cinacalcet	Pituitary	226256-56-0	Y	C <sub>22</sub> H <sub>22</sub> F <sub>3</sub> N
Cinalukast	Bronchodilator	128312-51-6		C <sub>23</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub> S
Cinametic Acid	Gastroprokinetic	35703-32-3		C <sub>12</sub> H <sub>14</sub> O <sub>5</sub>
Cinamolol	Antihypotensive	39099-98-4		C <sub>16</sub> H <sub>23</sub> NO <sub>4</sub>
Cinanserin	Antidepressant	1166-34-3		C <sub>20</sub> H <sub>24</sub> N <sub>2</sub> OS
Cinaproxen	Antiinflammatory	89163-44-0		C <sub>19</sub> H <sub>21</sub> NO <sub>5</sub> S
Cinchonidine	Antimalarial	485-71-2		C <sub>19</sub> H <sub>22</sub> N <sub>2</sub> O
Cinchonine	Antimalarial	118-10-5	Y	C <sub>19</sub> H <sub>22</sub> N <sub>2</sub> O
Cinchophen	Analgesic	132-60-5		C <sub>16</sub> H <sub>11</sub> NO <sub>2</sub>
Cinecromen	Antithrombotic	62380-23-8		C <sub>34</sub> H <sub>41</sub> N <sub>3</sub> O <sub>10</sub>
Cinepaxadil	Unclassified	69118-25-8		C <sub>29</sub> H <sub>36</sub> N <sub>2</sub> O <sub>9</sub>
Cinepazet	Antianginal	23887-41-4		C <sub>20</sub> H <sub>28</sub> N <sub>2</sub> O <sub>6</sub>
Cinepazic Acid	Unclassified	54063-23-9		C <sub>18</sub> H <sub>24</sub> N <sub>2</sub> O <sub>6</sub>
Cinepazide	Vasodilator	23887-46-9		C <sub>22</sub> H <sub>31</sub> N <sub>3</sub> O <sub>5</sub>
Cinfenine	Antispasmodic	54141-87-6		C <sub>25</sub> H <sub>27</sub> NO
Cinfeoac	Antiinflammatory	66984-59-6		C <sub>18</sub> H <sub>14</sub> O <sub>6</sub>
Cinlumide	Muscle Relaxant	64379-93-7		C <sub>12</sub> H <sub>12</sub> FNO
Cingestol	Progestogen	16915-71-2		C <sub>20</sub> H <sub>28</sub> O
Cinitapride	Gastroprokinetic	66564-14-5	Y	C <sub>21</sub> H <sub>30</sub> N <sub>4</sub> O <sub>4</sub>
Cinmetacin	Antiinflammatory	20168-99-4		C <sub>21</sub> H <sub>19</sub> NO <sub>4</sub>
Cinnamaverine	Analgesic	1679-75-0		C <sub>21</sub> H <sub>25</sub> NO <sub>2</sub>
Cinnamedrine	Antispasmodic	90-86-8		C <sub>19</sub> H <sub>23</sub> NO
Cinnarizine	Antihistaminic	298-57-7	Y	C <sub>26</sub> H <sub>28</sub> N <sub>2</sub>
Cinnofuradione	Unclassified	477-80-5		C <sub>20</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>
Cinocetamide	Anesthetic	28598-08-5		C <sub>19</sub> H <sub>27</sub> NO <sub>4</sub>
Cinolazepam	Sedative	75696-02-5	Y	C <sub>18</sub> H <sub>13</sub> ClFN <sub>3</sub> O <sub>2</sub>
Cinoquidox	Antibacterial	64557-97-7		C <sub>13</sub> H <sub>12</sub> N <sub>4</sub> O <sub>3</sub>
Cinoxacin	Antibiotic	28657-80-9		C <sub>12</sub> H <sub>10</sub> N <sub>2</sub> O <sub>5</sub>
Cinoxate	Dermatologic	104-28-9		C <sub>14</sub> H <sub>18</sub> O <sub>4</sub>
Cinoxolone	Antilulcerative	31581-02-9		C <sub>41</sub> H <sub>56</sub> O <sub>5</sub>
Cinoxopazide	Vasodilator	88053-05-8		C <sub>20</sub> H <sub>25</sub> N <sub>3</sub> O <sub>4</sub>
Cinperene	Antipsychotic	14796-24-8		C <sub>25</sub> H <sub>28</sub> N <sub>2</sub> O <sub>2</sub>
Cinprazole	Antilulcerative	51493-19-7		C <sub>30</sub> H <sub>32</sub> N <sub>4</sub> O
Cinpropazide	Vasodilator	23887-47-0		C <sub>21</sub> H <sub>31</sub> N <sub>3</sub> O <sub>5</sub>
Cinromide	Anticonvulsant	58473-74-8		C <sub>11</sub> H <sub>12</sub> BrNO
Cintazone	Antiinflammatory	2056-56-6		C <sub>22</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>
Cintramide	Antipsychotic	5588-21-6		C <sub>12</sub> H <sub>15</sub> NO <sub>4</sub>
Cinuperone	Antipsychotic	82117-51-9		C <sub>23</sub> H <sub>24</sub> FN <sub>3</sub> O
Cioteronel	Dermatologic	89672-11-7		C <sub>16</sub> H <sub>28</sub> O <sub>2</sub>
Cipamfylline	Antiviral	132210-43-6		C <sub>13</sub> H <sub>17</sub> N <sub>5</sub> O <sub>2</sub>
Cipemastat	Antirheumatic	190648-49-8		C <sub>22</sub> H <sub>36</sub> N <sub>4</sub> O <sub>5</sub>
Ciprafamide	Antiamoebic	35452-73-4		C <sub>21</sub> H <sub>24</sub> N <sub>2</sub> O
Cipralisant	Nootropic	213027-19-1		C <sub>14</sub> H <sub>20</sub> N <sub>2</sub>
Ciprazafone	Anticonvulsant	75616-03-4		C <sub>19</sub> H <sub>18</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Ciprefadol Succinate	Analgesic	59889-36-0		C <sub>19</sub> H <sub>27</sub> NO
Ciprocinnolone	Steroid	58524-83-7		C <sub>28</sub> H <sub>34</sub> F <sub>2</sub> O <sub>7</sub>
Ciprofibrate	Antihyperlipidemic	52214-84-3	Y	C <sub>13</sub> H <sub>14</sub> Cl <sub>2</sub> O <sub>3</sub>
Ciprofloxacin	Antibiotic	85721-33-1	Y	C <sub>17</sub> H <sub>18</sub> FN <sub>3</sub> O <sub>3</sub>
Ciprokiren	Antihypertensive	143631-62-3		C <sub>37</sub> H <sub>55</sub> N <sub>5</sub> O <sub>8</sub> S
Cipropride	Antiemetic	68475-40-1		C <sub>17</sub> H <sub>25</sub> N <sub>3</sub> O <sub>4</sub> S
Ciproquazone	Analgesic	33453-23-5		C <sub>19</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>
Ciprostene Calcium	Anticoagulant	81845-44-5		C <sub>22</sub> H <sub>36</sub> O <sub>4</sub>
Ciramadol	Analgesic	63269-31-8		C <sub>15</sub> H <sub>23</sub> NO <sub>2</sub>
Cirazoline	Antidepressant	59939-16-1		C <sub>13</sub> H <sub>16</sub> N <sub>2</sub> O
Cisapride	Gastroprokinetic	81098-60-4	Y	C <sub>23</sub> H <sub>29</sub> ClFN <sub>3</sub> O <sub>4</sub>
Cisconazole	Antifungal	104456-95-3		C <sub>19</sub> H <sub>15</sub> F <sub>3</sub> N <sub>2</sub> OS
Cismadinone	Progestogen	54063-31-9		C <sub>21</sub> H <sub>27</sub> ClO <sub>3</sub>
Citalopram	Antidepressant	59729-33-8	Y	C <sub>20</sub> H <sub>21</sub> FN <sub>2</sub> O
Citatepine	Antipsychotic	65509-66-2		C <sub>20</sub> H <sub>18</sub> N <sub>2</sub> S

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Citenamide	Anticonvulsant	10423-37-7		C <sub>16</sub> H <sub>13</sub> NO
Citenazone	Antiviral	21512-15-2		C <sub>7</sub> H <sub>6</sub> N <sub>4</sub> S <sub>2</sub>
Citicoline Sodium	Nootropic	987-78-0	Y	C <sub>14</sub> H <sub>26</sub> N <sub>4</sub> O <sub>11</sub> P <sub>2</sub>
Citolone	Hepatic Protectant	1195-16-0		C <sub>6</sub> H <sub>9</sub> NO <sub>2</sub> S
Citric Acid	Anticoagulant	77-92-9	Y	C <sub>6</sub> H <sub>8</sub> O <sub>7</sub>
Cizolirtine	Antipsychotic	142155-43-9		C <sub>15</sub> H <sub>21</sub> N <sub>3</sub> O
Cladribine	Antineoplastic	4291-63-8		C <sub>10</sub> H <sub>12</sub> ClN <sub>5</sub> O <sub>3</sub>
Clamidoxic Acid	Antibiotic	6170-69-0		C <sub>15</sub> H <sub>11</sub> Cl <sub>2</sub> NO <sub>4</sub>
Clamikalant	Antiarrhythmic	158751-64-5		C <sub>19</sub> H <sub>22</sub> ClN <sub>3</sub> O <sub>5</sub> S <sub>2</sub>
Clamoxyquin	Antiamoebic	2545-39-3		C <sub>17</sub> H <sub>24</sub> ClN <sub>3</sub> O
Clanfenuur	Antineoplastic	51213-99-1		C <sub>16</sub> H <sub>15</sub> ClFN <sub>3</sub> O <sub>2</sub>
Clanobutin	Choleretic	30544-61-7		C <sub>18</sub> H <sub>18</sub> ClNO <sub>4</sub>
Clantifen	Antihistaminic	16562-98-4		C <sub>11</sub> H <sub>7</sub> Cl <sub>2</sub> NO <sub>2</sub> S
Clarithromycin	Antibiotic	81103-11-9	Y	C <sub>38</sub> H <sub>69</sub> NO <sub>13</sub>
Clavulanic Acid	Antibiotic	58001-44-8		C <sub>8</sub> H <sub>9</sub> NO <sub>5</sub>
Clazolam	Anxiolytic	7492-29-7		C <sub>18</sub> H <sub>17</sub> ClN <sub>2</sub> O
Clazolimine	Diuretic	40828-44-2		C <sub>10</sub> H <sub>10</sub> ClN <sub>3</sub> O
Clazosentan	Antihistaminic	180384-56-9		C <sub>25</sub> H <sub>23</sub> N <sub>9</sub> O <sub>6</sub> S
Clazuril	Antibacterial	101831-36-1		C <sub>17</sub> H <sub>10</sub> Cl <sub>2</sub> N <sub>4</sub> O <sub>2</sub>
Clebopride	Antiemetic	55905-53-8		C <sub>20</sub> H <sub>24</sub> ClN <sub>3</sub> O <sub>2</sub>
Clefamide	Antiamoebic	3576-64-5		C <sub>17</sub> H <sub>16</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>5</sub>
Clemastine	Antihistaminic	15686-51-8	Y	C <sub>21</sub> H <sub>26</sub> ClNO
Clemeprol	Choleretic	71827-56-0		C <sub>17</sub> H <sub>20</sub> ClNO
Clemizole	Antihistaminic	442-52-4		C <sub>19</sub> H <sub>20</sub> ClN <sub>3</sub>
Clenbuterol	Bronchodilator	37148-27-9	Y	C <sub>12</sub> H <sub>18</sub> Cl <sub>2</sub> N <sub>2</sub> O
Clenpirin	Analgesic	27050-41-5		C <sub>14</sub> H <sub>18</sub> Cl <sub>2</sub> N <sub>2</sub>
Clentiazem Maleate	Antihypertensive	96125-53-0		C <sub>22</sub> H <sub>25</sub> ClN <sub>2</sub> O <sub>4</sub> S
Cletoquine	Antibiotic	4298-15-1		C <sub>16</sub> H <sub>22</sub> ClN <sub>3</sub> O
Clevidipine	Antihypertensive	167221-71-8		C <sub>21</sub> H <sub>23</sub> Cl <sub>2</sub> NO <sub>6</sub>
Clevudine	Antiviral	163252-36-6	Y	C <sub>10</sub> H <sub>13</sub> FN <sub>2</sub> O <sub>5</sub>
Clibucaine	Analgesic	15302-10-0		C <sub>15</sub> H <sub>20</sub> Cl <sub>2</sub> N <sub>2</sub> O
Clidafidine	Sedative	33588-20-4		C <sub>9</sub> H <sub>8</sub> Cl <sub>2</sub> N <sub>2</sub> O
Clidanac	Antiinflammatory	34148-01-1		C <sub>16</sub> H <sub>19</sub> ClO <sub>2</sub>
Clidinium	Antispasmodic	7020-55-5		C <sub>22</sub> H <sub>26</sub> NO <sub>3</sub>
Climazolam	Anesthetic	59467-77-5		C <sub>18</sub> H <sub>13</sub> Cl <sub>2</sub> N <sub>3</sub>
Climbazole	Antifungal	38083-17-9		C <sub>15</sub> H <sub>17</sub> ClN <sub>2</sub> O <sub>2</sub>
Climiqualine	Anxiolytic	55150-67-9		C <sub>18</sub> H <sub>12</sub> ClN <sub>3</sub>
Clinafloxacin	Antibiotic	105956-97-6		C <sub>17</sub> H <sub>17</sub> ClFN <sub>3</sub> O <sub>3</sub>
Clindamycin	Antibiotic	18323-44-9	Y	C <sub>18</sub> H <sub>33</sub> ClN <sub>2</sub> O <sub>5</sub> S
Clindamycin Palmitate	Antibiotic	36688-78-5		C <sub>34</sub> H <sub>63</sub> ClN <sub>2</sub> O <sub>6</sub> S
Clindamycin Phosphate	Antibiotic	24729-96-2		C <sub>18</sub> H <sub>34</sub> ClN <sub>2</sub> O <sub>8</sub> PS
Clinofibrate	Antihyperlipidemic	30299-08-2	Y	C <sub>28</sub> H <sub>36</sub> O <sub>6</sub>
Clinolamide	Diuretic	3207-50-9		C <sub>24</sub> H <sub>43</sub> NO
Clinprost	Anticoagulant	88931-51-5		C <sub>22</sub> H <sub>36</sub> O <sub>4</sub>
Clioquinol	Antibacterial	130-26-7		C <sub>9</sub> H <sub>5</sub> ClINO
Clixanide	Anthelmintic	14437-41-3		C <sub>15</sub> H <sub>10</sub> Cl <sub>2</sub> NO <sub>3</sub>
Cliprofen	Antiinflammatory	51022-75-4		C <sub>14</sub> H <sub>11</sub> ClO <sub>3</sub> S
Cliropamine	Cardiotonic	109525-44-2		C <sub>19</sub> H <sub>25</sub> NO <sub>2</sub>
Clobazam	Anxiolytic	22316-47-8	Y	C <sub>16</sub> H <sub>13</sub> ClN <sub>2</sub> O <sub>2</sub>
Clobenoxide	Capillary Protectant	29899-95-4		C <sub>25</sub> H <sub>32</sub> Cl <sub>2</sub> O <sub>6</sub>
Clobenzepam	Antihistaminic	1159-93-9		C <sub>17</sub> H <sub>18</sub> ClN <sub>3</sub> O
Clobenzorex	Anorexic	13364-32-4		C <sub>16</sub> H <sub>18</sub> ClN
Clobenztropine	Antihistaminic	5627-46-3		C <sub>21</sub> H <sub>24</sub> ClNO
Clobetasol Propionate	Glucocorticoid	25122-46-7		C <sub>25</sub> H <sub>32</sub> ClFO <sub>5</sub>
Clobetasone Butyrate	Glucocorticoid	25122-57-0		C <sub>26</sub> H <sub>32</sub> ClFO <sub>5</sub>
Clobutinol	Antitussive	14860-49-2		C <sub>14</sub> H <sub>22</sub> ClNO
Clobuzarit	Antirheumatic	22494-47-9		C <sub>17</sub> H <sub>17</sub> ClO <sub>3</sub>
Clocanfamide	Antineoplastic	18966-32-0		C <sub>18</sub> H <sub>24</sub> ClNO <sub>2</sub>
Clocapramine	Antipsychotic	47739-98-0		C <sub>28</sub> H <sub>37</sub> ClN <sub>4</sub> O
Clociguanil	Antimalarial	3378-93-6		C <sub>13</sub> H <sub>16</sub> Cl <sub>2</sub> N <sub>4</sub> O
Clocinazine	Antihistaminic	298-55-5		C <sub>26</sub> H <sub>27</sub> ClN <sub>2</sub>
Clocortolone Acetate	Glucocorticoid	4258-85-9		C <sub>24</sub> H <sub>30</sub> ClFO <sub>5</sub>
Clocortolone Pivalate	Glucocorticoid	34097-16-0		C <sub>27</sub> H <sub>36</sub> ClFO <sub>5</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Clocoumarol	Anticoagulant	35838-63-2		C <sub>21</sub> H <sub>21</sub> ClO <sub>3</sub>
Clodacaine	Anesthetic	5626-25-5		C <sub>16</sub> H <sub>26</sub> ClN <sub>3</sub> O
Clodanolene	Muscle Relaxant	14796-28-2		C <sub>14</sub> H <sub>9</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>3</sub>
Clodazon	Antidepressant	4755-59-3		C <sub>18</sub> H <sub>20</sub> ClN <sub>3</sub> O
Clodoxopone	Antiparkinsonian	71923-34-7		C <sub>21</sub> H <sub>21</sub> ClN <sub>2</sub> O <sub>3</sub>
Clofarabine	Antineoplastic	123318-82-1		C <sub>10</sub> H <sub>11</sub> ClFN <sub>5</sub> O <sub>3</sub>
Clofazimine	Antibacterial	2030-63-9		C <sub>22</sub> H <sub>27</sub> Cl <sub>2</sub> N <sub>4</sub>
Clofenamic Acid	Antiinflammatory	4295-55-0		C <sub>13</sub> H <sub>9</sub> Cl <sub>2</sub> NO <sub>2</sub>
Clofenamide	Diuretic	671-95-4		C <sub>6</sub> H <sub>7</sub> ClN <sub>2</sub> O <sub>4</sub> S <sub>2</sub>
Clofenciclan	Unclassified	5632-52-0		C <sub>18</sub> H <sub>28</sub> ClNO
Clofenetamine	Decongestant	511-46-6		C <sub>20</sub> H <sub>26</sub> ClNO
Clofenoxyde	Unclassified	3030-53-3		C <sub>16</sub> H <sub>12</sub> Cl <sub>2</sub> O <sub>3</sub>
Clofeverine	Analgesic	54340-63-5		C <sub>16</sub> H <sub>16</sub> ClNO <sub>3</sub>
Clofexamide	Antiinflammatory	1223-36-5		C <sub>14</sub> H <sub>21</sub> ClN <sub>2</sub> O <sub>2</sub>
Clofibrate	Antihyperlipidemic	637-07-0	Y	C <sub>12</sub> H <sub>15</sub> ClO <sub>3</sub>
Clofibrilic Acid	Antihyperlipidemic	882-09-7		C <sub>10</sub> H <sub>11</sub> ClO <sub>3</sub>
Clofibrilide	Antihyperlipidemic	26717-47-5		C <sub>16</sub> H <sub>22</sub> ClNO <sub>4</sub>
Clofilium Phosphate	Antiarrhythmic	68379-03-3		C <sub>21</sub> H <sub>37</sub> ClN.H <sub>2</sub> O <sub>4</sub> P
Clofoctol	Antibiotic	37693-01-9		C <sub>21</sub> H <sub>26</sub> Cl <sub>2</sub> O
Cloforex	Anorexic	14261-75-7		C <sub>13</sub> H <sub>18</sub> ClNO <sub>2</sub>
Clofurac	Analgesic	60986-89-2		C <sub>14</sub> H <sub>15</sub> ClO <sub>2</sub>
Clogestone Acetate	Progestogen	3044-32-4		C <sub>25</sub> H <sub>33</sub> ClO <sub>5</sub>
Cloguanamil	Muscle Relaxant	21702-93-2		C <sub>9</sub> H <sub>8</sub> ClN <sub>5</sub> O
Clomacran Phosphate	Antipsychotic	5310-55-4		C <sub>18</sub> H <sub>21</sub> ClN <sub>2</sub>
Clomegestone Acetate	Progestogen	424-89-5		C <sub>24</sub> H <sub>31</sub> ClO <sub>4</sub>
Clometacin	Analgesic	25803-14-9		C <sub>19</sub> H <sub>16</sub> ClNO <sub>4</sub>
Clometherone	Pituitary	5591-27-5		C <sub>22</sub> H <sub>31</sub> ClO <sub>2</sub>
Clomethiazole	Sedative	533-45-9		C <sub>6</sub> H <sub>8</sub> ClNS
Clometocillin	Antibiotic	1926-49-4		C <sub>17</sub> H <sub>18</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>5</sub> S
Clomifenoxide	Antidepressant	97642-74-5		C <sub>26</sub> H <sub>28</sub> ClNO <sub>2</sub>
Clominorex	Anorexic	3876-10-6		C <sub>9</sub> H <sub>9</sub> ClN <sub>2</sub> O
Clomiphene	Estrogen	911-45-5	Y	C <sub>26</sub> H <sub>28</sub> ClNO
Clomipramine	Antidepressant	303-49-1	Y	C <sub>19</sub> H <sub>23</sub> ClN <sub>2</sub>
Clomocycline	Antibiotic	1181-54-0		C <sub>23</sub> H <sub>25</sub> ClN <sub>2</sub> O <sub>9</sub>
Clomoxir	Antidiabetic	88431-47-4		C <sub>14</sub> H <sub>17</sub> O <sub>3</sub> Cl
Clonazepam	Anticonvulsant	1622-61-3	Y	C <sub>15</sub> H <sub>10</sub> ClN <sub>3</sub> O <sub>3</sub>
Clonazoline	Decongestant	17692-28-3		C <sub>14</sub> H <sub>13</sub> ClN <sub>2</sub>
Clonidine	Antihypertensive	4205-90-7	Y	C <sub>9</sub> H <sub>9</sub> Cl <sub>2</sub> N <sub>3</sub>
Clonitazene	Analgesic	3861-76-5		C <sub>20</sub> H <sub>23</sub> ClN <sub>4</sub> O <sub>2</sub>
Clonitrate	Vasodilator	2612-33-1		C <sub>3</sub> H <sub>5</sub> ClN <sub>2</sub> O <sub>6</sub>
Clonixeril	Analgesic	21829-22-1		C <sub>16</sub> H <sub>17</sub> ClN <sub>2</sub> O <sub>4</sub>
Clonixin	Analgesic	17737-65-4		C <sub>13</sub> H <sub>11</sub> ClN <sub>2</sub> O <sub>2</sub>
Cloпамide	Antihypertensive	636-54-4	Y	C <sub>14</sub> H <sub>20</sub> ClN <sub>3</sub> O <sub>5</sub> S
Cloпenthixol	Antipsychotic	982-24-1	Y	C <sub>22</sub> H <sub>25</sub> ClN <sub>2</sub> OS
Cloperastine	Antitussive	3703-76-2		C <sub>20</sub> H <sub>24</sub> ClNO
Cloperidone	Sedative	4052-13-5		C <sub>21</sub> H <sub>23</sub> ClN <sub>4</sub> O <sub>2</sub>
Clopidogrel Sulfate	Anticoagulant	113665-84-2		C <sub>16</sub> H <sub>16</sub> ClNO <sub>2</sub> S
Clopidol	Antibacterial	2971-90-6		C <sub>7</sub> H <sub>7</sub> Cl <sub>2</sub> NO
Cloпimozide	Antipsychotic	53179-12-7		C <sub>28</sub> H <sub>28</sub> ClF <sub>2</sub> N <sub>3</sub> O
Cloпipazan Mesylate	Antipsychotic	60085-78-1		C <sub>19</sub> H <sub>18</sub> ClNO
Clopirac	Antiinflammatory	42779-82-8		C <sub>14</sub> H <sub>14</sub> ClNO <sub>2</sub>
Cloponone	Respiratory Stimulant	85409-44-5		C <sub>11</sub> H <sub>9</sub> Cl <sub>4</sub> NO <sub>2</sub>
Cloprednol	Glucocorticoid	5251-34-3	Y	C <sub>21</sub> H <sub>25</sub> ClO <sub>5</sub>
Cloprostenoл	Prostaglandin	40665-92-7		C <sub>22</sub> H <sub>29</sub> ClO <sub>6</sub>
Cloprothiazole	Antibiotic	6469-36-9		C <sub>7</sub> H <sub>10</sub> ClNS
Cloquinozine	Diuretic	5220-68-8		C <sub>16</sub> H <sub>22</sub> ClN
Cloracetadol	Analgesic	15687-05-5		C <sub>10</sub> H <sub>10</sub> Cl <sub>3</sub> NO <sub>3</sub>
Cloranolol	Antiarrhythmic	39563-28-5		C <sub>13</sub> H <sub>19</sub> Cl <sub>2</sub> NO <sub>2</sub>
Clorazepate	Anxiolytic	23887-31-2	Y	C <sub>16</sub> H <sub>11</sub> ClN <sub>2</sub> O <sub>3</sub>
Clorethate	Sedative	5634-37-7		C <sub>5</sub> H <sub>4</sub> Cl <sub>6</sub> O <sub>3</sub>
Clorexolone	Diuretic	2127-01-7		C <sub>14</sub> H <sub>17</sub> ClN <sub>2</sub> O <sub>3</sub> S
Clorgiline	Antidepressant	17780-72-2		C <sub>13</sub> H <sub>15</sub> Cl <sub>2</sub> NO
Cloricromen	Antithrombotic	68206-94-0		C <sub>20</sub> H <sub>26</sub> ClNO <sub>5</sub>



Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Cloridarol	Vasodilator	3611-72-1		C <sub>15</sub> H <sub>11</sub> ClO <sub>2</sub>
Clorindanic Acid	Antibiotic	153-43-5		C <sub>10</sub> H <sub>9</sub> ClO <sub>3</sub>
Clorindione	Anticonvulsant	1146-99-2		C <sub>15</sub> H <sub>9</sub> ClO <sub>2</sub>
Clormecaine	Analgesic	13930-34-2		C <sub>11</sub> H <sub>15</sub> ClN <sub>2</sub> O <sub>2</sub>
Cloroperone	Antipsychotic	61764-61-2		C <sub>22</sub> H <sub>23</sub> ClFNO <sub>2</sub>
Cloroqualone	Sedative	25509-07-3		C <sub>16</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>2</sub> O
Clorotepine	Antipsychotic	13448-22-1		C <sub>19</sub> H <sub>21</sub> ClN <sub>2</sub> S
Clorprenaline	Bronchodilator	3811-25-4		C <sub>11</sub> H <sub>16</sub> ClNO
Clorsulon	Anthelmintic	60200-06-8		C <sub>8</sub> H <sub>8</sub> Cl <sub>3</sub> N <sub>3</sub> O <sub>4</sub> S <sub>2</sub>
Clortermine	Anorexic	10389-73-8		C <sub>10</sub> H <sub>14</sub> ClN
Closantel	Anthelmintic	57808-65-8		C <sub>22</sub> H <sub>14</sub> Cl <sub>2</sub> I <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Closiramine Aceturate	Antihistaminic	47135-88-6		C <sub>18</sub> H <sub>21</sub> ClN <sub>2</sub>
Clostebol	Steroid	1093-58-9		C <sub>19</sub> H <sub>27</sub> ClO <sub>2</sub>
Clothiapine	Antipsychotic	2058-52-8		C <sub>18</sub> H <sub>18</sub> ClN <sub>3</sub> S
Clothixamide Maleate	Antipsychotic	4177-58-6		C <sub>24</sub> H <sub>28</sub> ClN <sub>3</sub> OS
Clotiazepam	Anxiolytic	33671-46-4	Y	C <sub>16</sub> H <sub>15</sub> ClN <sub>2</sub> OS
Cloticasone Propionate	Antiinflammatory	80486-69-7		C <sub>25</sub> H <sub>31</sub> ClF <sub>2</sub> O <sub>5</sub> S
Clotioxone	Analgesic	1856-34-4		C <sub>9</sub> H <sub>5</sub> Cl <sub>3</sub> N <sub>2</sub> O <sub>2</sub> S
Clotrimazole	Antifungal	23593-75-1	Y	C <sub>22</sub> H <sub>17</sub> ClN <sub>2</sub>
Clovoxamine	Antidepressant	54739-19-4		C <sub>14</sub> H <sub>21</sub> ClN <sub>2</sub> O <sub>2</sub>
Cloxacepride	Antihistaminic	65569-29-1		C <sub>22</sub> H <sub>27</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>4</sub>
Cloxacillin	Antibiotic	61-72-3	Y	C <sub>19</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>5</sub> S
Cloxazolam	Anxiolytic	24166-13-0		C <sub>17</sub> H <sub>14</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Cloxestradiol	Estrogen	54063-33-1		C <sub>20</sub> H <sub>25</sub> Cl <sub>3</sub> O <sub>3</sub>
Cloximate	Antiinflammatory	58832-68-1		C <sub>14</sub> H <sub>19</sub> ClN <sub>2</sub> O <sub>3</sub>
Cloxtotestosterone	Androgen	53608-96-1		C <sub>21</sub> H <sub>29</sub> Cl <sub>3</sub> O <sub>3</sub>
Cloxypendyl	Antipsychotic	15311-77-0		C <sub>20</sub> H <sub>25</sub> ClN <sub>4</sub> OS
Cloxyquin	Antibacterial	130-16-5		C <sub>9</sub> H <sub>6</sub> ClNO
Clozapine	Antipsychotic	5786-21-0	Y	C <sub>18</sub> H <sub>19</sub> ClN <sub>4</sub>
Cocaine	Anesthetic	50-36-2		C <sub>17</sub> H <sub>21</sub> NO <sub>4</sub>
Codeine	Antitussive	76-57-3	Y	C <sub>18</sub> H <sub>21</sub> NO <sub>3</sub>
Codoxime	Antitussive	7125-76-0		C <sub>20</sub> H <sub>24</sub> N <sub>2</sub> O <sub>5</sub>
Co Fluampicil	Antibiotic	5250-39-5		C <sub>19</sub> H <sub>17</sub> ClFN <sub>3</sub> O <sub>5</sub> S
Cogazocine	Analgesic	57653-29-9		C <sub>21</sub> H <sub>32</sub> NO
Colchicine	Anticholelithogenic	64-86-8	Y	C <sub>22</sub> H <sub>25</sub> NO <sub>6</sub>
Colestolone	Antihyperlipidemic	50673-97-7		C <sub>27</sub> H <sub>44</sub> O <sub>2</sub>
Colfenamate	Antiinflammatory	30531-86-3		C <sub>16</sub> H <sub>13</sub> F <sub>3</sub> N <sub>2</sub> O <sub>3</sub>
Colforsin	Bronchodilator	66575-29-9		C <sub>22</sub> H <sub>34</sub> O <sub>7</sub>
Colfosceril Palmitate	Respiratory Stimulant	63-89-8		C <sub>40</sub> H <sub>80</sub> NO <sub>8</sub> P
Colterol Mesylate	Bronchodilator	18866-78-9		C <sub>12</sub> H <sub>19</sub> NO <sub>3</sub>
Coluracetam	Nootropic	135463-81-9		C <sub>19</sub> H <sub>23</sub> N <sub>3</sub> O <sub>3</sub>
Conessine Hydrobromide	Analgesic	546-06-5		C <sub>24</sub> H <sub>40</sub> N <sub>2</sub>
Conivaptan	Cardiotonic	210101-16-9		C <sub>32</sub> H <sub>26</sub> N <sub>4</sub> O <sub>2</sub>
Conorphone	Analgesic	72060-05-0		C <sub>23</sub> H <sub>29</sub> NO <sub>3</sub>
Cormethasone Acetate	Antiinflammatory	35135-67-2		C <sub>24</sub> H <sub>29</sub> F <sub>3</sub> O <sub>6</sub>
Cortisone Acetate	Glucocorticoid	50-04-4		C <sub>23</sub> H <sub>30</sub> O <sub>6</sub>
Cortisuzol	Glucocorticoid	50801-44-0		C <sub>37</sub> H <sub>40</sub> N <sub>2</sub> O <sub>8</sub> S
Cortivazol	Glucocorticoid	1110-40-3		C <sub>32</sub> H <sub>38</sub> N <sub>2</sub> O <sub>5</sub>
Cortodoxone	Antiinflammatory	152-58-9		C <sub>21</sub> H <sub>30</sub> O <sub>4</sub>
Cotarnine Chloride	Hemostatic	10018-19-6		C <sub>12</sub> H <sub>14</sub> NO <sub>3</sub> .Cl
Cotinine	Antidepressant	486-56-6		C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> O
Cotriptyline	Antidepressant	34662-67-4		C <sub>21</sub> H <sub>20</sub> NO
Coumaphos	Antineoplastic	56-72-4		C <sub>14</sub> H <sub>16</sub> ClO <sub>5</sub> PS
Coumarin	Anticoagulant	91-64-5		C <sub>9</sub> H <sub>6</sub> O <sub>2</sub>
Coumazoline	Anticholelithogenic	37681-00-8		C <sub>14</sub> H <sub>16</sub> N <sub>2</sub> O
Coumetarol	Anticoagulant	4366-18-1		C <sub>21</sub> H <sub>16</sub> O <sub>7</sub>
Creatinolfosfate	Bone Resorption Inhibitor	6903-79-3		C <sub>4</sub> H <sub>12</sub> N <sub>3</sub> O <sub>4</sub> P
Crilvastatin	Antihyperlipidemic	120551-59-9		C <sub>14</sub> H <sub>23</sub> NO <sub>3</sub>
Crisnatol Mesylate	Antineoplastic	96389-68-3		C <sub>23</sub> H <sub>23</sub> NO <sub>2</sub>
Crobenetine	Analgesic	221019-25-6		C <sub>25</sub> H <sub>33</sub> NO <sub>2</sub>
Croconazole	Antifungal	77175-51-0		C <sub>18</sub> H <sub>15</sub> ClN <sub>2</sub> O
Cromakalim	Antihypertensive	94470-67-4		C <sub>16</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>
Cromitrile Sodium	Bronchodilator	53736-51-9		C <sub>20</sub> H <sub>15</sub> N <sub>5</sub> O <sub>5</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Cromoglicate Lisetil	Bronchodilator	110816-79-0		C <sub>33</sub> H <sub>36</sub> N <sub>2</sub> O <sub>12</sub>
Cromolyn	Bronchodilator	16110-51-3	Y	C <sub>23</sub> H <sub>16</sub> O <sub>11</sub>
Cronidipine	Antihypertensive	113759-50-5		C <sub>30</sub> H <sub>32</sub> ClN <sub>3</sub> O <sub>8</sub>
Cropropamide	Analgesic	633-47-6		C <sub>13</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub>
Crotamiton	Dermatologic	483-63-6		C <sub>13</sub> H <sub>17</sub> NO
Crotetamide	Analgesic	6168-76-9		C <sub>12</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>
Crotoniazide	Antibiotic	7007-96-7		C <sub>10</sub> H <sub>11</sub> N <sub>3</sub> O
Crotoxyfos	Antineoplastic	7700-17-6		C <sub>14</sub> H <sub>19</sub> O <sub>6</sub> P
Crufomate	Anthelminthic	299-86-5		C <sub>12</sub> H <sub>19</sub> ClNO <sub>3</sub> P
Cyacetacide	Antibacterial	140-87-4		C <sub>3</sub> H <sub>5</sub> N <sub>3</sub> O
Cyamemazine	Antipsychotic	3546-03-0	Y	C <sub>19</sub> H <sub>21</sub> N <sub>3</sub> S
Cyclacillin	Antibiotic	3485-14-1		C <sub>15</sub> H <sub>23</sub> N <sub>3</sub> O <sub>4</sub> S
Cyclandelate	Vasodilator	456-59-7	Y	C <sub>17</sub> H <sub>24</sub> O <sub>3</sub>
Cyclarbamate	Anxiolytic	5779-54-4		C <sub>21</sub> H <sub>24</sub> N <sub>2</sub> O <sub>4</sub>
Cyclazocine	Antidote	3572-80-3		C <sub>18</sub> H <sub>25</sub> NO
Cyclazodone	Antidepressant	14461-91-7		C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>
Cyclexanone	Antitussive	15301-52-7		C <sub>16</sub> H <sub>25</sub> NO <sub>2</sub>
Cyclindole	Antidepressant	32211-97-5		C <sub>14</sub> H <sub>18</sub> N <sub>2</sub>
Cycliramine Maleate	Antihistaminic	47128-12-1		C <sub>18</sub> H <sub>19</sub> ClN <sub>2</sub>
Cyclizine	Antiemetic	82-92-8		C <sub>18</sub> H <sub>22</sub> N <sub>2</sub>
Cyclobarbitol	Sedative	52-31-3		C <sub>12</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>
Cyclobendazole	Anthelminthic	31431-43-3		C <sub>13</sub> H <sub>13</sub> N <sub>3</sub> O <sub>3</sub>
Cyclobenzaprine	Muscle Relaxant	303-53-7	Y	C <sub>20</sub> H <sub>21</sub> N
Cyclobutyrol	Choleretic	512-16-3		C <sub>10</sub> H <sub>18</sub> O <sub>3</sub>
Cyclocumarol	Anticoagulant	518-20-7		C <sub>20</sub> H <sub>18</sub> O <sub>4</sub>
Cyclofenil	Androgen	2624-43-3		C <sub>23</sub> H <sub>24</sub> O <sub>4</sub>
Cycloguanil Pamoate	Antimalarial	516-21-2		C <sub>11</sub> H <sub>14</sub> ClN <sub>5</sub>
Cycloheximide	Antineoplastic	66-81-9		C <sub>15</sub> H <sub>23</sub> NO <sub>4</sub>
Cyclomenol	Antiarrhythmic	5591-47-9		C <sub>14</sub> H <sub>20</sub> O
Cyclomethycaine Sulfate	Analgesic	139-62-8		C <sub>22</sub> H <sub>33</sub> NO <sub>3</sub>
Cyclopentamine	Decongestant	102-45-4		C <sub>9</sub> H <sub>19</sub> N
Cyclopenthiiazide	Antihypertensive	742-20-1	Y	C <sub>13</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>4</sub> S <sub>2</sub>
Cyclopentobarbital sodium	Sedative	76-68-6		C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>
Cyclopentolate	Mydriatic	512-15-2		C <sub>17</sub> H <sub>25</sub> NO <sub>3</sub>
Cyclophenazine	Antipsychotic	17692-26-1		C <sub>23</sub> H <sub>26</sub> F <sub>3</sub> N <sub>3</sub> S
Cyclophosphamide	Antineoplastic	50-18-0		C <sub>7</sub> H <sub>15</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub> P
Cyclopregnol	Progestogen	465-53-2		C <sub>21</sub> H <sub>32</sub> O <sub>2</sub>
Cyclopropane	Anesthetic	75-19-4		C <sub>3</sub> H <sub>6</sub>
Cycloserine	Antibacterial	68-41-7	Y	C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>
Cyclothiazide	Diuretic	2259-96-3		C <sub>14</sub> H <sub>16</sub> ClN <sub>3</sub> O <sub>4</sub> S <sub>2</sub>
Cyclovalone	Choleretic	579-23-7		C <sub>22</sub> H <sub>22</sub> O <sub>5</sub>
Cycrimine	Antispasmodic	77-39-4		C <sub>19</sub> H <sub>29</sub> NO
Cyheptamide	Anticonvulsant	7199-29-3		C <sub>16</sub> H <sub>15</sub> NO
Cyheptropine	Antihypotensive	602-40-4		C <sub>24</sub> H <sub>27</sub> NO <sub>2</sub>
Cynarine	Choleretic	30964-13-7		C <sub>25</sub> H <sub>24</sub> O <sub>12</sub>
Cypenammine	Antidepressant	15301-54-9		C <sub>11</sub> H <sub>15</sub> N
Cyprazepam	Sedative	15687-07-7		C <sub>19</sub> H <sub>18</sub> ClN <sub>3</sub> O
Cyprenorphine	Analgesic	4406-22-8		C <sub>26</sub> H <sub>33</sub> NO <sub>4</sub>
Cyprodenate	Antipsychotic	15585-86-1		C <sub>13</sub> H <sub>25</sub> NO <sub>2</sub>
Cyproheptadine	Antihistaminic	129-03-3	Y	C <sub>21</sub> H <sub>21</sub> N
Cyprolidol	Antidepressant	4904-00-1		C <sub>21</sub> H <sub>19</sub> NO
Cyproquinat	Antibacterial	19485-08-6		C <sub>20</sub> H <sub>23</sub> NO <sub>5</sub>
Cyproterone Acetate	Antineoplastic	427-51-0	Y	C <sub>24</sub> H <sub>29</sub> ClO <sub>4</sub>
Cyproximide	Antipsychotic	66537-94-8		C <sub>11</sub> H <sub>8</sub> ClNO <sub>2</sub>
Cyromazine	Antihistaminic	66215-27-8		C <sub>6</sub> H <sub>10</sub> N <sub>6</sub>
Cysteamine	Antidote	60-23-1	Y	C <sub>2</sub> H <sub>7</sub> NS
Cytarabine	Antineoplastic	147-94-4		C <sub>9</sub> H <sub>13</sub> N <sub>5</sub> O <sub>5</sub>
Cyverine	Antispasmodic	4432-75-1		C <sub>17</sub> H <sub>33</sub> N
Dabelotine	Nootropic	118976-38-8		C <sub>15</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>
Dabigatran	Antithrombotic	211914-51-1	Y	C <sub>25</sub> H <sub>25</sub> N <sub>7</sub> O <sub>3</sub>
Dabigatran Etxilate	Antithrombotic	211915-06-9	Y	C <sub>34</sub> H <sub>41</sub> N <sub>7</sub> O <sub>5</sub>
Dabuzalgron	Antispasmodic	219311-44-1		C <sub>12</sub> H <sub>16</sub> ClN <sub>3</sub> O <sub>3</sub> S
Dacarbazine	Antineoplastic	4342-03-4		C <sub>6</sub> H <sub>10</sub> N <sub>6</sub> O

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Dacemazine	Antihistaminic	518-61-6		C <sub>16</sub> H <sub>16</sub> N <sub>2</sub> O <sub>5</sub>
Dacinostat	Antineoplastic	404951-53-7		C <sub>22</sub> H <sub>25</sub> N <sub>3</sub> O <sub>3</sub>
Dacisteine	Unclassified	18725-37-6		C <sub>7</sub> H <sub>11</sub> NO <sub>4</sub> S
Dacopafant	Antithrombotic	125372-33-0		C <sub>12</sub> H <sub>11</sub> N <sub>3</sub> O <sub>5</sub>
Dacuronium Bromide	Muscle Relaxant	27115-86-2		C <sub>33</sub> H <sub>58</sub> N <sub>2</sub> O <sub>3</sub> Br <sub>2</sub>
Dagapamil	Vasodilator	85247-76-3		C <sub>36</sub> H <sub>56</sub> N <sub>2</sub> O <sub>4</sub>
Daglutril	Antihypertensive	182821-27-8		C <sub>31</sub> H <sub>38</sub> N <sub>2</sub> O <sub>6</sub>
Dalbraminol	Cardiotonic	81528-80-5		C <sub>17</sub> H <sub>26</sub> N <sub>4</sub> O <sub>2</sub>
Dalcotidine	Antiulcerative	120958-90-9		C <sub>18</sub> H <sub>29</sub> N <sub>3</sub> O <sub>2</sub>
Daledalin Tosylate	Antidepressant	22136-27-2		C <sub>19</sub> H <sub>24</sub> N <sub>2</sub>
Dalfopristin	Antibacterial	112362-50-2		C <sub>34</sub> H <sub>50</sub> N <sub>4</sub> O <sub>9</sub> S
Daltroban	Immunosuppressant	79094-20-5		C <sub>16</sub> H <sub>16</sub> ClNO <sub>4</sub> S
Dalvastatin	Antihyperlipidemic	132100-55-1		C <sub>24</sub> H <sub>31</sub> FO <sub>3</sub>
Dametralast	Vasodilator	71680-63-2		C <sub>6</sub> H <sub>8</sub> N <sub>6</sub>
Damotepine	Antipsychotic	1469-07-4		C <sub>17</sub> H <sub>17</sub> NS
Danazol	Steroid	17230-88-5	Y	C <sub>22</sub> H <sub>27</sub> NO <sub>2</sub>
Daniquidone	Antineoplastic	67199-66-0		C <sub>15</sub> H <sub>11</sub> N <sub>3</sub> O
Danitracen	Antidepressant	31232-26-5		C <sub>20</sub> H <sub>21</sub> NO
Danofloxacin Mesylate	Antibacterial	112398-08-0		C <sub>19</sub> H <sub>20</sub> FN <sub>3</sub> O <sub>3</sub>
Danosteine	Antitussive	4938-00-5		C <sub>5</sub> H <sub>8</sub> O <sub>4</sub> S
Danthron	Laxative	117-10-2		C <sub>14</sub> H <sub>8</sub> O <sub>4</sub>
Dantrolene	Muscle Relaxant	7261-97-4	Y	C <sub>14</sub> H <sub>10</sub> N <sub>4</sub> O <sub>5</sub>
Dapabutan	Unclassified	6582-31-6		C <sub>19</sub> H <sub>40</sub> N <sub>2</sub> O <sub>2</sub>
Dapiprazole	Antiglaucoma	72822-12-9		C <sub>19</sub> H <sub>27</sub> N <sub>5</sub>
Dapitant	Antiemetic	153438-49-4		C <sub>37</sub> H <sub>39</sub> NO <sub>4</sub>
Dapivirine	Antiviral	244767-67-7		C <sub>20</sub> H <sub>19</sub> N <sub>5</sub>
Dapoxetine	Antidepressant	119356-77-3	Y	C <sub>21</sub> H <sub>23</sub> NO
Dapsone	Antibiotic	80-08-0	Y	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> S
Darapladib	Antihyperlipidemic	356057-34-6	Y	C <sub>36</sub> H <sub>38</sub> F <sub>4</sub> N <sub>4</sub> O <sub>2</sub> S
Darbufelone	Antiinflammatory	139226-28-1		C <sub>18</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub> S
Darenzepine	Antiulcerative	84629-61-8		C <sub>21</sub> H <sub>21</sub> N <sub>3</sub> O <sub>2</sub>
Darglitazone Sodium	Antidiabetic	141200-24-0		C <sub>23</sub> H <sub>20</sub> N <sub>2</sub> O <sub>4</sub> S
Darifenacin	Antispasmodic	133099-04-4	Y	C <sub>28</sub> H <sub>30</sub> N <sub>2</sub> O <sub>2</sub>
Darodipine	Antihypertensive	72803-02-2		C <sub>19</sub> H <sub>21</sub> N <sub>3</sub> O <sub>5</sub>
Darsidomine	Vasodilator	137500-42-6		C <sub>9</sub> H <sub>16</sub> N <sub>4</sub> O
Darunavir	Antiviral	206361-99-1	Y	C <sub>27</sub> H <sub>37</sub> N <sub>3</sub> O <sub>7</sub> S
Darusentan	Anesthetic	171714-84-4		C <sub>22</sub> H <sub>22</sub> N <sub>2</sub> O <sub>6</sub>
Dasantafil	Erectile Dysfunction	569351-91-3		C <sub>22</sub> H <sub>28</sub> BrN <sub>5</sub> O <sub>5</sub>
Dasatinib	Antineoplastic	302962-49-8	Y	C <sub>22</sub> H <sub>26</sub> ClN <sub>7</sub> O <sub>2</sub> S
Datelliptium Chloride	Antineoplastic	105118-14-7		C <sub>23</sub> H <sub>28</sub> N <sub>3</sub> O.Cl
Daunorubicin	Antineoplastic	20830-81-3		C <sub>27</sub> H <sub>29</sub> NO <sub>10</sub>
Davasaicin	Analgesic	147497-64-1		C <sub>22</sub> H <sub>30</sub> N <sub>2</sub> O <sub>3</sub>
Daxalipram	Antidepressant	189940-24-7		C <sub>14</sub> H <sub>19</sub> NO <sub>4</sub>
Dazadrol Maleate	Antidepressant	47029-84-5		C <sub>15</sub> H <sub>14</sub> ClN <sub>3</sub> O
Dazepinil	Antidepressant	75991-50-3		C <sub>17</sub> H <sub>18</sub> N <sub>2</sub>
Dazidamine	Antineoplastic	75522-73-5		C <sub>19</sub> H <sub>23</sub> N <sub>3</sub> S
Dazmegrel	Anticoagulant	76894-77-4		C <sub>16</sub> H <sub>17</sub> N <sub>3</sub> O <sub>2</sub>
Dazolicine	Antiarrhythmic	61477-97-2		C <sub>17</sub> H <sub>24</sub> ClN <sub>3</sub> S
Dazopride Fumarate	Gastroprokinetic	70181-03-2		C <sub>15</sub> H <sub>23</sub> ClN <sub>4</sub> O <sub>2</sub>
Dazoquinast	Bronchodilator	76002-75-0		C <sub>11</sub> H <sub>7</sub> N <sub>3</sub> O <sub>2</sub>
Dazoxiben	Antithrombotic	78218-09-4		C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>
Deanol Aceglumate	Nootropic	1188-37-0		C <sub>7</sub> H <sub>11</sub> NO <sub>5</sub>
Deboxamet	Antiulcerative	34024-41-4		C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>
Debrisoquin Sulfate	Antihypertensive	1131-64-2		C <sub>10</sub> H <sub>13</sub> N <sub>3</sub>
Debropol	Unclassified	24403-04-1		C <sub>3</sub> H <sub>6</sub> BrNO <sub>3</sub>
Decamethonium Bromide	Muscle Relaxant	541-22-0		C <sub>16</sub> H <sub>38</sub> Br <sub>2</sub> N <sub>2</sub>
Decimemide	Anticonvulsant	14817-09-5		C <sub>19</sub> H <sub>31</sub> NO <sub>4</sub>
Decitabine	Antineoplastic	2353-33-5		C <sub>8</sub> H <sub>12</sub> N <sub>4</sub> O <sub>4</sub>
Decitropine	Antihypotensive	1242-69-9		C <sub>23</sub> H <sub>25</sub> NO
Declenperone	Sedative	63388-37-4		C <sub>22</sub> H <sub>24</sub> FN <sub>3</sub> O <sub>2</sub>
Declopramide	Antiemetic	891-60-1		C <sub>13</sub> H <sub>20</sub> ClN <sub>3</sub> O
Decloxizine	Sedative	3733-63-9		C <sub>21</sub> H <sub>28</sub> N <sub>2</sub> O <sub>2</sub>
Decominol	Antihypotensive	60812-35-3		C <sub>13</sub> H <sub>29</sub> NO <sub>2</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Decoquinat	Antibacterial	18507-89-6		C <sub>24</sub> H <sub>35</sub> NO <sub>5</sub>
Dectaflur	Antibacterial	36505-83-6		C <sub>18</sub> H <sub>37</sub> N.FH
Deditonium Bromide	Antispasmodic	2401-56-1		C <sub>38</sub> H <sub>66</sub> Br <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Deferasirox	Antidote	201530-41-8	Y	C <sub>21</sub> H <sub>15</sub> N <sub>3</sub> O <sub>4</sub>
Deferiprone	Antidote	30652-11-0	Y	C <sub>7</sub> H <sub>9</sub> NO <sub>2</sub>
Deferitritin	Antidote	239101-33-8		C <sub>11</sub> H <sub>11</sub> NO <sub>4</sub> S
Deferoxamine Mesylate	Antidote	70-51-9		C <sub>25</sub> H <sub>48</sub> N <sub>6</sub> O <sub>8</sub>
Deflazacort	Antiinflammatory	14484-47-0	Y	C <sub>25</sub> H <sub>31</sub> NO <sub>6</sub>
Defosfamide	Antineoplastic	3733-81-1		C <sub>9</sub> H <sub>20</sub> Cl <sub>3</sub> N <sub>2</sub> O <sub>5</sub> P
Dehydrocholic Acid	Choleretic	81-23-2		C <sub>24</sub> H <sub>34</sub> O <sub>5</sub>
Dehydroemetine	Antiamoebic	4914-30-1		C <sub>29</sub> H <sub>38</sub> N <sub>2</sub> O <sub>4</sub>
Delanterone	Antineoplastic	63014-96-0		C <sub>20</sub> H <sub>28</sub> O
Delapril	Antihypertensive	83435-66-9	Y	C <sub>26</sub> H <sub>32</sub> N <sub>2</sub> O <sub>5</sub>
Delavirdine	Antiviral	136817-59-9	Y	C <sub>22</sub> H <sub>28</sub> N <sub>6</sub> O <sub>3</sub> S
Delequamine	Erectile Dysfunction	119905-05-4		C <sub>18</sub> H <sub>26</sub> N <sub>2</sub> O <sub>3</sub> S
Delergotril	Antibiotic	59091-65-5		C <sub>17</sub> H <sub>19</sub> N <sub>3</sub>
Delfantrine	Antimalarial	3436-11-1		C <sub>14</sub> H <sub>22</sub> N <sub>4</sub> O <sub>3</sub> S
Delfaprazine	Antipsychotic	117827-81-3		C <sub>18</sub> H <sub>22</sub> N <sub>2</sub>
Delmadinone Acetate	Progestogen	13698-49-2		C <sub>23</sub> H <sub>27</sub> ClO <sub>4</sub>
Delmetacin	Antiinflammatory	16401-80-2		C <sub>18</sub> H <sub>15</sub> NO <sub>3</sub>
Delmopinol	Antibiotic	79874-76-3	Y	C <sub>16</sub> H <sub>33</sub> NO <sub>2</sub>
Delorazepam	Sedative	2894-67-9		C <sub>15</sub> H <sub>10</sub> Cl <sub>2</sub> N <sub>2</sub> O
Deloxolone	Dermatologic	68635-50-7		C <sub>34</sub> H <sub>52</sub> O <sub>6</sub>
Delprostenate	Prostaglandin	62524-99-6		C <sub>23</sub> H <sub>29</sub> ClO <sub>6</sub>
Delucemine	Nootropic	186495-49-8		C <sub>16</sub> H <sub>17</sub> F <sub>2</sub> N
Dembrexine	Antidepressant	83200-09-3		C <sub>13</sub> H <sub>17</sub> Br <sub>2</sub> NO <sub>2</sub>
Demecarium Bromide	Cholinergic	56-94-0		C <sub>32</sub> H <sub>52</sub> Br <sub>2</sub> N <sub>4</sub> O <sub>4</sub>
Demeclocycline	Antibiotic	127-33-3	Y	C <sub>21</sub> H <sub>21</sub> ClN <sub>2</sub> O <sub>8</sub>
Demecolcine	Antineoplastic	477-30-5		C <sub>21</sub> H <sub>25</sub> NO <sub>5</sub>
Demecycline	Antibacterial	987-02-0		C <sub>21</sub> H <sub>22</sub> N <sub>2</sub> O <sub>8</sub>
Demegestone	Progestogen	10116-22-0		C <sub>21</sub> H <sub>28</sub> O <sub>2</sub>
Demelverine	Antispasmodic	13977-33-8		C <sub>17</sub> H <sub>21</sub> N
Demexiptiline	Antidepressant	24701-51-7		C <sub>18</sub> H <sub>18</sub> N <sub>2</sub> O
Democonazole	Antifungal	70161-09-0		C <sub>19</sub> H <sub>15</sub> Cl <sub>3</sub> N <sub>2</sub> O <sub>2</sub>
Demoxepam	Anxiolytic	963-39-3		C <sub>15</sub> H <sub>11</sub> ClN <sub>2</sub> O <sub>2</sub>
Demoxytocin	Oxytocic	113-78-0		C <sub>43</sub> H <sub>65</sub> N <sub>11</sub> O <sub>12</sub> S <sub>2</sub>
Denaverine	Analgesic	3579-62-2		C <sub>24</sub> H <sub>33</sub> NO <sub>3</sub>
Denbufylline	Bronchodilator	57076-71-8		C <sub>16</sub> H <sub>24</sub> N <sub>4</sub> O <sub>3</sub>
Denipride	Gastroprokinetic	106972-33-2		C <sub>18</sub> H <sub>26</sub> N <sub>4</sub> O <sub>5</sub>
Denopamine	Cardiotonic	71771-90-9		C <sub>18</sub> H <sub>23</sub> NO <sub>4</sub>
Denotivir	Antiviral	51287-57-1		C <sub>18</sub> H <sub>14</sub> ClN <sub>3</sub> O <sub>2</sub> S
Denpidazone	Unclassified	42438-73-3		C <sub>20</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub>
Denufosol Tetrasodium	Decongestant	211448-85-0		C <sub>18</sub> H <sub>27</sub> N <sub>5</sub> O <sub>21</sub> P <sub>4</sub>
Denzimol	Anticonvulsant	73931-96-1		C <sub>19</sub> H <sub>20</sub> N <sub>2</sub> O
Deoxycholic Acid	Choleretic	83-44-3		C <sub>24</sub> H <sub>40</sub> O <sub>4</sub>
Depramine	Antidepressant	303-54-8		C <sub>19</sub> H <sub>22</sub> N <sub>2</sub>
Deprodone	Antidepressant	20423-99-8		C <sub>21</sub> H <sub>28</sub> O <sub>4</sub>
Deprostit	Antiulcerative	33813-84-2		C <sub>21</sub> H <sub>28</sub> O <sub>4</sub>
Deptropine Citrate	Antihistaminic	604-51-3		C <sub>23</sub> H <sub>27</sub> NO
Deracoxib	Antiinflammatory	169590-41-4		C <sub>17</sub> H <sub>14</sub> F <sub>3</sub> N <sub>3</sub> O <sub>3</sub> S
Deramciclone	Vasodilator	120444-71-5		C <sub>20</sub> H <sub>31</sub> NO
Derigidole	Antidiabetic	122830-14-2		C <sub>16</sub> H <sub>21</sub> N <sub>3</sub>
Derpanicate	Estrogen	99518-29-3		C <sub>46</sub> H <sub>54</sub> N <sub>8</sub> O <sub>12</sub> S <sub>2</sub>
Dersalazine	Antiinflammatory	188913-58-8	Y	C <sub>35</sub> H <sub>32</sub> N <sub>6</sub> O <sub>4</sub>
Desciclovir	Antiviral	84408-37-7		C <sub>8</sub> H <sub>11</sub> N <sub>5</sub> O <sub>2</sub>
Descinolone Acetonide	Glucocorticoid	2135-14-0		C <sub>24</sub> H <sub>31</sub> FO <sub>5</sub>
Deserpidine	Antihypertensive	131-01-1		C <sub>32</sub> H <sub>38</sub> N <sub>2</sub> O <sub>8</sub>
Desflurane	Anesthetic	57041-67-5		C <sub>3</sub> H <sub>2</sub> F <sub>6</sub> O
Desglugastrin	Antispasmodic	51987-65-6		C <sub>49</sub> H <sub>61</sub> N <sub>9</sub> O <sub>13</sub>
Desipramine	Antidepressant	50-47-5	Y	C <sub>18</sub> H <sub>22</sub> N <sub>2</sub>
Deslanoside	Cardiotonic	17598-65-1		C <sub>47</sub> H <sub>74</sub> O <sub>19</sub>
Desloratadine	Antihistaminic	100643-71-8	Y	C <sub>19</sub> H <sub>19</sub> ClN <sub>2</sub>
Desmeninol	Unclassified	583-91-5		C <sub>5</sub> H <sub>10</sub> O <sub>3</sub> S

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Desmethylmoramide	Analgesic	1767-88-0		C <sub>24</sub> H <sub>30</sub> N <sub>2</sub> O <sub>2</sub>
Descriptine	Pituitary	66759-48-6		C <sub>32</sub> H <sub>45</sub> N <sub>5</sub> O <sub>4</sub>
Desogestrel	Progestogen	54024-22-5	Y	C <sub>22</sub> H <sub>30</sub> O
Desomorphine	Analgesic	427-00-9		C <sub>17</sub> H <sub>21</sub> NO <sub>2</sub>
Desonide	Antiinflammatory	638-94-8		C <sub>24</sub> H <sub>32</sub> O <sub>6</sub>
Desoximetasone	Antiinflammatory	382-67-2		C <sub>22</sub> H <sub>29</sub> FO <sub>4</sub>
Desoxycorticosterone Acetate	Steroid	56-47-3		C <sub>23</sub> H <sub>32</sub> O <sub>4</sub>
Desoxycorticosterone Pivalate	Steroid	808-48-0		C <sub>26</sub> H <sub>38</sub> O <sub>4</sub>
Desvenlafaxine Succinate	Antidepressant	93413-62-8	Y	C <sub>16</sub> H <sub>25</sub> NO <sub>2</sub>
Detanosal	Unclassified	23573-66-2		C <sub>13</sub> H <sub>19</sub> NO <sub>3</sub>
Deterenol	Adrenergic	7376-66-1		C <sub>11</sub> H <sub>17</sub> NO <sub>2</sub>
Detivaciclovir	Antiviral	220984-26-9		C <sub>9</sub> H <sub>13</sub> N <sub>5</sub> O <sub>2</sub>
Detomidine	Analgesic	76631-46-4		C <sub>12</sub> H <sub>14</sub> N <sub>2</sub>
Detorubicin	Antineoplastic	66211-92-5		C <sub>33</sub> H <sub>39</sub> NO <sub>14</sub>
Detrothyronine	Pituitary	5714-08-9		C <sub>15</sub> H <sub>12</sub> I <sub>3</sub> NO <sub>4</sub>
Deutolperisone	Muscle Relaxant	474641-19-5		C <sub>17</sub> H <sub>18</sub> D <sub>7</sub> NO
Devapamil	Antianginal	92302-55-1		C <sub>26</sub> H <sub>36</sub> N <sub>2</sub> O <sub>3</sub>
Devazepide	Antispasmodic	103420-77-5		C <sub>25</sub> H <sub>20</sub> N <sub>4</sub> O <sub>2</sub>
Dexamethasone	Glucocorticoid	50-02-2	Y	C <sub>22</sub> H <sub>29</sub> FO <sub>5</sub>
Dexamethasone Acefurate	Steroid	83880-70-0		C <sub>29</sub> H <sub>33</sub> FO <sub>8</sub>
Dexamethasone Acetate	Glucocorticoid	1177-87-3		C <sub>24</sub> H <sub>31</sub> FO <sub>6</sub>
Dexamethasone Beloxil	Antiinflammatory	150587-07-8		C <sub>29</sub> H <sub>35</sub> FO <sub>5</sub>
Dexamethasone Dipropionate	Antiinflammatory	55541-30-5		C <sub>28</sub> H <sub>37</sub> FO <sub>7</sub>
Dexamethasone Sodium Phosphate	Glucocorticoid	2392-39-4		C <sub>22</sub> H <sub>28</sub> FN <sub>2</sub> O <sub>8</sub> P
Dexamisole	Antidepressant	14769-74-5		C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> S
Dexbrompheniramine Maleate	Antihistaminic	132-21-8	Y	C <sub>16</sub> H <sub>19</sub> BrN <sub>2</sub>
Dexbudesonide	Glucocorticoid	51372-29-3		C <sub>25</sub> H <sub>34</sub> O <sub>6</sub>
Dexchlorpheniramine Maleate	Antihistaminic	25523-97-1	Y	C <sub>16</sub> H <sub>19</sub> ClN <sub>2</sub>
Dexclamol	Sedative	52340-25-7		C <sub>24</sub> H <sub>29</sub> NO
Dexecadotril	Antihypotensive	112573-72-5		C <sub>21</sub> H <sub>23</sub> NO <sub>4</sub> S
Dexefaroxan	Antihypertensive	143249-88-1		C <sub>13</sub> H <sub>16</sub> N <sub>2</sub> O
Dexetimide	Antiparkinsonian	21888-98-2		C <sub>23</sub> H <sub>26</sub> N <sub>2</sub> O <sub>2</sub>
Dexetozoline	Decongestant	77519-25-6		C <sub>13</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> S
Dexfenfluramine	Anorexic	3239-44-9		C <sub>12</sub> H <sub>16</sub> F <sub>3</sub> N
Dexfosfoserine	Antifungal	407-41-0		C <sub>3</sub> H <sub>8</sub> NO <sub>6</sub> P
Dexibuprofen	Analgesic	51146-56-6		C <sub>13</sub> H <sub>18</sub> O <sub>2</sub>
Deximafen	Antidepressant	42116-77-8		C <sub>11</sub> H <sub>13</sub> N <sub>3</sub>
Dexindoprofen	Analgesic	53086-13-8		C <sub>17</sub> H <sub>15</sub> NO <sub>3</sub>
Dexivacaine	Anesthetic	24358-84-7		C <sub>15</sub> H <sub>22</sub> N <sub>2</sub> O
Dexketoprofen	Analgesic	22161-81-5	Y	C <sub>16</sub> H <sub>14</sub> O <sub>3</sub>
Dexlansoprazole	Antiulcerative	138530-94-6	Y	C <sub>16</sub> H <sub>14</sub> F <sub>3</sub> N <sub>3</sub> O <sub>2</sub> S
Dexlofedidine	Antihypertensive	81447-79-2		C <sub>11</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>2</sub> O
Dexloxiglumide	Antispasmodic	119817-90-2	Y	C <sub>21</sub> H <sub>30</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>5</sub>
Dexmedetomidine	Anxiolytic	113775-47-6		C <sub>13</sub> H <sub>16</sub> N <sub>2</sub>
Dexmethylphenidate	Nootropic	40431-64-9	Y	C <sub>14</sub> H <sub>19</sub> NO <sub>2</sub>
Dexnafenodone	Sedative	92629-87-3		C <sub>20</sub> H <sub>23</sub> NO
Dexniguldipine	Antihypertensive	120054-86-6		C <sub>36</sub> H <sub>39</sub> N <sub>3</sub> O <sub>6</sub>
Dexoxadrol	Analgesic	4741-41-7		C <sub>20</sub> H <sub>23</sub> NO <sub>2</sub>
Dexpanthenol	Cholinergic	81-13-0		C <sub>9</sub> H <sub>19</sub> NO <sub>4</sub>
Dexpemedolac	Analgesic	114030-44-3		C <sub>22</sub> H <sub>23</sub> NO <sub>3</sub>
Dexpropranolol	Antiarrhythmic	5051-22-9		C <sub>16</sub> H <sub>21</sub> NO <sub>2</sub>
Dexproxibutene	Analgesic	47419-52-3		C <sub>22</sub> H <sub>27</sub> NO <sub>2</sub>
Dextrazoxane	Antianginal	24584-09-6		C <sub>11</sub> H <sub>16</sub> N <sub>4</sub> O <sub>4</sub>
Dexsecoverine	Antispasmodic	90237-04-0		C <sub>22</sub> H <sub>35</sub> NO <sub>2</sub>
Dexsotalol	Antiarrhythmic	30236-32-9		C <sub>12</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> S
Dextilidine	Antihistaminic	32447-90-8		C <sub>17</sub> H <sub>23</sub> NO <sub>2</sub>
Dextiopronin	Antidote	29335-92-0		C <sub>5</sub> H <sub>9</sub> NO <sub>3</sub> S
Dextofisopam	Antispasmodic	82059-50-5		C <sub>22</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub>
Dextroamphetamine	Nootropic	51-64-9	Y	C <sub>9</sub> H <sub>13</sub> N
Dextrofemine	Antispasmodic	15687-08-8		C <sub>18</sub> H <sub>23</sub> NO
Dextromethorphan Hydrobromide	Antitussive	125-71-3	Y	C <sub>18</sub> H <sub>25</sub> NO
Dextromoramide	Analgesic	357-56-2	Y	C <sub>25</sub> H <sub>32</sub> N <sub>2</sub> O <sub>2</sub>
Dextrorphan	Analgesic	125-73-5		C <sub>17</sub> H <sub>23</sub> NO

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Dextrothyroxine	Antihyperlipidemic	51-49-0		C <sub>15</sub> H <sub>11</sub> I <sub>4</sub> NO <sub>4</sub>
Dexverapamil	Antianginal	38321-02-7		C <sub>27</sub> H <sub>38</sub> N <sub>2</sub> O <sub>4</sub>
Dezaguanine	Antineoplastic	41729-52-6		C <sub>6</sub> H <sub>6</sub> N <sub>4</sub> O
Dezinamide	Anticonvulsant	91077-32-6		C <sub>11</sub> H <sub>11</sub> F <sub>3</sub> N <sub>2</sub> O <sub>2</sub>
Dezocine	Analgesic	53648-55-8		C <sub>16</sub> H <sub>23</sub> NO
Diacerein	Antirheumatic	13739-02-1	Y	C <sub>19</sub> H <sub>12</sub> O <sub>8</sub>
Diacetamate	Analgesic	2623-33-8		C <sub>10</sub> H <sub>11</sub> NO <sub>3</sub>
Diacetolol	Antihypertensive	22568-64-5		C <sub>16</sub> H <sub>24</sub> N <sub>2</sub> O <sub>4</sub>
Diacetylmorphine	Analgesic	561-27-3		C <sub>21</sub> H <sub>23</sub> NO <sub>5</sub>
Diacetylnalorphine	Analgesic	2748-74-5		C <sub>23</sub> H <sub>25</sub> NO <sub>5</sub>
Diamfenetide	Anthelmintic	36141-82-9		C <sub>20</sub> H <sub>24</sub> N <sub>2</sub> O <sub>5</sub>
Diamocaine Cyclamate	Anesthetic	27112-37-4		C <sub>25</sub> H <sub>37</sub> N <sub>3</sub> O
Diampromide	Analgesic	552-25-0		C <sub>21</sub> H <sub>28</sub> N <sub>2</sub> O
Diamthazole	Antifungal	95-27-2		C <sub>15</sub> H <sub>23</sub> N <sub>3</sub> OS
Dianicline	Antidepressant	292634-27-6		C <sub>13</sub> H <sub>16</sub> N <sub>2</sub> O
Diapamide	Diuretic	3688-85-5		C <sub>9</sub> H <sub>11</sub> ClN <sub>2</sub> O <sub>3</sub> S
Diaplasinin	Anticoagulant	481631-45-2		C <sub>32</sub> H <sub>31</sub> N <sub>5</sub> O
Diarbarone	Unclassified	1233-70-1		C <sub>16</sub> H <sub>20</sub> N <sub>2</sub> O <sub>4</sub>
Diathymosulfone	Antibacterial	5964-62-5		C <sub>32</sub> H <sub>34</sub> N <sub>4</sub> O <sub>4</sub> S
Diaveridine	Antibacterial	5355-16-8		C <sub>13</sub> H <sub>16</sub> N <sub>4</sub> O <sub>2</sub>
Diazepam	Anxiolytic	439-14-5	Y	C <sub>16</sub> H <sub>13</sub> ClN <sub>2</sub> O
Diaziquone	Antineoplastic	57998-68-2		C <sub>16</sub> H <sub>20</sub> N <sub>4</sub> O <sub>6</sub>
Diazoxide	Antihypertensive	364-98-7	Y	C <sub>8</sub> H <sub>7</sub> ClN <sub>2</sub> O <sub>2</sub> S
Dibekacin	Antibiotic	34493-98-6		C <sub>18</sub> H <sub>37</sub> N <sub>5</sub> O <sub>8</sub>
Dibemethine	Antineoplastic	102-05-6		C <sub>15</sub> H <sub>17</sub> N
Dibenzepin	Antidepressant	4498-32-2		C <sub>18</sub> H <sub>21</sub> N <sub>3</sub> O
Dibenzothiophene	Dermatologic	132-65-0		C <sub>12</sub> H <sub>8</sub> S
Dibrospidium Chloride	Antibiotic	86641-76-1		C <sub>18</sub> H <sub>32</sub> Br <sub>2</sub> Cl <sub>2</sub> N <sub>4</sub> O <sub>2</sub>
Dibucaine	Anesthetic	85-79-0		C <sub>20</sub> H <sub>29</sub> N <sub>3</sub> O <sub>2</sub>
Dibuprol	Choleretic	2216-77-5		C <sub>11</sub> H <sub>24</sub> O <sub>3</sub>
Dibupyrone	Analgesic	772990-64-4		C <sub>16</sub> H <sub>23</sub> N <sub>3</sub> O <sub>4</sub> S
Dibusadol	Unclassified	24353-45-5		C <sub>17</sub> H <sub>26</sub> N <sub>2</sub> O <sub>3</sub>
Dibutoline Sulfate	Antispasmodic	532-49-0		C <sub>15</sub> H <sub>33</sub> N <sub>2</sub> O <sub>2</sub> .1/2O <sub>4</sub> S
Dicarbene	Antidepressant	17411-19-7		C <sub>13</sub> H <sub>18</sub> N <sub>2</sub>
Dicarfen	Antiinflammatory	15585-88-3		C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub>
Dichlorisone Acetate	Dermatologic	79-61-8		C <sub>23</sub> H <sub>28</sub> Cl <sub>2</sub> O <sub>5</sub>
Dichlormezanone	Anxiolytic	114676-16-3		C <sub>11</sub> H <sub>11</sub> Cl <sub>2</sub> NO <sub>3</sub> S
Dichlorophene	Anthelmintic	97-23-4		C <sub>13</sub> H <sub>10</sub> Cl <sub>2</sub> O <sub>2</sub>
Dichlorophenarsine	Antibacterial	455-83-4		C <sub>6</sub> H <sub>6</sub> AsCl <sub>2</sub> NO
Dichloroxylenol	Anesthetic	133-53-9		C <sub>8</sub> H <sub>8</sub> Cl <sub>2</sub> O
Dichlorphenamide	Antiglaucoma	120-97-8	Y	C <sub>6</sub> H <sub>6</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>4</sub> S <sub>2</sub>
Dichlorvos	Anthelmintic	62-73-7		C <sub>4</sub> H <sub>7</sub> Cl <sub>2</sub> O <sub>4</sub> P
Dicrenone	Antihypertensive	41020-79-5		C <sub>26</sub> H <sub>36</sub> O <sub>5</sub>
Diclazuril	Antibacterial	101831-37-2	Y	C <sub>17</sub> H <sub>9</sub> Cl <sub>3</sub> N <sub>4</sub> O <sub>2</sub>
Diclofenac	Antiinflammatory	15307-86-5	Y	C <sub>14</sub> H <sub>11</sub> Cl <sub>2</sub> NO <sub>2</sub>
Diclofensine	Antidepressant	67165-56-4		C <sub>17</sub> H <sub>17</sub> Cl <sub>2</sub> NO
Diclofurime	Antihypertensive	64743-08-4		C <sub>18</sub> H <sub>22</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>3</sub>
Diclometide	Antipsychotic	17243-49-1		C <sub>14</sub> H <sub>20</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Diclounixin	Analgesic	17737-68-7		C <sub>12</sub> H <sub>8</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Dicloralurea	Antibacterial	116-52-9		C <sub>5</sub> H <sub>6</sub> Cl <sub>6</sub> N <sub>2</sub> O <sub>3</sub>
Dicloxacillin	Antibiotic	3116-76-5	Y	C <sub>19</sub> H <sub>17</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>5</sub> S
Dicolinium Iodide	Muscle Relaxant	382-82-1		C <sub>16</sub> H <sub>34</sub> I <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Dicresulene	Unclassified	78480-14-5		C <sub>15</sub> H <sub>16</sub> O <sub>8</sub> S <sub>2</sub>
Dicumarol	Anticoagulant	66-76-2		C <sub>19</sub> H <sub>12</sub> O <sub>6</sub>
Dicyclomine	Antispasmodic	77-19-0	Y	C <sub>19</sub> H <sub>35</sub> NO <sub>2</sub>
Didanosine	Antiviral	69655-05-6	Y	C <sub>10</sub> H <sub>12</sub> N <sub>4</sub> O <sub>3</sub>
Didrovaltrate	Sedative	18296-45-2		C <sub>22</sub> H <sub>32</sub> O <sub>8</sub>
Dieldrin	Dermatologic	60-57-1		C <sub>12</sub> H <sub>8</sub> Cl <sub>6</sub> O
Dienestrol	Estrogen	84-17-3		C <sub>18</sub> H <sub>18</sub> O <sub>2</sub>
Dienogest	Contraceptive	65928-58-7	Y	C <sub>20</sub> H <sub>25</sub> NO <sub>2</sub>
Diethadione	Anticonvulsant	702-54-5		C <sub>8</sub> H <sub>13</sub> NO <sub>3</sub>
Diethazine	Antiparkinsonian	60-91-3		C <sub>18</sub> H <sub>22</sub> N <sub>2</sub> S
Diethyl Oxalate	Anorexic	95-92-1		C <sub>6</sub> H <sub>10</sub> O <sub>4</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Diethylcarbamazine	Anthelmintic	90-89-1	Y	C <sub>10</sub> H <sub>21</sub> N <sub>3</sub> O
Diethylpropion	Anorexic	90-84-6	Y	C <sub>13</sub> H <sub>19</sub> NO
Diethylstilbestrol	Antineoplastic	56-53-1	Y	C <sub>18</sub> H <sub>20</sub> O <sub>2</sub>
Diethylstilbestrol Dipalmitate	Antineoplastic	6533-53-5		C <sub>50</sub> H <sub>80</sub> O <sub>4</sub>
Diethylstilbestrol Dipropionate	Antineoplastic	130-80-3		C <sub>24</sub> H <sub>28</sub> O <sub>4</sub>
Diethylthiambutene	Analgesic	86-14-6		C <sub>16</sub> H <sub>21</sub> NS <sub>2</sub>
Dietifen	Antihistaminic	3686-78-0		C <sub>21</sub> H <sub>27</sub> NO <sub>2</sub>
Difebarbamate	Sedative	15687-09-9		C <sub>28</sub> H <sub>42</sub> N <sub>4</sub> O <sub>9</sub>
Difemerine	Antispasmodic	80387-96-8		C <sub>20</sub> H <sub>25</sub> NO <sub>3</sub>
Difemetorex	Anorexic	13862-07-2		C <sub>20</sub> H <sub>25</sub> NO
Difenamizole	Analgesic	20170-20-1		C <sub>20</sub> H <sub>22</sub> N <sub>4</sub> O
Difenclozaxine	Antidepressant	5617-26-5		C <sub>19</sub> H <sub>22</sub> ClNO <sub>2</sub>
Difenoximide	Antispasmodic	47806-92-8		C <sub>32</sub> H <sub>31</sub> N <sub>5</sub> O <sub>4</sub>
Difenoxin	Antidiarrheal	28782-42-5	Y	C <sub>28</sub> H <sub>28</sub> N <sub>2</sub> O <sub>2</sub>
Difetarsone	Antiamebic	3639-19-8		C <sub>14</sub> H <sub>18</sub> As <sub>2</sub> N <sub>2</sub> O <sub>6</sub>
Difeterol	Adrenergic	14587-50-9		C <sub>25</sub> H <sub>29</sub> NO <sub>2</sub>
Diflomotecan	Antineoplastic	220997-97-7		C <sub>21</sub> H <sub>16</sub> F <sub>2</sub> N <sub>2</sub> O <sub>4</sub>
Diflorasone Diacetate	Antiinflammatory	33564-31-7		C <sub>26</sub> H <sub>32</sub> F <sub>2</sub> O <sub>7</sub>
Difloxacin	Antibiotic	98106-17-3		C <sub>21</sub> H <sub>19</sub> F <sub>2</sub> N <sub>3</sub> O <sub>3</sub>
Difluanine	Nootropic	5522-39-4		C <sub>28</sub> H <sub>33</sub> F <sub>2</sub> N <sub>3</sub>
Diflucortolone	Glucocorticoid	2607-06-9		C <sub>22</sub> H <sub>28</sub> F <sub>2</sub> O <sub>4</sub>
Diflucortolone Pivalate	Antiinflammatory	15845-96-2		C <sub>27</sub> H <sub>36</sub> F <sub>2</sub> O <sub>5</sub>
Diflumidone Sodium	Antiinflammatory	22736-85-2		C <sub>14</sub> H <sub>11</sub> F <sub>2</sub> NO <sub>3</sub> S
Diflunisal	Antiinflammatory	22494-42-4	Y	C <sub>13</sub> H <sub>8</sub> F <sub>2</sub> O <sub>3</sub>
Difluprednate	Antiinflammatory	23674-86-4		C <sub>27</sub> H <sub>34</sub> F <sub>2</sub> O <sub>7</sub>
Difalone	Antiinflammatory	21626-89-1		C <sub>16</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>
Digitoxin	Cardiotonic	71-63-6		C <sub>41</sub> H <sub>64</sub> O <sub>13</sub>
Digoxin	Cardiotonic	20830-75-5	Y	C <sub>41</sub> H <sub>64</sub> O <sub>14</sub>
Dihexyverine	Anticholelithogenic	561-77-3		C <sub>20</sub> H <sub>35</sub> NO <sub>2</sub>
Dihydralazine	Vasodilator	484-23-1		C <sub>8</sub> H <sub>10</sub> N <sub>6</sub>
Dihydrocodeine Bitartrate	Analgesic	125-28-0	Y	C <sub>18</sub> H <sub>23</sub> NO <sub>3</sub>
Dihydroergotamine Mesylate	Antimigraine	511-12-6		C <sub>33</sub> H <sub>37</sub> N <sub>5</sub> O <sub>5</sub>
Dihydrostreptomycin Sulfate	Antibacterial	128-46-1		C <sub>21</sub> H <sub>41</sub> N <sub>7</sub> O <sub>12</sub>
Dihydrotachysterol	Steroid	67-96-9		C <sub>28</sub> H <sub>46</sub> O
Diisopromine	Antidepressant	5966-41-6		C <sub>21</sub> H <sub>29</sub> N
Diisopropanolamine	Decongestant	110-97-4		C <sub>6</sub> H <sub>15</sub> NO <sub>2</sub>
Diisopropylamine Dichloroacetate	Vasodilator	108-18-9		C <sub>6</sub> H <sub>15</sub> N
Dilazep	Vasodilator	35898-87-4		C <sub>31</sub> H <sub>44</sub> N <sub>2</sub> O <sub>10</sub>
Dilevalol	Antihypertensive	75659-07-3		C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> O <sub>3</sub>
Dilmefone	Anticonvulsant	37398-31-5		C <sub>16</sub> H <sub>15</sub> NO <sub>3</sub>
Diloxanide	Antiamebic	579-38-4		C <sub>9</sub> H <sub>9</sub> Cl <sub>2</sub> NO <sub>2</sub>
Diloxanide Furoate	Antiamebic	3736-81-0		C <sub>14</sub> H <sub>11</sub> Cl <sub>2</sub> NO <sub>4</sub>
Diltiazem	Antianginal	42399-41-7	Y	C <sub>22</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub> S
Dimabefylline	Bronchodilator	1703-48-6		C <sub>16</sub> H <sub>19</sub> N <sub>5</sub> O <sub>2</sub>
Dimecamine	Muscle Relaxant	3570-07-8		C <sub>12</sub> H <sub>23</sub> N
Dimecolonium Iodide	Antispasmodic	3425-97-6		C <sub>14</sub> H <sub>30</sub> I <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Dimecrotic Acid	Choleretic	7706-67-4		C <sub>12</sub> H <sub>14</sub> O <sub>4</sub>
Dimefadane	Analgesic	5581-40-8		C <sub>17</sub> H <sub>19</sub> N
Dimeflin	Nootropic	1165-48-6		C <sub>20</sub> H <sub>21</sub> NO <sub>3</sub>
Dimelazine	Antihypotensive	15302-12-2		C <sub>19</sub> H <sub>22</sub> N <sub>2</sub> S
Dimemorfan	Antitussive	36309-01-0		C <sub>18</sub> H <sub>25</sub> N
Dimenhydrinate	Antiemetic	85-18-7	Y	C <sub>7</sub> H <sub>7</sub> ClN <sub>4</sub> O <sub>2</sub>
Dimenoxadol	Analgesic	509-78-4		C <sub>20</sub> H <sub>25</sub> NO <sub>3</sub>
Dimepheptanol	Analgesic	545-90-4		C <sub>21</sub> H <sub>29</sub> NO
Dimepregnen	Progestogen	21208-26-4		C <sub>23</sub> H <sub>36</sub> O <sub>2</sub>
Dimeprozan	Antipsychotic	6538-22-3		C <sub>19</sub> H <sub>21</sub> NO <sub>2</sub>
Dimercaprol	Antidote	59-52-9		C <sub>3</sub> H <sub>8</sub> OS <sub>2</sub>
Dimesna	Mucolytic	45127-11-5		C <sub>4</sub> H <sub>10</sub> O <sub>6</sub> S <sub>4</sub>
Dimesone	Unclassified	25092-07-3		C <sub>23</sub> H <sub>31</sub> FO <sub>4</sub>
Dimestrol	Estrogen	130-79-0		C <sub>20</sub> H <sub>24</sub> O <sub>2</sub>
Dimetacrine	Antidepressant	4757-55-5		C <sub>20</sub> H <sub>26</sub> N <sub>2</sub>
Dimetamfetamine	Anorexic	17279-39-9		C <sub>11</sub> H <sub>17</sub> N
Dimethadione	Anticonvulsant	695-53-4		C <sub>5</sub> H <sub>7</sub> NO <sub>3</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Dimethazan	Antidepressant	519-30-2		C <sub>11</sub> H <sub>17</sub> N <sub>5</sub> O <sub>2</sub>
Dimethindene Maleate	Antihistaminic	5636-83-9		C <sub>20</sub> H <sub>24</sub> N <sub>2</sub>
Dimethisoquin	Anesthetic	86-80-6		C <sub>17</sub> H <sub>24</sub> N <sub>2</sub> O
Dimethisterone	Progestogen	79-64-1		C <sub>23</sub> H <sub>32</sub> O <sub>2</sub>
Dimetholizine	Unclassified	7008-00-6		C <sub>15</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub>
Dimethoxanate	Antitussive	477-93-0		C <sub>19</sub> H <sub>22</sub> N <sub>2</sub> O <sub>5</sub> S
1,3-Dimethylbutyl Salicylate	Antiinflammatory	22490-72-8	Y	C <sub>15</sub> H <sub>33</sub> N <sub>3</sub>
Dimethyl Fumarate	Immunomodulator	624-49-7	Y	C <sub>6</sub> H <sub>8</sub> O <sub>4</sub>
Dimethyl Sulfoxide	Urologic	67-68-5		C <sub>2</sub> H <sub>6</sub> OS
Dimethylaminoethyl Reserpilate Di	Antihypertensive	5585-67-1		C <sub>26</sub> H <sub>35</sub> N <sub>3</sub> O <sub>5</sub>
Dimethylthiambutene	Analgesic	524-84-5		C <sub>14</sub> H <sub>17</sub> NS <sub>2</sub>
Dimethyltubocurarinium Chloride	Neuromuscular Blocking Agent	33335-58-9Y		C <sub>40</sub> H <sub>48</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>6</sub>
Dimetipirium Bromide	Antihypertensive	51047-24-6		C <sub>23</sub> H <sub>30</sub> BrNO <sub>3</sub>
Dimetofrine	Antihypotensive	22950-29-4		C <sub>11</sub> H <sub>17</sub> NO <sub>4</sub>
Dimetridazole	Antiprotozoal	551-92-8		C <sub>5</sub> H <sub>7</sub> N <sub>3</sub> O <sub>2</sub>
Diminazene	Analgesic	536-71-0		C <sub>14</sub> H <sub>15</sub> N <sub>7</sub>
Dimiracetam	Anticonvulsant	126100-97-8		C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>
Dimorpholamine	Nootropic	119-48-2		C <sub>20</sub> H <sub>38</sub> N <sub>4</sub> O <sub>4</sub>
Dimoxamine	Nootropic	52842-59-8		C <sub>13</sub> H <sub>21</sub> NO <sub>2</sub>
Dimoxaprost	Prostaglandin	90243-98-4		C <sub>21</sub> H <sub>34</sub> O <sub>6</sub>
Dimpylate	Ectoparasiticide	333-41-5		C <sub>12</sub> H <sub>21</sub> N <sub>2</sub> O <sub>3</sub> PS
Dinaline	Bronchodilator	58338-59-3		C <sub>13</sub> H <sub>13</sub> N <sub>3</sub> O
Dinazafone	Anticonvulsant	71119-12-5		C <sub>20</sub> H <sub>21</sub> ClN <sub>2</sub> O <sub>2</sub>
Diniprophylline	Bronchodilator	17692-30-7		C <sub>22</sub> H <sub>20</sub> N <sub>6</sub> O <sub>6</sub>
Dinitolmide	Antibacterial	148-01-6		C <sub>8</sub> H <sub>7</sub> N <sub>3</sub> O <sub>5</sub>
Dinoprost	Oxytocic	551-11-1	Y	C <sub>20</sub> H <sub>34</sub> O <sub>5</sub>
Dinoprostone	Oxytocic	363-24-6		C <sub>20</sub> H <sub>32</sub> O <sub>5</sub>
Dinsed	Antibacterial	96-62-8		C <sub>14</sub> H <sub>14</sub> N <sub>4</sub> O <sub>8</sub> S <sub>2</sub>
Diosmin	Capillary Protectant	520-27-4	Y	C <sub>28</sub> H <sub>32</sub> O <sub>15</sub>
Dioxadilol	Antihypertensive	80743-08-4		C <sub>16</sub> H <sub>25</sub> NO <sub>4</sub>
Dioxadrol	Antidepressant	6495-46-1		C <sub>20</sub> H <sub>23</sub> NO <sub>2</sub>
Dioxamate	Antihistaminic	3567-40-6		C <sub>15</sub> H <sub>29</sub> NO <sub>4</sub>
Dioxaphetyl Butyrate	Antispasmodic	467-86-7		C <sub>22</sub> H <sub>27</sub> NO <sub>3</sub>
Dioxethedrin	Bronchodilator	497-75-6		C <sub>11</sub> H <sub>17</sub> NO <sub>3</sub>
Dioxifedrine	Adrenergic	10329-60-9		C <sub>10</sub> H <sub>15</sub> NO <sub>3</sub>
Dioxybenzone	Dermatologic	131-53-3		C <sub>14</sub> H <sub>12</sub> O <sub>4</sub>
Dioxyline Phosphate	Cardiotonic	147-27-3		C <sub>22</sub> H <sub>25</sub> NO <sub>4</sub>
Dipenine Bromide	Antispasmodic	2001-81-2		C <sub>20</sub> H <sub>38</sub> BrNO <sub>2</sub>
Diperodon	Anesthetic	101-08-6		C <sub>22</sub> H <sub>27</sub> N <sub>3</sub> O <sub>4</sub>
Diphenhydramine	Antihistaminic	58-73-1	Y	C <sub>17</sub> H <sub>21</sub> NO
Diphenidol	Antiemetic	972-02-1	Y	C <sub>21</sub> H <sub>27</sub> NO
Diphenoxylate /Atropine Sulfate	Antispasmodic	915-30-0		C <sub>30</sub> H <sub>32</sub> N <sub>2</sub> O <sub>2</sub>
Diphenylpyraline	Antihistaminic	147-20-6		C <sub>19</sub> H <sub>23</sub> NO
Diphoxazide	Antibacterial	511-41-1		C <sub>17</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>
Dipipanone	Analgesic	467-83-4	Y	C <sub>24</sub> H <sub>31</sub> NO
Dipiproverine	Antispasmodic	117-30-6		C <sub>20</sub> H <sub>30</sub> N <sub>2</sub> O <sub>2</sub>
Dipivefrin	Mydriatic	52365-63-6	Y	C <sub>19</sub> H <sub>29</sub> NO <sub>5</sub>
Diprafenone	Antiarrhythmic	81447-80-5		C <sub>23</sub> H <sub>31</sub> NO <sub>3</sub>
Diprenorphine	Antidote	14357-78-9		C <sub>26</sub> H <sub>35</sub> NO <sub>4</sub>
Diprobutine	Antiparkinsonian	61822-36-4		C <sub>10</sub> H <sub>23</sub> N
Diprofene	Antihypertensive	5835-72-3		C <sub>22</sub> H <sub>29</sub> NOS
Diproleandomycin	Antibiotic	14289-25-9		C <sub>41</sub> H <sub>69</sub> NO <sub>14</sub>
Diproqualone	Sedative	36518-02-2		C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>
Diproteverine	Antihypertensive	69373-95-1		C <sub>26</sub> H <sub>35</sub> NO <sub>4</sub>
Diproxadol	Analgesic	52042-24-7		C <sub>12</sub> H <sub>14</sub> ClNO <sub>4</sub>
Dipyridamole	Antithrombotic	58-32-2	Y	C <sub>24</sub> H <sub>40</sub> N <sub>8</sub> O <sub>4</sub>
Dipyrrithione	Antibacterial	3696-28-4		C <sub>10</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> S <sub>2</sub>
Dipyrocetyl	Analgesic	486-79-3		C <sub>11</sub> H <sub>10</sub> O <sub>6</sub>
Dipyrone	Analgesic	50567-35-6		C <sub>13</sub> H <sub>17</sub> N <sub>3</sub> O <sub>4</sub> S
Diquafosol Tetrasodium	Mucolytic	59985-21-6		C <sub>18</sub> H <sub>26</sub> N <sub>4</sub> O <sub>23</sub> P <sub>4</sub>
Dirithromycin	Antibiotic	62013-04-1	Y	C <sub>42</sub> H <sub>78</sub> N <sub>2</sub> O <sub>14</sub>



Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Dirlotapide	Antihyperlipidemic	481658-94-0		C <sub>40</sub> H <sub>33</sub> F <sub>3</sub> N <sub>4</sub> O <sub>3</sub>
Disermolide	Antiparkinsonian	127943-53-7		C <sub>33</sub> H <sub>55</sub> NO <sub>8</sub>
Disobutamide	Antiarrhythmic	68284-69-5		C <sub>23</sub> H <sub>38</sub> ClN <sub>3</sub> O
Disogluside	Unclassified	14144-06-0		C <sub>33</sub> H <sub>52</sub> O <sub>8</sub>
Disopyramide	Antiarrhythmic	3737-09-5	Y	C <sub>21</sub> H <sub>29</sub> N <sub>3</sub> O
Disoxaril	Antiviral	87495-31-6		C <sub>20</sub> H <sub>26</sub> N <sub>2</sub> O <sub>3</sub>
Distigmine Bromide	Muscle Relaxant	15876-67-2	Y	C <sub>22</sub> H <sub>32</sub> Br <sub>2</sub> N <sub>4</sub> O <sub>4</sub>
Disufenton Sodium	Nootropic	168021-77-0		C <sub>11</sub> H <sub>15</sub> NO <sub>7</sub> S <sub>2</sub>
Disulergine	Urologic	59032-40-5		C <sub>17</sub> H <sub>24</sub> N <sub>4</sub> O <sub>2</sub> S
Disulfiram	Alcohol Deterrant	97-77-8	Y	C <sub>10</sub> H <sub>20</sub> N <sub>2</sub> S <sub>4</sub>
Disuprazole	Ant ulcerative	99499-40-8		C <sub>16</sub> H <sub>17</sub> N <sub>3</sub> OS <sub>2</sub>
Ditazole	Antiinflammatory	18471-20-0		C <sub>19</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub>
Ditekiren	Antihypertensive	103336-05-6		C <sub>50</sub> H <sub>75</sub> N <sub>9</sub> O <sub>8</sub>
Ditercalinium Chloride	Antihypertensive	74517-42-3		C <sub>46</sub> H <sub>50</sub> Cl <sub>2</sub> N <sub>6</sub> O <sub>2</sub>
Dithiazanine Iodide	Anthelminthic	514-73-8		C <sub>23</sub> H <sub>23</sub> N <sub>2</sub> S <sub>2</sub>
Ditiocarb	Immunomodulator	147-84-2		C <sub>5</sub> H <sub>11</sub> NS <sub>2</sub>
Ditiomustine	Antineoplastic	82599-22-2		C <sub>10</sub> H <sub>18</sub> Cl <sub>2</sub> N <sub>6</sub> O <sub>4</sub> S <sub>2</sub>
Ditolamide	Antibiotic	723-42-2		C <sub>13</sub> H <sub>21</sub> NO <sub>2</sub> S
Ditophal	Antibiotic	584-69-0		C <sub>12</sub> H <sub>14</sub> O <sub>2</sub> S <sub>2</sub>
Divabuterol	Bronchodilator	54592-27-7		C <sub>22</sub> H <sub>35</sub> NO <sub>5</sub>
Divaplon	Anxiolytic	90808-12-1		C <sub>17</sub> H <sub>17</sub> N <sub>3</sub> O <sub>2</sub>
Dixanthogen	Ectoparasiticide	502-55-6		C <sub>6</sub> H <sub>10</sub> O <sub>2</sub> S <sub>4</sub>
Dizatrifone	Nootropic	92257-40-4		C <sub>21</sub> H <sub>21</sub> N <sub>3</sub> O <sub>3</sub>
Dizocilpine Maleate	Nootropic	77086-21-6		C <sub>16</sub> H <sub>15</sub> N
Dobupride	Gastroprokinetic	106707-51-1		C <sub>20</sub> H <sub>30</sub> ClN <sub>3</sub> O <sub>4</sub>
Dobutamine	Cardiotonic	34368-04-2		C <sub>18</sub> H <sub>23</sub> NO <sub>3</sub>
Docarpamine	Cardiotonic	74639-40-0		C <sub>21</sub> H <sub>30</sub> N <sub>2</sub> O <sub>8</sub> S
Docebenone	Antiinflammatory	80809-81-0		C <sub>21</sub> H <sub>26</sub> O <sub>3</sub>
Docetaxel	Antineoplastic	114977-28-5		C <sub>43</sub> H <sub>53</sub> NO <sub>14</sub>
Doconazole	Antifungal	59831-63-9		C <sub>26</sub> H <sub>22</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>3</sub>
Doconexent	Unclassified	6217-54-5		C <sub>22</sub> H <sub>32</sub> O <sub>2</sub>
Docusate Sodium	Laxative	10041-19-7		C <sub>20</sub> H <sub>38</sub> O <sub>7</sub> S
Dodeclonium Bromide	Antibiotic	15687-13-5		C <sub>22</sub> H <sub>39</sub> BrClNO
Dodicin	Antibacterial	6843-97-6		C <sub>18</sub> H <sub>39</sub> N <sub>3</sub> O <sub>2</sub>
Dofamium Chloride	Antihistaminic	54063-35-3		C <sub>25</sub> H <sub>44</sub> ClN <sub>3</sub> O <sub>2</sub>
Dofequidar	Antineoplastic	129716-58-1		C <sub>30</sub> H <sub>31</sub> N <sub>3</sub> O <sub>3</sub>
Dofetilide	Antiarrhythmic	115256-11-6	Y	C <sub>19</sub> H <sub>27</sub> N <sub>3</sub> O <sub>5</sub> S <sub>2</sub>
Dolasetron	Antiemetic	115956-12-2	Y	C <sub>19</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub>
Doliracetam	Anticonvulsant	84901-45-1		C <sub>16</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Domazoline Fumarate	Anticholelithogenic	6043-01-2		C <sub>14</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>
Domiodol	Mucolytic	61869-07-6		C <sub>5</sub> H <sub>9</sub> IO <sub>3</sub>
Domiphen Bromide	Antibacterial	538-71-6		C <sub>22</sub> H <sub>40</sub> BrNO
Domipizone	Bronchodilator	95355-10-5		C <sub>13</sub> H <sub>16</sub> N <sub>2</sub> O <sub>4</sub>
Domitroban	Antithrombotic	112966-96-8		C <sub>20</sub> H <sub>27</sub> NO <sub>4</sub> S
Domoprednate	Dermatologic	66877-67-6		C <sub>26</sub> H <sub>36</sub> O <sub>5</sub>
Domoxin	Antidepressant	61-74-5		C <sub>16</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>
Domperidone	Antiemetic	57808-66-9	Y	C <sub>22</sub> H <sub>24</sub> ClN <sub>5</sub> O <sub>2</sub>
Donepezil	Nootropic	120014-06-4	Y	C <sub>24</sub> H <sub>29</sub> NO <sub>3</sub>
Donetidine	Antihistaminic	99248-32-5		C <sub>20</sub> H <sub>25</sub> N <sub>5</sub> O <sub>3</sub> S
Donitriptan	Antimigraine	170912-52-4		C <sub>23</sub> H <sub>25</sub> N <sub>5</sub> O <sub>2</sub>
Dopamantine	Antiparkinsonian	39907-68-1		C <sub>19</sub> H <sub>25</sub> NO <sub>3</sub>
Dopamine	Cardiotonic	51-61-6	Y	C <sub>8</sub> H <sub>11</sub> NO <sub>2</sub>
Dopexamine	Cardiotonic	86197-47-9		C <sub>22</sub> H <sub>32</sub> N <sub>2</sub> O <sub>2</sub>
Dopropidil	Antianginal	79700-61-1		C <sub>20</sub> H <sub>35</sub> NO <sub>2</sub>
Doqualast	Antihistaminic	64019-03-0		C <sub>13</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub>
Doramapimod	Antirheumatic	285983-48-4		C <sub>31</sub> H <sub>37</sub> N <sub>5</sub> O <sub>3</sub>
Doramectin	Antibacterial	117704-25-3		C <sub>50</sub> H <sub>74</sub> O <sub>14</sub>
Doranidazole	Antiprotozoal	149838-23-3		C <sub>8</sub> H <sub>13</sub> N <sub>3</sub> O <sub>6</sub>
Dorastine	Antihistaminic	21228-13-7		C <sub>20</sub> H <sub>22</sub> ClN <sub>3</sub>
Doreptide	Antiparkinsonian	90104-48-6		C <sub>17</sub> H <sub>24</sub> N <sub>4</sub> O <sub>3</sub>
Doretinel	Dermatologic	104561-36-6		C <sub>24</sub> H <sub>30</sub> O <sub>2</sub>
Doripenem	Antibiotic	148016-81-3		C <sub>15</sub> H <sub>24</sub> N <sub>4</sub> O <sub>6</sub> S <sub>2</sub>
Dorzolamide	Antiglaucoma	120279-96-1		C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O <sub>4</sub> S <sub>3</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Dosergoside	Antiinflammatory	87178-42-5		C <sub>34</sub> H <sub>53</sub> N <sub>3</sub> O <sub>3</sub>
Dotarizine	Vasodilator	84625-59-2		C <sub>29</sub> H <sub>34</sub> N <sub>2</sub> O <sub>2</sub>
Dotefonium Bromide	Antispasmodic	26058-50-4		C <sub>20</sub> H <sub>27</sub> BrN <sub>2</sub> O <sub>2</sub> S
Dothiepin	Antidepressant	113-53-1	Y	C <sub>19</sub> H <sub>21</sub> NS
Doxaminol	Cardiotonic	55286-56-1		C <sub>26</sub> H <sub>29</sub> NO <sub>3</sub>
Doxapram	Respiratory Stimulant	309-29-5		C <sub>24</sub> H <sub>30</sub> N <sub>2</sub> O <sub>2</sub>
Doxaprost	Bronchodilator	51953-95-8		C <sub>21</sub> H <sub>36</sub> O <sub>4</sub>
Doxazosin	Antihypertensive	74191-85-8	Y	C <sub>23</sub> H <sub>25</sub> N <sub>5</sub> O <sub>5</sub>
Doxefazepam	Sedative	40762-15-0		C <sub>17</sub> H <sub>14</sub> ClFN <sub>2</sub> O <sub>3</sub>
Doxenitoin	Anticonvulsant	3254-93-1		C <sub>15</sub> H <sub>14</sub> N <sub>2</sub> O
Doxepin	Antidepressant	1668-19-5	Y	C <sub>19</sub> H <sub>21</sub> NO
Doxercalciferol	Thyroid	54573-75-0	Y	C <sub>28</sub> H <sub>44</sub> O <sub>2</sub>
Doxibetasol	Glucocorticoid	1879-77-2		C <sub>22</sub> H <sub>29</sub> FO <sub>4</sub>
Doxifluridine	Antineoplastic	3094-09-5	Y	C <sub>9</sub> H <sub>11</sub> FN <sub>2</sub> O <sub>5</sub>
Doxofylline	Bronchodilator	69975-86-6	Y	C <sub>11</sub> H <sub>14</sub> N <sub>4</sub> O <sub>4</sub>
Doxorubicin	Antineoplastic	23214-92-8	Y	C <sub>27</sub> H <sub>29</sub> NO <sub>11</sub>
Doxpicomine	Analgesic	62904-71-6		C <sub>12</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>
Doxycycline	Antibiotic	564-25-0	Y	C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>8</sub>
Doxylamine	Antihistaminic	469-21-6	Y	C <sub>17</sub> H <sub>22</sub> N <sub>2</sub> O
Draflazine	Cardiotonic	120770-34-5		C <sub>30</sub> H <sub>33</sub> Cl <sub>2</sub> F <sub>2</sub> N <sub>5</sub> O <sub>2</sub>
Dramedilol	Antihypertensive	76953-65-6		C <sub>20</sub> H <sub>29</sub> N <sub>5</sub> O <sub>4</sub>
Draquinolol	Antihyperlipidemic	67793-71-9		C <sub>24</sub> H <sub>30</sub> N <sub>2</sub> O <sub>4</sub>
Drazidox	Antibacterial	27314-77-8		C <sub>10</sub> H <sub>10</sub> N <sub>4</sub> O <sub>3</sub>
Dribendazole	Anthelminthic	63667-16-3		C <sub>15</sub> H <sub>19</sub> N <sub>3</sub> O <sub>2</sub> S
Drinidene	Analgesic	53394-92-6		C <sub>10</sub> H <sub>9</sub> NO
Drobuline	Antiarrhythmic	58473-73-7		C <sub>19</sub> H <sub>25</sub> NO
Drocarbil	Anthelminthic	63-75-2		C <sub>8</sub> H <sub>13</sub> NO <sub>2</sub>
Drocinonide	Antiinflammatory	2355-59-1		C <sub>24</sub> H <sub>35</sub> FO <sub>6</sub>
Droclidinium Bromide	Antihypertensive	29125-56-2		C <sub>22</sub> H <sub>32</sub> BrNO <sub>3</sub>
Drofenine	Antispasmodic	1679-76-1		C <sub>20</sub> H <sub>31</sub> NO <sub>2</sub>
Droloxifene	Antineoplastic	82413-20-5		C <sub>26</sub> H <sub>29</sub> NO <sub>2</sub>
Drometrizole	Dermatologic	2440-22-4		C <sub>13</sub> H <sub>11</sub> N <sub>3</sub> O
Dromostanolone Propionate	Antineoplastic	521-12-0		C <sub>23</sub> H <sub>36</sub> O <sub>3</sub>
Dronabinol	Antiemetic	1972-08-3	Y	C <sub>21</sub> H <sub>30</sub> O <sub>2</sub>
Dronedarone	Antiarrhythmic	141626-36-0	Y	C <sub>31</sub> H <sub>44</sub> N <sub>2</sub> O <sub>5</sub> S
Dropempine	Unclassified	34703-49-6		C <sub>10</sub> H <sub>19</sub> N
Droperidol	Antipsychotic	548-73-2		C <sub>22</sub> H <sub>22</sub> FN <sub>3</sub> O <sub>2</sub>
Droprenilamine	Vasodilator	57653-27-7		C <sub>24</sub> H <sub>33</sub> N
Dropropizine	Antitussive	17692-31-8		C <sub>13</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>
Drospirenone	Contraceptive	67392-87-4	Y	C <sub>24</sub> H <sub>30</sub> O <sub>3</sub>
Drotaverine	Antispasmodic	14009-24-6	Y	C <sub>24</sub> H <sub>31</sub> NO <sub>4</sub>
Drotebanol	Antitussive	3176-03-2	Y	C <sub>19</sub> H <sub>27</sub> NO <sub>4</sub>
Droxacin Sodium	Antibacterial	35067-47-1		C <sub>14</sub> H <sub>13</sub> NO <sub>4</sub>
Droxicainide	Antiarrhythmic	78289-26-6		C <sub>16</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub>
Droxicam	Antiinflammatory	90101-16-9		C <sub>16</sub> H <sub>11</sub> N <sub>3</sub> O <sub>5</sub> S
Droxidopa	Antiparkinsonian	23651-95-8	Y	C <sub>9</sub> H <sub>11</sub> NO <sub>5</sub>
Droxinavir	Antiviral	159910-86-8		C <sub>29</sub> H <sub>51</sub> N <sub>5</sub> O <sub>4</sub>
Droxypropine	Mydriatic	15599-26-5		C <sub>18</sub> H <sub>27</sub> NO <sub>3</sub>
Duazomycin	Antineoplastic	2508-89-6		C <sub>8</sub> H <sub>15</sub> N <sub>3</sub> O <sub>4</sub>
Dulofibrate	Antihyperlipidemic	61887-16-9		C <sub>16</sub> H <sub>14</sub> Cl <sub>2</sub> O <sub>3</sub>
Duloxetine	Antidepressant	116539-59-4	Y	C <sub>18</sub> H <sub>19</sub> NOS
Dulozafone	Anticonvulsant	75616-02-3		C <sub>20</sub> H <sub>22</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>4</sub>
Duometacin	Antiinflammatory	25771-23-7		C <sub>20</sub> H <sub>19</sub> NO <sub>5</sub>
Duoperone Fumarate	Nootropic	62030-88-0		C <sub>28</sub> H <sub>26</sub> F <sub>4</sub> N <sub>2</sub> O <sub>5</sub>
Dupracetam	Nootropic	59776-90-8		C <sub>12</sub> H <sub>18</sub> N <sub>4</sub> O <sub>4</sub>
Dyclonine	Anesthetic	586-60-7	Y	C <sub>18</sub> H <sub>27</sub> NO <sub>2</sub>
Dutasteride	Steroid	164656-23-9	Y	C <sub>27</sub> H <sub>30</sub> F <sub>6</sub> N <sub>2</sub> O <sub>2</sub>
Dydrogesterone	Progestogen	152-62-5	Y	C <sub>21</sub> H <sub>28</sub> O <sub>2</sub>
Dymanthine	Anthelminthic	124-28-7	Y	C <sub>20</sub> H <sub>43</sub> N
Dyphylline	Bronchodilator	479-18-5		C <sub>10</sub> H <sub>14</sub> N <sub>4</sub> O <sub>4</sub>
Ebalzotan	Antidepressant	149494-37-1	Y	C <sub>19</sub> H <sub>30</sub> N <sub>2</sub> O <sub>2</sub>
Ebastine	Antihistaminic	90729-43-4	Y	C <sub>32</sub> H <sub>39</sub> NO <sub>2</sub>
Eberconazole	Antifungal	128326-82-9		C <sub>18</sub> H <sub>14</sub> Cl <sub>2</sub> N <sub>2</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Ebiratide	Steroid	105250-86-0		C <sub>48</sub> H <sub>73</sub> N <sub>11</sub> O <sub>10</sub> S
Ebrotidine	Antiulcerative	100981-43-9	Y	C <sub>14</sub> H <sub>17</sub> BrN <sub>6</sub> O <sub>2</sub> S <sub>3</sub>
Ebselen	Nootropic	60940-34-3	Y	C <sub>13</sub> H <sub>9</sub> NOSe
Ecabapide	Antiulcerative	104775-36-2		C <sub>20</sub> H <sub>25</sub> N <sub>3</sub> O <sub>4</sub>
Ecabet	Antiulcerative	33159-27-2	Y	C <sub>20</sub> H <sub>28</sub> O <sub>5</sub> S
Ecadotril	Antihypotensive	112573-73-6		C <sub>21</sub> H <sub>23</sub> NO <sub>4</sub> S
Ecalcidene	Dermatologic	150337-94-3		C <sub>29</sub> H <sub>45</sub> NO <sub>3</sub>
Ecamsule	Dermatologic	92761-26-7		C <sub>28</sub> H <sub>34</sub> O <sub>8</sub> S <sub>2</sub>
Ecastolol	Antianginal	77695-52-4		C <sub>26</sub> H <sub>33</sub> N <sub>3</sub> O <sub>6</sub>
Ecenofloxacin	Antibiotic	162301-05-5		C <sub>19</sub> H <sub>21</sub> FN <sub>4</sub> O <sub>3</sub>
Echothiophate Iodide	Cholinergic	513-10-0		C <sub>9</sub> H <sub>23</sub> INO <sub>3</sub> PS
Ecipramidil	Antihypotensive	64552-16-5		C <sub>29</sub> H <sub>33</sub> NO <sub>5</sub>
Eclanamine Maleate	Antidepressant	67450-44-6		C <sub>16</sub> H <sub>22</sub> Cl <sub>2</sub> N <sub>2</sub> O
Eclazolast	Antihistaminic	80263-73-6		C <sub>12</sub> H <sub>12</sub> ClNO <sub>4</sub>
Ecomustine	Antineoplastic	98383-18-7		C <sub>10</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>6</sub>
Econazole	Antifungal	27220-47-9	Y	C <sub>18</sub> H <sub>15</sub> Cl <sub>3</sub> N <sub>2</sub> O
Ecopipam	Sedative	112108-01-7	Y	C <sub>19</sub> H <sub>20</sub> ClNO
Ecopladib	Analgesic	381683-92-7		C <sub>39</sub> H <sub>33</sub> Cl <sub>3</sub> N <sub>2</sub> O <sub>5</sub> S
Ecraprost	Anticoagulant	136892-64-3		C <sub>28</sub> H <sub>48</sub> O <sub>6</sub>
Ectylurea	Sedative	95-04-5		C <sub>7</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>
Edaglitazone	Antidiabetic	213411-83-7		C <sub>24</sub> H <sub>20</sub> N <sub>2</sub> O <sub>4</sub> S <sub>2</sub>
Edaravone	Nootropic	89-25-8		C <sub>10</sub> H <sub>10</sub> N <sub>2</sub> O
Edatrexate	Antineoplastic	80576-83-6		C <sub>22</sub> H <sub>25</sub> N <sub>7</sub> O <sub>5</sub>
Edelfosine	Antineoplastic	70641-51-9	Y	C <sub>27</sub> H <sub>58</sub> NO <sub>6</sub> P
Edetate	Antidote	60-00-4		C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O <sub>8</sub>
Edifolone Acetate	Antiarrhythmic	90733-40-7		C <sub>24</sub> H <sub>37</sub> NO <sub>4</sub>
Edogestrone	Progestogen	809-01-8		C <sub>26</sub> H <sub>38</sub> O <sub>5</sub>
Edonentan	Cardiotonic	210891-04-6		C <sub>28</sub> H <sub>32</sub> N <sub>4</sub> O <sub>5</sub> S
Edotecarin	Antineoplastic	174402-32-5		C <sub>29</sub> H <sub>28</sub> N <sub>4</sub> O <sub>11</sub>
Edoxudine	Antiviral	15176-29-1		C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> O <sub>5</sub>
Edronocaine	Analgesic	190258-12-9		C <sub>15</sub> H <sub>25</sub> NO <sub>2</sub>
Edrophonium	Cholinergic	312-48-1		C <sub>10</sub> H <sub>16</sub> NO+
Efaproxiral	Antihypotensive	131179-95-8		C <sub>20</sub> H <sub>23</sub> NO <sub>4</sub>
Efaroxan	Antihypertensive	89197-32-0	Y	C <sub>13</sub> H <sub>16</sub> N <sub>2</sub> O
Efavirenz	Antiviral	154598-52-4	Y	C <sub>14</sub> H <sub>9</sub> ClF <sub>3</sub> NO <sub>2</sub>
Efegatran Sulfate	Antithrombotic	105806-65-3		C <sub>21</sub> H <sub>32</sub> N <sub>6</sub> O <sub>3</sub>
Efepristin	Antibiotic	57206-54-9		C <sub>44</sub> H <sub>52</sub> N <sub>8</sub> O <sub>10</sub>
Efetzole	Antidepressant	90408-21-2		C <sub>12</sub> H <sub>14</sub> N <sub>2</sub>
Efipladib	Antihypotensive	381683-94-9		C <sub>40</sub> H <sub>35</sub> Cl <sub>3</sub> N <sub>2</sub> O <sub>4</sub> S
Efletirizine	Antihistaminic	150756-35-7		C <sub>21</sub> H <sub>24</sub> F <sub>2</sub> N <sub>2</sub> O <sub>3</sub>
Eflornithine	Antineoplastic	70052-12-9	Y	C <sub>6</sub> H <sub>12</sub> F <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Efloxate	Vasodilator	119-41-5		C <sub>19</sub> H <sub>16</sub> O <sub>5</sub>
Eflucimibe	Antihyperlipidemic	202340-45-2		C <sub>29</sub> H <sub>43</sub> NO <sub>2</sub> S
Eflumast	Antihistaminic	70977-46-7		C <sub>10</sub> H <sub>18</sub> FN <sub>3</sub> O <sub>3</sub>
Efonidipine	Antihypertensive	111011-63-3	Y	C <sub>34</sub> H <sub>38</sub> N <sub>3</sub> O <sub>7</sub> P
Eglumetad	Anxiolytic	176199-48-7		C <sub>8</sub> H <sub>11</sub> NO <sub>4</sub>
Egualen	Antiulcerative	99287-30-6	Y	C <sub>15</sub> H <sub>18</sub> O <sub>3</sub> S
Elacridar	Antineoplastic	143664-11-3		C <sub>34</sub> H <sub>33</sub> N <sub>3</sub> O <sub>5</sub>
Elantrine	Anticholelithogenic	1232-85-5		C <sub>20</sub> H <sub>24</sub> N <sub>2</sub>
Elanzepine	Anticonvulsant	6196-08-3		C <sub>19</sub> H <sub>21</sub> ClN <sub>2</sub>
Elarofiban	Anticoagulant	198958-88-2		C <sub>22</sub> H <sub>32</sub> N <sub>4</sub> O <sub>4</sub>
Elbanizine	Antihistaminic	110629-41-9		C <sub>26</sub> H <sub>31</sub> N <sub>5</sub> O <sub>2</sub>
Eldacimibe	Antihyperlipidemic	141993-70-6		C <sub>39</sub> H <sub>58</sub> N <sub>2</sub> O <sub>5</sub>
Eletriptan	Antimigraine	143322-58-1	Y	C <sub>22</sub> H <sub>26</sub> N <sub>2</sub> O <sub>2</sub> S
Elfazepam	Anxiolytic	52042-01-0		C <sub>19</sub> H <sub>18</sub> ClFN <sub>2</sub> O <sub>3</sub> S
Elgodipine	Antianginal	119413-55-7		C <sub>29</sub> H <sub>33</sub> FN <sub>2</sub> O <sub>6</sub>
Elinafide	Antineoplastic	162706-37-8		C <sub>31</sub> H <sub>28</sub> N <sub>4</sub> O <sub>4</sub>
Eliprodil	Antiparkinsonian	119431-25-3		C <sub>20</sub> H <sub>23</sub> ClFNO
Elisartan	Antihypertensive	149968-26-3		C <sub>27</sub> H <sub>29</sub> ClN <sub>6</sub> O <sub>5</sub>
Ellagic Acid	Hemostatic	476-66-4		C <sub>14</sub> H <sub>6</sub> O <sub>8</sub>
Elliptinium Acetate	Antineoplastic	58337-35-2		C <sub>20</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub>
Elmustine	Antineoplastic	60784-46-5		C <sub>5</sub> H <sub>10</sub> ClN <sub>3</sub> O <sub>3</sub>
Elnadipine	Antiparkinsonian	103946-15-2		C <sub>19</sub> H <sub>19</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>3</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Elomotecan	Antineoplastic	220998-10-7		C <sub>29</sub> H <sub>32</sub> ClN <sub>3</sub> O <sub>4</sub>
Elopirazole	Antipsychotic	115464-77-2		C <sub>23</sub> H <sub>22</sub> FN <sub>3</sub> O
Elsamitrucin	Antineoplastic	97068-30-9		C <sub>33</sub> H <sub>35</sub> NO <sub>13</sub>
Eltanolone	Anesthetic	128-20-1		C <sub>21</sub> H <sub>34</sub> O <sub>2</sub>
Eltenac	Antiinflammatory	72895-88-6		C <sub>12</sub> H <sub>9</sub> Cl <sub>2</sub> NO <sub>2</sub> S
Eltoprazine	Antipsychotic	98224-03-4	Y	C <sub>12</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>
Eltrombopag Olamine	Hematinic	496775-61-2	Y	C <sub>25</sub> H <sub>22</sub> N <sub>4</sub> O <sub>4</sub>
Elucaine	Anticholelithogenic	25314-87-8		C <sub>19</sub> H <sub>23</sub> NO <sub>2</sub>
Elvucitabine	Antiviral	181785-84-2		C <sub>9</sub> H <sub>10</sub> FN <sub>3</sub> O <sub>3</sub>
Elzasonan Citrate	Antidepressant	361343-19-3		C <sub>22</sub> H <sub>23</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>5</sub>
Elziverine	Antispasmodic	95520-81-3		C <sub>32</sub> H <sub>37</sub> N <sub>3</sub> O <sub>5</sub>
Emakalim	Antihypertensive	129729-66-4		C <sub>17</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>
Emapunil	Unclassified	226954-04-7		C <sub>23</sub> H <sub>23</sub> N <sub>5</sub> O <sub>2</sub>
Embeconazole	Antifungal	329744-44-7		C <sub>27</sub> H <sub>25</sub> F <sub>3</sub> N <sub>4</sub> O <sub>5</sub> S
Embramine	Antihistaminic	3565-72-8		C <sub>18</sub> H <sub>22</sub> BrNO
Embusartan	Antihypertensive	156001-18-2		C <sub>25</sub> H <sub>24</sub> FN <sub>3</sub> O <sub>3</sub>
Embutramide	Anesthetic	15687-14-6		C <sub>17</sub> H <sub>27</sub> NO <sub>3</sub>
Emedastine	Antihistaminic	87233-61-2	Y	C <sub>17</sub> H <sub>26</sub> N <sub>4</sub> O
Emetine	Antiamoebic	483-18-1		C <sub>29</sub> H <sub>40</sub> N <sub>2</sub> O <sub>4</sub>
Emideltide	Unclassified	62568-57-4		C <sub>35</sub> H <sub>48</sub> N <sub>10</sub> O <sub>15</sub>
Emiglitate	Antidiabetic	80879-63-6		C <sub>17</sub> H <sub>25</sub> NO <sub>7</sub>
Emilium Tosylate	Antiarrhythmic	30716-01-9		C <sub>19</sub> H <sub>27</sub> NO <sub>4</sub> S
Emitefur	Antineoplastic	110690-43-2		C <sub>28</sub> H <sub>19</sub> FN <sub>4</sub> O <sub>8</sub>
Emivirine	Antiviral	149950-60-7		C <sub>17</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub>
Emopamil	Vasodilator	78370-13-5		C <sub>23</sub> H <sub>30</sub> N <sub>2</sub>
Emorfazone	Antiinflammatory	38957-41-4		C <sub>11</sub> H <sub>17</sub> N <sub>3</sub> O <sub>3</sub>
Emylcamate	Anxiolytic	78-28-4		C <sub>7</sub> H <sub>15</sub> NO <sub>2</sub>
Enadoline	Analgesic	124378-77-4		C <sub>24</sub> H <sub>32</sub> N <sub>2</sub> O <sub>3</sub>
Enalapril	Antihypertensive	75847-73-3	Y	C <sub>20</sub> H <sub>28</sub> N <sub>2</sub> O <sub>5</sub>
Enalaprilat	Antihypertensive	76420-72-9		C <sub>18</sub> H <sub>24</sub> N <sub>2</sub> O <sub>5</sub>
Enalkiren	Antihypertensive	113082-98-7		C <sub>35</sub> H <sub>56</sub> N <sub>6</sub> O <sub>6</sub>
Enazadrem Phosphate	Dermatologic	107361-33-1		C <sub>18</sub> H <sub>25</sub> N <sub>3</sub> O
Enbucrilate	Dermatologic	6606-65-1		C <sub>8</sub> H <sub>11</sub> NO <sub>2</sub>
Encainide	Antiarrhythmic	66778-36-7		C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> O <sub>2</sub>
Enciprazine	Anxiolytic	68576-86-3		C <sub>23</sub> H <sub>32</sub> N <sub>2</sub> O <sub>6</sub>
Enclomiphene	Steroid	15690-57-0	Y	C <sub>26</sub> H <sub>28</sub> ClNO
Encyprate	Antidepressant	2521-01-9		C <sub>13</sub> H <sub>17</sub> NO <sub>2</sub>
Endixaprine	Antineoplastic	93181-85-2		C <sub>15</sub> H <sub>15</sub> Cl <sub>2</sub> N <sub>3</sub> O
Endobenzyl Bromide	Mydriatic	52080-56-5		C <sub>20</sub> H <sub>28</sub> NO <sub>3</sub> .Br
Endomide	Immunomodulator	4582-18-7		C <sub>17</sub> H <sub>28</sub> N <sub>2</sub> O <sub>2</sub>
Endralazine Mesylate	Antihypertensive	39715-02-1		C <sub>14</sub> H <sub>15</sub> N <sub>3</sub> O
Endrysone	Antiinflammatory	35100-44-8		C <sub>22</sub> H <sub>30</sub> O <sub>3</sub>
Enecadin	Nootropic	259525-01-4		C <sub>21</sub> H <sub>28</sub> FN <sub>3</sub> O
Enefexine	Antidepressant	67765-04-2		C <sub>13</sub> H <sub>19</sub> N
Enestebol	Androgen	2320-86-7		C <sub>20</sub> H <sub>28</sub> O <sub>3</sub>
Enfenamic Acid	Antiinflammatory	23049-93-6		C <sub>15</sub> H <sub>15</sub> NO <sub>2</sub>
Enflurane	Anesthetic	13838-16-9		C <sub>3</sub> H <sub>2</sub> ClF <sub>5</sub> O
Englitzone Sodium	Antidiabetic	109229-58-5		C <sub>20</sub> H <sub>19</sub> NO <sub>3</sub> S
Eniclobrate	Antihyperlipidemic	81126-88-7		C <sub>24</sub> H <sub>24</sub> ClNO <sub>3</sub>
Enilconazole	Antifungal	35554-44-0		C <sub>14</sub> H <sub>14</sub> Cl <sub>2</sub> N <sub>2</sub> O
Enilospirone	Anxiolytic	59798-73-1		C <sub>15</sub> H <sub>18</sub> ClNO <sub>3</sub>
Eniluracil	Antineoplastic	59989-18-3	Y	C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>
Eniporide	Cardiotonic	176644-21-6		C <sub>14</sub> H <sub>16</sub> N <sub>4</sub> O <sub>3</sub> S
Enisoprost	Anticlerative	81026-63-3		C <sub>22</sub> H <sub>36</sub> O <sub>5</sub>
Enocitabine	Antineoplastic	55726-47-1		C <sub>31</sub> H <sub>55</sub> N <sub>3</sub> O <sub>6</sub>
Enofelast	Bronchodilator	125722-16-9		C <sub>16</sub> H <sub>15</sub> FO
Enolicam Sodium	Antiinflammatory	59755-82-7		C <sub>17</sub> H <sub>12</sub> Cl <sub>3</sub> NO <sub>4</sub> S
Enoxacin	Antibiotic	74011-58-8	Y	C <sub>15</sub> H <sub>17</sub> FN <sub>4</sub> O <sub>3</sub>
Enoxamast	Antibacterial	74604-76-5		C <sub>13</sub> H <sub>10</sub> N <sub>2</sub> O <sub>5</sub> S
Enoximone	Cardiotonic	77671-31-9		C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> S
Enoxolone	Antiinflammatory	471-53-4		C <sub>30</sub> H <sub>46</sub> O <sub>4</sub>
Enpiprazole	Anxiolytic	31729-24-5		C <sub>16</sub> H <sub>21</sub> ClN <sub>4</sub>
Enpiroline Phosphate	Antimalarial	66364-73-6		C <sub>19</sub> H <sub>18</sub> F <sub>6</sub> N <sub>2</sub> O

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Enprazepine	Anticonvulsant	47206-15-5		C <sub>20</sub> H <sub>24</sub> N <sub>2</sub>
Enprofylline	Bronchodilator	41078-02-8		C <sub>8</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub>
Enpromate	Antineoplastic	10087-89-5		C <sub>22</sub> H <sub>23</sub> NO <sub>2</sub>
Enprostil	Antiulcerative	73121-56-9		C <sub>23</sub> H <sub>26</sub> O <sub>6</sub>
Enrasentan	Anesthetic	167256-08-8		C <sub>29</sub> H <sub>30</sub> O <sub>8</sub>
Enrofloxacin	Antibiotic	93106-60-6		C <sub>19</sub> H <sub>22</sub> FN <sub>3</sub> O <sub>3</sub>
Ensaculin	Nootropic	155773-59-4		C <sub>26</sub> H <sub>32</sub> N <sub>2</sub> O <sub>5</sub>
Ensulizole	Dermatologic	27503-81-7		C <sub>13</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> S
Entacapone	Antiparkinsonian	130929-57-6	Y	C <sub>14</sub> H <sub>15</sub> N <sub>3</sub> O <sub>5</sub>
Entecavir	Antiviral	142217-69-4	Y	C <sub>12</sub> H <sub>15</sub> N <sub>5</sub> O <sub>3</sub>
Enviomycin	Antibiotic	33103-22-9		C <sub>25</sub> H <sub>43</sub> N <sub>13</sub> O <sub>10</sub>
Enviradene	Antiviral	80883-55-2		C <sub>19</sub> H <sub>21</sub> N <sub>3</sub> O <sub>2</sub> S
Enviroxime	Antiviral	72301-79-2		C <sub>17</sub> H <sub>18</sub> N <sub>4</sub> O <sub>3</sub> S
Enzacamene	Dermatologic	36861-47-9		C <sub>18</sub> H <sub>22</sub> O
Enzastaurin	Antineoplastic	170364-57-5	Y	C <sub>32</sub> H <sub>29</sub> N <sub>5</sub> O <sub>2</sub>
Epalrestat	Antidiabetic	82159-09-9	Y	C <sub>15</sub> H <sub>13</sub> NO <sub>3</sub> S <sub>2</sub>
Epanolol	Antianginal	86880-51-5		C <sub>20</sub> H <sub>23</sub> N <sub>3</sub> O <sub>4</sub>
Eperezolid	Antibacterial	165800-04-4		C <sub>18</sub> H <sub>23</sub> FN <sub>4</sub> O <sub>5</sub>
Eperisone	Muscle Relaxant	64840-90-0		C <sub>17</sub> H <sub>25</sub> NO
Epervudine	Antiviral	60136-25-6		C <sub>12</sub> H <sub>18</sub> N <sub>2</sub> O <sub>5</sub>
Ephedrine	Bronchodilator	299-42-3	Y	C <sub>10</sub> H <sub>15</sub> NO
Ephedrine Camphorate	Antihypotensive	124-83-4		C <sub>10</sub> H <sub>16</sub> O <sub>4</sub>
Epicainide	Antiarrhythmic	66304-03-8		C <sub>21</sub> H <sub>26</sub> N <sub>2</sub> O <sub>2</sub>
Epicillin	Antibiotic	26774-90-3		C <sub>16</sub> H <sub>21</sub> N <sub>3</sub> O <sub>4</sub> S
Epicriptine	Pituitary	88660-47-3		C <sub>32</sub> H <sub>43</sub> N <sub>5</sub> O <sub>5</sub>
Epiestriol	Steroid	547-81-9		C <sub>18</sub> H <sub>24</sub> O <sub>3</sub>
Epimestrol	Pituitary	7004-98-0		C <sub>19</sub> H <sub>26</sub> O <sub>3</sub>
Epinastine	Antihistaminic	80012-43-7	Y	C <sub>16</sub> H <sub>15</sub> N <sub>3</sub>
Epinephrine	Bronchodilator	51-43-4		C <sub>9</sub> H <sub>13</sub> NO <sub>3</sub>
Epinephryl Borate	Adrenergic	5579-16-8		C <sub>9</sub> H <sub>12</sub> BNO <sub>4</sub>
Epipropidine	Antineoplastic	5696-17-3		C <sub>16</sub> H <sub>28</sub> N <sub>2</sub> O <sub>2</sub>
Epirizole	Analgesic	18694-40-1		C <sub>11</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub>
Epiroprim	Antibiotic	73090-70-7		C <sub>19</sub> H <sub>23</sub> N <sub>5</sub> O <sub>2</sub>
Epirubicin	Antineoplastic	56420-45-2		C <sub>27</sub> H <sub>29</sub> NO <sub>11</sub>
Epitetracycline	Antibacterial	79-85-6		C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>8</sub>
Epithiazide	Antihypertensive	1764-85-8		C <sub>10</sub> H <sub>11</sub> ClF <sub>3</sub> N <sub>3</sub> O <sub>4</sub> S <sub>3</sub>
Epitiostanol	Antineoplastic	2363-58-8		C <sub>19</sub> H <sub>30</sub> OS
Eplerenone	Antihypertensive	107724-20-9	Y	C <sub>24</sub> H <sub>30</sub> O <sub>6</sub>
Eplivanserin	Anxiolytic	130579-75-8		C <sub>19</sub> H <sub>21</sub> FN <sub>2</sub> O <sub>2</sub>
Epoprostenol	Antithrombotic	35121-78-9		C <sub>20</sub> H <sub>32</sub> O <sub>5</sub>
Epostane	Oxytocic	80471-63-2		C <sub>22</sub> H <sub>31</sub> NO <sub>3</sub>
Eprazinone	Antitussive	10402-90-1		C <sub>24</sub> H <sub>32</sub> N <sub>2</sub> O <sub>2</sub>
Epristeride	Steroid	119169-78-7		C <sub>25</sub> H <sub>37</sub> NO <sub>3</sub>
Eprobemide	Antiparkinsonian	87940-60-1		C <sub>14</sub> H <sub>19</sub> ClN <sub>2</sub> O <sub>2</sub>
Eprodissate Disodium	Nootropic	21668-77-9	Y	C <sub>3</sub> H <sub>8</sub> O <sub>6</sub> S <sub>2</sub>
Eprosartan	Antihypertensive	133040-01-4	Y	C <sub>23</sub> H <sub>24</sub> N <sub>2</sub> O <sub>4</sub> S
Eprovafen	Antidepressant	101335-99-3		C <sub>18</sub> H <sub>22</sub> O <sub>2</sub> S
Eproxindine	Antiarrhythmic	85793-29-9		C <sub>23</sub> H <sub>29</sub> N <sub>3</sub> O <sub>3</sub>
Eprozinol	Bronchodilator	32665-36-4		C <sub>22</sub> H <sub>30</sub> N <sub>2</sub> O <sub>2</sub>
Epsiprantel	Anthelmintic	98123-83-2		C <sub>20</sub> H <sub>26</sub> N <sub>2</sub> O <sub>2</sub>
Eptaloprost	Prostaglandin	90693-76-8		C <sub>24</sub> H <sub>34</sub> O <sub>5</sub>
Eptapirone	Anxiolytic	179756-58-2		C <sub>16</sub> H <sub>23</sub> N <sub>7</sub> O <sub>2</sub>
Eptastigmine	Cholinergic	101246-68-8		C <sub>21</sub> H <sub>33</sub> N <sub>3</sub> O <sub>2</sub>
Eptazocine	Analgesic	72522-13-5		C <sub>15</sub> H <sub>21</sub> NO
Eptifibatide	Antithrombotic	188627-80-7		C <sub>35</sub> H <sub>49</sub> N <sub>11</sub> O <sub>5</sub> S <sub>2</sub>
Equilin	Estrogen	474-86-2		C <sub>18</sub> H <sub>20</sub> O <sub>2</sub>
Erbulozole	Antineoplastic	124784-31-2		C <sub>24</sub> H <sub>27</sub> N <sub>3</sub> O <sub>5</sub> S
Erdosteine	Mucolytic	84611-23-4	Y	C <sub>8</sub> H <sub>11</sub> NO <sub>4</sub> S <sub>2</sub>
Ergonovine	Antihypertensive	60-79-7	Y	C <sub>19</sub> H <sub>23</sub> N <sub>3</sub> O <sub>2</sub>
Ergotamine	Analgesic	113-15-5		C <sub>33</sub> H <sub>35</sub> N <sub>5</sub> O <sub>5</sub>
Eriocolol	Antihypertensive	85320-67-8		C <sub>18</sub> H <sub>24</sub> ClNO <sub>3</sub>
Erizepine	Anticonvulsant	96645-87-3		C <sub>20</sub> H <sub>22</sub> N <sub>2</sub>
Erlotinib	Antineoplastic	183321-74-6	Y	C <sub>22</sub> H <sub>23</sub> N <sub>3</sub> O <sub>4</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Erocainide	Antiarrhythmic	85750-38-5		C <sub>22</sub> H <sub>33</sub> ClN <sub>2</sub> O
Ersentilide	Antiarrhythmic	125279-79-0		C <sub>21</sub> H <sub>26</sub> N <sub>4</sub> O <sub>5</sub> S
Ertapenem	Antibacterial	153832-46-3		C <sub>22</sub> H <sub>25</sub> N <sub>3</sub> O <sub>7</sub> S
Ertiprotafib	Antidiabetic	251303-04-5		C <sub>31</sub> H <sub>27</sub> BrO <sub>3</sub> S
Erythrityl Tetranitrate	Vasodilator	7297-25-8		C <sub>4</sub> H <sub>6</sub> N <sub>4</sub> O <sub>12</sub>
Erythromycin	Antibiotic	114-07-8	Y	C <sub>37</sub> H <sub>67</sub> NO <sub>13</sub>
Erythromycin Acistrate	Antibiotic	992-69-8		C <sub>39</sub> H <sub>69</sub> NO <sub>14</sub>
Erythromycin Ethylsuccinate	Antibiotic	1264-62-6	Y	C <sub>43</sub> H <sub>75</sub> NO <sub>16</sub>
Erythromycin Propionate	Antibiotic	134-36-1		C <sub>40</sub> H <sub>71</sub> NO <sub>14</sub>
Erythromycin Salnacedin	Antibiotic	87573-04-4		C <sub>12</sub> H <sub>13</sub> NO <sub>5</sub> S
Esafloxacin	Antibiotic	129672-09-9		C <sub>15</sub> H <sub>17</sub> FN <sub>4</sub> O <sub>3</sub>
Esaprazole	Antiulcerative	64204-55-3		C <sub>12</sub> H <sub>23</sub> N <sub>3</sub> O
Esatenolol	Adrenergic	93379-54-5		C <sub>14</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub>
Escitalopram Oxalate	Antidepressant	128196-01-0	Y	C <sub>20</sub> H <sub>21</sub> FN <sub>2</sub> O
Esculamine	Antiinflammatory	2908-75-0		C <sub>15</sub> H <sub>19</sub> NO <sub>6</sub>
Esculin	Dermatologic	531-75-9		C <sub>15</sub> H <sub>16</sub> O <sub>9</sub>
Eseridine	Cholinergic	25573-43-7		C <sub>15</sub> H <sub>21</sub> N <sub>3</sub> O <sub>3</sub>
Esflurbiprofen	Antiinflammatory	51543-39-6		C <sub>15</sub> H <sub>13</sub> FO <sub>2</sub>
Esketamine	Sedative	33643-46-8		C <sub>13</sub> H <sub>16</sub> ClNO
Eslicarbazepine	Antipsychotic	104746-04-5	Y	C <sub>15</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Esmirtazapine	Antidepressant	61337-87-9		C <sub>17</sub> H <sub>19</sub> N <sub>3</sub>
Esmolol	Antiarrhythmic	81147-92-4		C <sub>16</sub> H <sub>25</sub> NO <sub>4</sub>
Esomeprazole	Antiulcerative	119141-88-7	Y	C <sub>17</sub> H <sub>19</sub> N <sub>3</sub> O <sub>3</sub> S
Esonarimod	Antiarrhythmic	101973-77-7		C <sub>14</sub> H <sub>16</sub> O <sub>4</sub> S
Esorubicin	Antineoplastic	63521-85-7		C <sub>27</sub> H <sub>29</sub> NO <sub>10</sub>
Esoxybutynin Chloride	Antispasmodic	119618-22-3		C <sub>22</sub> H <sub>31</sub> NO <sub>3</sub>
Espatropate	Bronchodilator	132829-83-5		C <sub>19</sub> H <sub>23</sub> N <sub>3</sub> O <sub>3</sub>
Esproquin	Adrenergic	37517-33-2		C <sub>14</sub> H <sub>21</sub> NOS
Estazolam	Sedative	29975-16-4	Y	C <sub>16</sub> H <sub>11</sub> ClN <sub>4</sub>
Estradiol	Estrogen	50-28-2	Y	C <sub>18</sub> H <sub>24</sub> O <sub>2</sub>
Estradiol 17 Propionate	Estrogen	3758-34-7	Y	C <sub>21</sub> H <sub>28</sub> O <sub>3</sub>
Estradiol Acetate	Estrogen	4245-41-4		C <sub>20</sub> H <sub>26</sub> O <sub>3</sub>
Estradiol Benzoate	Estrogen	50-50-0		C <sub>25</sub> H <sub>28</sub> O <sub>3</sub>
Estradiol Cypionate	Estrogen	313-06-4		C <sub>26</sub> H <sub>36</sub> O <sub>3</sub>
Estradiol Dipropionate	Estrogen	113-38-2		C <sub>24</sub> H <sub>32</sub> O <sub>4</sub>
Estradiol Enanthate	Estrogen	4956-37-0		C <sub>25</sub> H <sub>36</sub> O <sub>3</sub>
Estradiol Undecylate	Estrogen	3571-53-7		C <sub>29</sub> H <sub>44</sub> O <sub>3</sub>
Estradiol Valerate	Estrogen	979-32-8	Y	C <sub>23</sub> H <sub>32</sub> O <sub>3</sub>
Estramustine	Antineoplastic	2998-57-4	Y	C <sub>23</sub> H <sub>31</sub> Cl <sub>2</sub> NO <sub>3</sub>
Estramustine Phosphate	Antineoplastic	4891-15-0		C <sub>23</sub> H <sub>32</sub> Cl <sub>2</sub> NO <sub>6</sub> P
Estrapronicate	Estrogen	4140-20-9		C <sub>27</sub> H <sub>31</sub> NO <sub>4</sub>
Estrazolinol Hydrobromide	Estrogen	5941-36-6		C <sub>20</sub> H <sub>25</sub> NO <sub>2</sub>
Estriol	Estrogen	50-27-1	Y	C <sub>18</sub> H <sub>24</sub> O <sub>3</sub>
Estrofurate	Estrogen	10322-73-3		C <sub>24</sub> H <sub>26</sub> O <sub>4</sub>
Estrone	Estrogen	53-16-7		C <sub>18</sub> H <sub>22</sub> O <sub>2</sub>
Estrone Sodium Sulfate	Estrogen	481-97-0	Y	C <sub>18</sub> H <sub>22</sub> O <sub>5</sub> S
Esuprone	Anticonvulsant	91406-11-0		C <sub>13</sub> H <sub>14</sub> O <sub>5</sub> S
Eszopiclone	Anxiolytic	138729-47-2	Y	C <sub>17</sub> H <sub>17</sub> ClN <sub>6</sub> O <sub>3</sub>
Etabenzarone	Capillary Protectant	15686-63-2		C <sub>23</sub> H <sub>27</sub> NO <sub>3</sub>
Etacepride	Antiprotozoal	68788-56-7		C <sub>17</sub> H <sub>24</sub> N <sub>2</sub> O <sub>3</sub>
Etafedrine	Adrenergic	7681-79-0		C <sub>12</sub> H <sub>19</sub> NO
Etafenone	Vasodilator	90-54-0		C <sub>21</sub> H <sub>27</sub> NO <sub>2</sub>
Etalocib	Antineoplastic	161172-51-6		C <sub>33</sub> H <sub>33</sub> FO <sub>6</sub>
Etaminile	Antitussive	15599-27-6		C <sub>15</sub> H <sub>22</sub> N <sub>2</sub>
Etamiphyllin	Bronchodilator	314-35-2		C <sub>13</sub> H <sub>21</sub> N <sub>5</sub> O <sub>2</sub>
Etanidazole	Antineoplastic	22668-01-5		C <sub>7</sub> H <sub>10</sub> N <sub>4</sub> O <sub>4</sub>
Etanterol	Bronchodilator	93047-39-3		C <sub>18</sub> H <sub>24</sub> N <sub>2</sub> O <sub>3</sub>
Etaqualone	Sedative	7432-25-9		C <sub>17</sub> H <sub>16</sub> N <sub>2</sub> O
Etarotene	Dermatologic	87719-32-2		C <sub>25</sub> H <sub>32</sub> O <sub>2</sub> S
Etasuline	Antiarrhythmic	16781-39-8		C <sub>16</sub> H <sub>15</sub> ClN <sub>2</sub> S
Etazepine	Anticonvulsant	88124-27-0		C <sub>17</sub> H <sub>17</sub> NO <sub>2</sub>
Etazolate	Antipsychotic	51022-77-6	Y	C <sub>14</sub> H <sub>19</sub> N <sub>5</sub> O <sub>2</sub>
Etebenecid	Uricosuric	1213-06-5		C <sub>11</sub> H <sub>15</sub> NO <sub>4</sub> S

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Eterobarb	Anticonvulsant	27511-99-5		C <sub>16</sub> H <sub>20</sub> N <sub>2</sub> O <sub>5</sub>
Etersalate	Analgesic	62992-61-4		C <sub>19</sub> H <sub>19</sub> NO <sub>6</sub>
Ethacrynic Acid	Diuretic	58-54-8	Y	C <sub>13</sub> H <sub>12</sub> Cl <sub>2</sub> O <sub>4</sub>
Ethambutol	Antibacterial	74-55-5	Y	C <sub>10</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub>
Ethamivan	Nootropic	304-84-7		C <sub>12</sub> H <sub>17</sub> NO <sub>3</sub>
1,2-Ethanedisulfonic Acid	Sedative	110-04-3	Y	C <sub>2</sub> H <sub>6</sub> O <sub>6</sub> S <sub>2</sub>
Ethanolamine Hydrofluoride	Dermatologic	111-42-2		C <sub>4</sub> H <sub>11</sub> NO <sub>2</sub>
Ethaverine	Antispasmodic	486-47-5		C <sub>24</sub> H <sub>29</sub> NO <sub>4</sub>
Ethchlorvynol	Sedative	113-18-8	Y	C <sub>7</sub> H <sub>9</sub> ClO
Ethenzamide	Analgesic	938-73-8		C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>
Ether	Anesthetic	60-29-7		C <sub>4</sub> H <sub>10</sub> O
Ethiazide	Diuretic	1824-58-4	Y	C <sub>9</sub> H <sub>12</sub> ClN <sub>3</sub> O <sub>4</sub> S <sub>2</sub>
Ethinamate	Sedative	126-52-3	Y	C <sub>9</sub> H <sub>13</sub> NO <sub>2</sub>
Ethinyl Estradiol	Estrogen	57-63-6	Y	C <sub>20</sub> H <sub>24</sub> O <sub>2</sub>
Ethionamide	Antibacterial	536-33-4	Y	C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> S
Ethisterone	Progestogen	434-03-7		C <sub>21</sub> H <sub>28</sub> O <sub>2</sub>
Ethoheptazine Citrate	Analgesic	77-15-6		C <sub>16</sub> H <sub>23</sub> NO <sub>2</sub>
Ethomoxane	Sedative	3570-46-5		C <sub>15</sub> H <sub>23</sub> NO <sub>3</sub>
Ethonam Nitrate	Antifungal	15037-44-2		C <sub>16</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>
Ethopabate	Antibacterial	59-06-3		C <sub>12</sub> H <sub>15</sub> NO <sub>4</sub>
Ethopropazine	Antiparkinsonian	522-00-9		C <sub>19</sub> H <sub>25</sub> ClN <sub>2</sub> S
Ethosuximide	Anticonvulsant	77-67-8	Y	C <sub>7</sub> H <sub>11</sub> NO <sub>2</sub>
Ethotoin	Anticonvulsant	86-35-1	Y	C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>
Ethoxazene	Analgesic	94-10-0		C <sub>14</sub> H <sub>16</sub> N <sub>4</sub> O
Ethoxazurutoside	Cardiotonic	30851-76-4		C <sub>33</sub> H <sub>41</sub> NO <sub>17</sub>
Ethoxzolamide	Diuretic	452-35-7	Y	C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> S <sub>2</sub>
Ethybenztropine	Antibacterial	524-83-4		C <sub>22</sub> H <sub>27</sub> NO
Ethyl Biscoumacetate	Anticoagulant	548-00-5		C <sub>22</sub> H <sub>16</sub> O <sub>8</sub>
Ethyl Carfluzepate	Anxiolytic	65400-85-3		C <sub>20</sub> H <sub>17</sub> ClFN <sub>3</sub> O <sub>4</sub>
Ethyl Chloride	Anesthetic	75-00-3		C <sub>2</sub> H <sub>5</sub> Cl
Ethyl Dibunate	Antitussive	5560-69-0		C <sub>20</sub> H <sub>28</sub> O <sub>3</sub> S
Ethyl Dirazepate	Anxiolytic	23980-14-5		C <sub>18</sub> H <sub>14</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>3</sub>
Ethyl Linoleate	Prostaglandin	544-35-4		C <sub>20</sub> H <sub>36</sub> O <sub>2</sub>
Ethyl Loflazepate	Anxiolytic	29177-84-2	Y	C <sub>18</sub> H <sub>14</sub> ClFN <sub>3</sub> O <sub>3</sub>
Ethyl Nitrite [Spirit]	Antihypertensive	109-95-5		C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub>
Ethyl Pyrophosphate	Unclassified	20680-55-1		C <sub>6</sub> H <sub>16</sub> O <sub>7</sub> P <sub>2</sub>
Ethyl Vinyl Ether	Anesthetic	109-92-2		C <sub>4</sub> H <sub>8</sub> O
Ethylamine Oleate	Dermatologic	112-80-1		C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>
Ethylamine	Dermatologic	75-04-7		C <sub>2</sub> H <sub>7</sub> N
Ethylenediamine	Urologic	107-15-3	Y	C <sub>2</sub> H <sub>8</sub> N <sub>2</sub>
Ethylestrenol	Steroid	965-90-2		C <sub>20</sub> H <sub>32</sub> O
Ethylmethylthiambutene	Analgesic	441-61-2		C <sub>15</sub> H <sub>19</sub> NS <sub>2</sub>
Ethylmorphine Methiodide	Analgesic	6696-59-9		C <sub>20</sub> H <sub>26</sub> INO <sub>3</sub>
Ethylnorepinephrine	Bronchodilator	536-24-3		C <sub>10</sub> H <sub>15</sub> NO <sub>3</sub>
Ethylstibamine	Antiprotozoal	554-76-7		C <sub>6</sub> H <sub>8</sub> NO <sub>3</sub> Sb
Ethynerone	Progestogen	3124-93-4		C <sub>20</sub> H <sub>23</sub> ClO <sub>2</sub>
Ethynodiol Diacetate	Anesthetic	297-76-7		C <sub>24</sub> H <sub>32</sub> O <sub>4</sub>
Ethypicone	Unclassified	467-90-3		C <sub>10</sub> H <sub>15</sub> NO <sub>2</sub>
Etibendazole	Anthelmintic	64420-40-2		C <sub>18</sub> H <sub>16</sub> FN <sub>3</sub> O <sub>4</sub>
Eticlopride	Gastroprokinetic	84226-12-0		C <sub>17</sub> H <sub>25</sub> ClN <sub>2</sub> O <sub>3</sub>
Eticyclidine	Antiparkinsonian	2201-15-2		C <sub>14</sub> H <sub>21</sub> N
Etidocaine	Anesthetic	36637-18-0		C <sub>17</sub> H <sub>28</sub> N <sub>2</sub> O
Etidronate	Bone Resorption Inhibitor	2809-21-4	Y	C <sub>2</sub> H <sub>8</sub> O <sub>7</sub> P <sub>2</sub>
Etifelmine	Antihypertensive	341-00-4	Y	C <sub>17</sub> H <sub>19</sub> N
Etifoxine	Anxiolytic	21715-46-8		C <sub>17</sub> H <sub>17</sub> ClN <sub>2</sub> O
Etilamfetamine	Anorexic	457-87-4		C <sub>11</sub> H <sub>17</sub> N
Etilefrine	Antihypotensive	709-55-7		C <sub>10</sub> H <sub>15</sub> NO <sub>2</sub>
Etilefrine Pivalate	Mydriatic	100696-30-8		C <sub>15</sub> H <sub>23</sub> NO <sub>3</sub>
Etilevodopa	Antiparkinsonian	37178-37-3		C <sub>11</sub> H <sub>15</sub> NO <sub>4</sub>
Etintidine	Antihistaminic	69539-53-3		C <sub>12</sub> H <sub>16</sub> N <sub>6</sub> S
Etipirium Iodide	Unclassified	3478-15-7		C <sub>21</sub> H <sub>26</sub> INO <sub>3</sub>
Etiprednol Dicoacetate	Antiinflammatory	199331-40-3		C <sub>24</sub> H <sub>30</sub> Cl <sub>2</sub> O <sub>6</sub>
Etiproston	Prostaglandin	59619-81-7		C <sub>24</sub> H <sub>32</sub> O <sub>7</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Etiracetam	Anticonvulsant	33996-58-6		C <sub>8</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Etiroxate	Nootropic	17365-01-4		C <sub>18</sub> H <sub>17</sub> I <sub>4</sub> NO <sub>4</sub>
Etisazole	Antifungal	7716-60-1		C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> S
Etisomicin	Antibiotic	70639-48-4		C <sub>20</sub> H <sub>39</sub> N <sub>5</sub> O <sub>7</sub>
Etisulergine	Antimigraine	64795-23-9		C <sub>19</sub> H <sub>28</sub> N <sub>4</sub> O <sub>2</sub> S
Etizolam	Anxiolytic	40054-69-1	Y	C <sub>17</sub> H <sub>15</sub> ClN <sub>4</sub> S
Etocarlide	Antibiotic	1234-30-6		C <sub>17</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub> S
Etocrylene	Dermatologic	5232-99-5		C <sub>18</sub> H <sub>15</sub> NO <sub>2</sub>
Etodolac	Antiinflammatory	41340-25-4	Y	C <sub>17</sub> H <sub>21</sub> NO <sub>3</sub>
Etodroxizine	Sedative	17692-34-1		C <sub>23</sub> H <sub>31</sub> ClN <sub>2</sub> O <sub>3</sub>
Etofamide	Antineoplastic	25287-60-9		C <sub>19</sub> H <sub>20</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>5</sub>
Etofenamate	Analgesic	30544-47-9		C <sub>18</sub> H <sub>18</sub> F <sub>3</sub> NO <sub>4</sub>
Etofenprox	Antiinflammatory	80844-07-1		C <sub>25</sub> H <sub>28</sub> O <sub>3</sub>
Etofibrate	Antihyperlipidemic	31637-97-5	Y	C <sub>18</sub> H <sub>18</sub> ClNO <sub>5</sub>
Etoformin	Antidiabetic	45086-03-1		C <sub>8</sub> H <sub>19</sub> N <sub>5</sub>
Etofuradine	Antianginal	17692-35-2		C <sub>18</sub> H <sub>21</sub> N <sub>3</sub> O
Etofylline	Bronchodilator	519-37-9		C <sub>9</sub> H <sub>12</sub> N <sub>4</sub> O <sub>3</sub>
Etoglucid	Antineoplastic	1954-28-5		C <sub>12</sub> H <sub>22</sub> O <sub>6</sub>
Etolorex	Anorexic	54063-36-4		C <sub>12</sub> H <sub>18</sub> ClNO
Etolotifen	Antihistaminic	82140-22-5		C <sub>24</sub> H <sub>29</sub> N <sub>4</sub> O <sub>5</sub>
Etoloxamine	Antihistaminic	1157-87-5		C <sub>19</sub> H <sub>25</sub> NO
Etomidate	Sedative	33125-97-2		C <sub>14</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>
Etomidoline	Antispasmodic	21590-92-1		C <sub>23</sub> H <sub>29</sub> N <sub>5</sub> O <sub>2</sub>
Etomoxir	Cardiotonic	124083-20-1		C <sub>17</sub> H <sub>23</sub> ClO <sub>4</sub>
Etonitazene	Analgesic	911-65-9		C <sub>22</sub> H <sub>28</sub> N <sub>4</sub> O <sub>3</sub>
Etonogestrel	Prostaglandin	54048-10-1		C <sub>22</sub> H <sub>28</sub> O <sub>2</sub>
Etoperidone	Antidepressant	52942-31-1		C <sub>19</sub> H <sub>28</sub> ClN <sub>5</sub> O
Etoposide	Antineoplastic	33419-42-0		C <sub>29</sub> H <sub>32</sub> O <sub>13</sub>
Etoposide Phosphate	Antineoplastic	117091-64-2		C <sub>29</sub> H <sub>33</sub> O <sub>16</sub> P
Etoprindole	Nootropic	54063-37-5		C <sub>15</sub> H <sub>21</sub> N <sub>3</sub> O
Etoprine	Antineoplastic	18588-57-3		C <sub>12</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>4</sub>
Etoricoxib	Antiinflammatory	202409-33-4	Y	C <sub>18</sub> H <sub>15</sub> ClN <sub>2</sub> O <sub>2</sub> S
Etorphine	Analgesic	14521-96-1		C <sub>25</sub> H <sub>33</sub> NO <sub>4</sub>
Etosalamide	Antifungal	15302-15-5		C <sub>11</sub> H <sub>15</sub> NO <sub>3</sub>
Etoxadrol	Anesthetic	28189-85-7		C <sub>16</sub> H <sub>23</sub> NO <sub>2</sub>
Etoxidrine	Analgesic	469-82-9		C <sub>18</sub> H <sub>27</sub> NO <sub>4</sub>
Etozolin	Diuretic	73-09-6	Y	C <sub>13</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> S
Etrabamine	Antidepressant	70590-58-8		C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> S
Etravirine	Antiviral	269055-15-4	Y	C <sub>20</sub> H <sub>15</sub> BrN <sub>6</sub> O
Etretinate	Dermatologic	54350-48-0		C <sub>23</sub> H <sub>30</sub> O <sub>3</sub>
Etriguat	Vasodilator	402595-29-3		C <sub>22</sub> H <sub>16</sub> FN <sub>7</sub>
Etryptamine Acetate	Nootropic	2235-90-7		C <sub>12</sub> H <sub>16</sub> N <sub>2</sub>
Etymemazine	Antihistaminic	523-54-6		C <sub>20</sub> H <sub>26</sub> N <sub>2</sub> S
Eucaïne	Analgesic	500-34-5		C <sub>15</sub> H <sub>21</sub> NO <sub>2</sub>
Eucatropine	Mydriatic	100-91-4		C <sub>17</sub> H <sub>25</sub> NO <sub>3</sub>
Eugenol	Analgesic	97-53-0		C <sub>10</sub> H <sub>12</sub> O <sub>2</sub>
Euprocín	Anesthetic	1301-42-4		C <sub>24</sub> H <sub>34</sub> N <sub>2</sub> O <sub>2</sub>
Evandamine	Antineoplastic	100035-75-4		C <sub>11</sub> H <sub>16</sub> N <sub>4</sub> S
Everolimus	Immunosuppressant	159351-69-6	Y	C <sub>53</sub> H <sub>83</sub> NO <sub>14</sub>
Exalamide	Antifungal	53370-90-4		C <sub>13</sub> H <sub>19</sub> NO <sub>2</sub>
Examorelin	Cardiotonic	140703-51-1		C <sub>47</sub> H <sub>58</sub> N <sub>12</sub> O <sub>6</sub>
Exaprolol	Adrenergic	55837-19-9		C <sub>18</sub> H <sub>29</sub> NO <sub>2</sub>
Exatecan	Antineoplastic	171335-80-1		C <sub>24</sub> H <sub>22</sub> FN <sub>3</sub> O <sub>4</sub>
Exemestane	Antineoplastic	107868-30-4	Y	C <sub>20</sub> H <sub>24</sub> O <sub>2</sub>
Exepanol	Antianginal	77416-65-0		C <sub>11</sub> H <sub>15</sub> NO <sub>2</sub>
Exifone	Nootropic	52479-85-3		C <sub>13</sub> H <sub>10</sub> O <sub>7</sub>
Exiproben	Choleretic	26281-69-6		C <sub>16</sub> H <sub>24</sub> O <sub>5</sub>
Exisulind	Antineoplastic	59973-80-7		C <sub>20</sub> H <sub>17</sub> FO <sub>4</sub> S
Ezetimibe	Antihyperlipidemic	163222-33-1	Y	C <sub>24</sub> H <sub>21</sub> F <sub>2</sub> NO <sub>3</sub>
Ezlopítant	Antiemetic	147116-64-1	Y	C <sub>31</sub> H <sub>38</sub> N <sub>2</sub> O
Fabesetron	Antiemetic	129300-27-2		C <sub>18</sub> H <sub>19</sub> N <sub>3</sub> O
Fadolmidine	Antidiabetic	189353-31-9		C <sub>13</sub> H <sub>14</sub> N <sub>2</sub> O
Fadrozole	Antineoplastic	102676-47-1	Y	C <sub>14</sub> H <sub>13</sub> N <sub>3</sub>



Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Falintolol	Antihypertensive	90581-63-8		C <sub>12</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub>
Falipamil	Antianginal	77862-92-1		C <sub>24</sub> H <sub>32</sub> N <sub>2</sub> O <sub>5</sub>
Falnidamol	Antineoplastic	196612-93-8		C <sub>18</sub> H <sub>19</sub> ClFN <sub>7</sub>
Famciclovir	Antiviral	104227-87-4	Y	C <sub>14</sub> H <sub>19</sub> N <sub>5</sub> O <sub>4</sub>
Famiraprinium Chloride	Unclassified	105538-42-9		C <sub>15</sub> H <sub>17</sub> N <sub>3</sub> O <sub>2</sub>
Famotidine	Ant ulcerative	76824-35-6	Y	C <sub>8</sub> H <sub>15</sub> N <sub>7</sub> O <sub>2</sub> S <sub>3</sub>
Fampridine	Nootropic	504-24-5	Y	C <sub>5</sub> H <sub>6</sub> N <sub>2</sub>
Famprofazone	Analgesic	22881-35-2		C <sub>24</sub> H <sub>31</sub> N <sub>3</sub> O
Famproniil	Unclassified	134183-95-2		C <sub>16</sub> H <sub>6</sub> Cl <sub>3</sub> F <sub>3</sub> N <sub>6</sub>
Fananserin	Antipsychotic	127625-29-0		C <sub>23</sub> H <sub>24</sub> FN <sub>3</sub> O <sub>2</sub> S
Fanapanel	Nootropic	161605-73-8		C <sub>14</sub> H <sub>15</sub> F <sub>3</sub> N <sub>3</sub> O <sub>6</sub> P
Fandofloxacin	Antibiotic	164150-99-6		C <sub>20</sub> H <sub>18</sub> F <sub>2</sub> N <sub>4</sub> O <sub>3</sub>
Fandosentan Potassium	Anticoagulant	221241-63-0		C <sub>25</sub> H <sub>18</sub> F <sub>3</sub> N <sub>6</sub> O <sub>6</sub> S
Fanetizole Mesylate	Immunomodulator	79069-94-6		C <sub>17</sub> H <sub>16</sub> N <sub>2</sub> S
Fantofarone	Antihypertensive	114432-13-2		C <sub>31</sub> H <sub>38</sub> N <sub>2</sub> O <sub>5</sub> S
Fantridone	Antidepressant	17692-37-4		C <sub>18</sub> H <sub>20</sub> N <sub>2</sub> O
Farampator	Antipsychotic	211735-76-1		C <sub>12</sub> H <sub>13</sub> N <sub>3</sub> O <sub>2</sub>
Farglitazar	Antidiabetic	196808-45-4		C <sub>34</sub> H <sub>30</sub> N <sub>2</sub> O <sub>5</sub>
Fasidotril	Antihypertensive	135038-57-2		C <sub>23</sub> H <sub>25</sub> NO <sub>6</sub> S
Fasiplon	Anxiolytic	106100-65-6		C <sub>13</sub> H <sub>15</sub> N <sub>5</sub> O <sub>2</sub>
Fasoracetam	Nootropic	110958-19-5		C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>
Fasudil	Vasodilator	103745-39-7	y	C <sub>14</sub> H <sub>17</sub> N <sub>3</sub> O <sub>2</sub> S
Fazadinium Bromide	Muscle Relaxant	49564-56-9		C <sub>28</sub> H <sub>24</sub> Br <sub>2</sub> N <sub>6</sub>
Fazarabine	Antineoplastic	65886-71-7		C <sub>8</sub> H <sub>12</sub> N <sub>4</sub> O <sub>5</sub>
Febantel	Anthelminthic	58306-30-2		C <sub>20</sub> H <sub>22</sub> N <sub>4</sub> O <sub>6</sub> S
Febarbamate	Antidepressant	13246-02-1		C <sub>20</sub> H <sub>27</sub> N <sub>3</sub> O <sub>6</sub>
Febuprol	Choleretic	3102-00-9		C <sub>13</sub> H <sub>20</sub> O <sub>3</sub>
Febuverine	Anesthetic	7077-33-0		C <sub>28</sub> H <sub>38</sub> N <sub>2</sub> O <sub>4</sub>
Febuxostat	Antiurolithic	144060-53-7	y	C <sub>16</sub> H <sub>16</sub> N <sub>2</sub> O <sub>5</sub> S
Feclimine	Unclassified	3590-16-7		C <sub>24</sub> H <sub>42</sub> N <sub>2</sub>
Feclobuzone	Antirheumatic	23111-34-4		C <sub>27</sub> H <sub>25</sub> ClN <sub>2</sub> O <sub>4</sub>
Fedotozine	Gastroprokinetic	123618-00-8		C <sub>22</sub> H <sub>31</sub> NO <sub>4</sub>
Fedrilate	Antiviral	23271-74-1		C <sub>20</sub> H <sub>29</sub> NO <sub>4</sub>
Felbamate	Anticonvulsant	25451-15-4	Y	C <sub>11</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub>
Felbinac	Antiinflammatory	5728-52-9		C <sub>14</sub> H <sub>12</sub> O <sub>2</sub>
Felipyrine	Antiinflammatory	1980-49-0		C <sub>15</sub> H <sub>20</sub> N <sub>2</sub> O
Felodipine	Antihypertensive	72509-76-3	Y	C <sub>18</sub> H <sub>19</sub> Cl <sub>2</sub> NO <sub>4</sub>
Feloprentan	Antimigraine	204267-33-4		C <sub>31</sub> H <sub>32</sub> N <sub>2</sub> O <sub>6</sub>
Femoxetine	Antidepressant	59859-58-4		C <sub>20</sub> H <sub>25</sub> NO <sub>2</sub>
Fenabutene	Analgesic	5984-83-8		C <sub>12</sub> H <sub>14</sub> O <sub>2</sub>
Fenacetinol	Unclassified	22521-79-5		C <sub>10</sub> H <sub>13</sub> NO <sub>3</sub>
Fenaclon	Antipsychotic	306-20-7		C <sub>11</sub> H <sub>14</sub> ClNO
Fenadiazole	Sedative	1008-65-7		C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>
Fenaftic Acid	Antifungal	27736-80-7		C <sub>24</sub> H <sub>31</sub> NO <sub>4</sub>
Fenalamide	Muscle Relaxant	4551-59-1		C <sub>19</sub> H <sub>30</sub> N <sub>2</sub> O <sub>3</sub>
Fenalcomine	Cardiotonic	34616-39-2		C <sub>20</sub> H <sub>27</sub> NO <sub>2</sub>
Fenamifuril	Unclassified	735-64-8		C <sub>14</sub> H <sub>17</sub> NO <sub>5</sub>
Fenamole	Antiinflammatory	5467-78-7		C <sub>7</sub> H <sub>7</sub> N <sub>5</sub>
Fenaperone	Antipsychotic	54063-38-6		C <sub>21</sub> H <sub>29</sub> FN <sub>2</sub> O <sub>3</sub>
Fenbendazole	Anthelminthic	43210-67-9		C <sub>15</sub> H <sub>13</sub> N <sub>3</sub> O <sub>2</sub> S
Fenbenicillin	Antibiotic	1926-48-3		C <sub>22</sub> H <sub>22</sub> N <sub>2</sub> O <sub>5</sub> S
Fenbufen	Antiinflammatory	36330-85-5	Y	C <sub>16</sub> H <sub>14</sub> O <sub>3</sub>
Fenbutrazate	Anorexic	4378-36-3		C <sub>23</sub> H <sub>29</sub> NO <sub>3</sub>
Fencamfamin	Nootropic	1209-98-9		C <sub>15</sub> H <sub>21</sub> N
Fencibutirol	Choleretic	5977-10-6		C <sub>16</sub> H <sub>22</sub> O <sub>3</sub>
Fenclofenac	Antiinflammatory	34645-84-6		C <sub>14</sub> H <sub>10</sub> Cl <sub>2</sub> O <sub>3</sub>
Fenclonine	Antidepressant	7424-00-2		C <sub>9</sub> H <sub>10</sub> ClNO <sub>2</sub>
Fenclorac	Antiinflammatory	36616-52-1		C <sub>14</sub> H <sub>16</sub> Cl <sub>2</sub> O <sub>2</sub>
Fenclozic Acid	Antiinflammatory	17969-20-9		C <sub>11</sub> H <sub>8</sub> ClNO <sub>2</sub> S
Fendiline	Vasodilator	13042-18-7		C <sub>23</sub> H <sub>25</sub> N
Fendizoate	Antipsychotic	84627-04-3		C <sub>20</sub> H <sub>14</sub> O <sub>4</sub>
Fendosal	Antiinflammatory	53597-27-6		C <sub>25</sub> H <sub>19</sub> NO <sub>3</sub>
Feneritrol	Antihypertensive	15301-67-4		C <sub>45</sub> H <sub>52</sub> O <sub>8</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Fenestrel	Estrogen	7698-97-7		C <sub>16</sub> H <sub>20</sub> O <sub>2</sub>
Fenethazine	Antihistaminic	522-24-7		C <sub>16</sub> H <sub>18</sub> N <sub>2</sub> S
Fenethylline	Nootropic	3736-08-1		C <sub>18</sub> H <sub>23</sub> N <sub>5</sub> O <sub>2</sub>
Fenetradil	Antihypertensive	54063-39-7		C <sub>22</sub> H <sub>36</sub> N <sub>2</sub> O <sub>3</sub>
Fenflumizole	Antiinflammatory	73445-46-2		C <sub>23</sub> H <sub>18</sub> F <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Fenfluramine	Anorexic	458-24-2		C <sub>12</sub> H <sub>16</sub> F <sub>3</sub> N
Fengabine	Antidepressant	80018-06-0		C <sub>17</sub> H <sub>17</sub> Cl <sub>2</sub> NO
Fenharmane	Unclassified	15301-68-5		C <sub>18</sub> H <sub>18</sub> N <sub>2</sub>
Fenimide	Antipsychotic	60-45-7		C <sub>13</sub> H <sub>15</sub> NO <sub>2</sub>
Feniodium Chloride	Antiprotozoal	71585-34-7		C <sub>12</sub> H <sub>6</sub> Cl <sub>5</sub> I
Fenipentol	Choleretic	583-03-9		C <sub>11</sub> H <sub>16</sub> O
Fenirofibrate	Antihyperlipidemic	54419-31-7		C <sub>17</sub> H <sub>17</sub> ClO <sub>4</sub>
Fenisorex	Anorexic	34887-52-0		C <sub>16</sub> H <sub>16</sub> FNO
Fenitrothion	Dermatologic	122-14-5		C <sub>9</sub> H <sub>12</sub> NO <sub>3</sub> PS
Fenleuton	Antiinflammatory	141579-54-6		C <sub>17</sub> H <sub>15</sub> FN <sub>2</sub> O <sub>3</sub>
Fenmetozole	Antidepressant	41473-09-0		C <sub>10</sub> H <sub>10</sub> Cl <sub>2</sub> N <sub>2</sub> O
Fenmetramide	Antidepressant	5588-29-4		C <sub>11</sub> H <sub>13</sub> NO <sub>2</sub>
Fenobam	Sedative	57653-26-6		C <sub>11</sub> H <sub>11</sub> ClN <sub>4</sub> O <sub>2</sub>
Fenocinol	Unclassified	3671-05-4		C <sub>16</sub> H <sub>18</sub> O <sub>3</sub>
Fenocitmine Sulfate	Antiulcerative	69365-65-7		C <sub>27</sub> H <sub>38</sub> N <sub>2</sub>
Fenofibrate	Antihyperlipidemic	49562-28-9	Y	C <sub>20</sub> H <sub>21</sub> ClO <sub>4</sub>
Fenoldopam	Antihypertensive	67227-56-9		C <sub>16</sub> H <sub>16</sub> ClNO <sub>3</sub>
Fenoprofen	Antiinflammatory	29679-58-1	Y	C <sub>15</sub> H <sub>14</sub> O <sub>3</sub>
Fenoterol	Bronchodilator	13392-18-2		C <sub>17</sub> H <sub>21</sub> NO <sub>4</sub>
Fenoverine	Antispasmodic	37561-27-6		C <sub>26</sub> H <sub>25</sub> N <sub>3</sub> O <sub>3</sub> S
Fenoxazoline	Nootropic	4846-91-7		C <sub>13</sub> H <sub>18</sub> N <sub>2</sub> O
Fenoxedil	Vasodilator	54063-40-0		C <sub>28</sub> H <sub>42</sub> N <sub>2</sub> O <sub>5</sub>
Fenozolone	Nootropic	15302-16-6		C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>
Fenpentadiol	Antidepressant	15687-18-0		C <sub>12</sub> H <sub>17</sub> ClO <sub>2</sub>
Fenperate	Unclassified	55837-26-8		C <sub>25</sub> H <sub>31</sub> NO <sub>4</sub>
Fenpipalone	Antiinflammatory	21820-82-6		C <sub>17</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>
Fenpipramide	Antispasmodic	77-01-0		C <sub>21</sub> H <sub>26</sub> N <sub>2</sub> O
Fenpiprane	Antispasmodic	3540-95-2		C <sub>20</sub> H <sub>25</sub> N
Fenpiverinium Bromide	Antispasmodic	258329-46-3		C <sub>22</sub> H <sub>29</sub> BrN <sub>2</sub> O
Fenprinast	Bronchodilator	75184-94-0		C <sub>16</sub> H <sub>16</sub> ClN <sub>5</sub> O
Fenproporex	Anorexic	16397-28-7		C <sub>12</sub> H <sub>16</sub> N <sub>2</sub>
Fenprostalene	Progestogen	69381-94-8		C <sub>23</sub> H <sub>30</sub> O <sub>6</sub>
Fenquizone	Diuretic	20287-37-0		C <sub>14</sub> H <sub>12</sub> ClN <sub>3</sub> O <sub>5</sub> S
Fenretinide	Antineoplastic	65646-68-6		C <sub>26</sub> H <sub>33</sub> NO <sub>2</sub>
Fenspiride	Bronchodilator	5053-06-5		C <sub>15</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>
Fentanyl	Analgesic	437-38-7		C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> O
Fenthion	Ectoparasiticide	55-38-9		C <sub>10</sub> H <sub>15</sub> O <sub>3</sub> PS <sub>2</sub>
Fentiazac	Antiinflammatory	18046-21-4		C <sub>17</sub> H <sub>12</sub> ClNO <sub>2</sub> S
Fenticlor	Antibacterial	97-24-5		C <sub>12</sub> H <sub>8</sub> Cl <sub>2</sub> O <sub>2</sub> S
Fenticonazole	Antifungal	72479-26-6		C <sub>24</sub> H <sub>20</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>5</sub> S
Fentonium Bromide	Antibiotic	34786-74-8		C <sub>31</sub> H <sub>34</sub> BrNO <sub>4</sub>
Fenyripol	Muscle Relaxant	3607-24-7		C <sub>12</sub> H <sub>13</sub> N <sub>3</sub> O
Fepentolic Acid	Unclassified	17243-33-3		C <sub>12</sub> H <sub>16</sub> O <sub>4</sub>
Fepitrizol	Unclassified	53415-46-6		C <sub>15</sub> H <sub>14</sub> N <sub>4</sub> O
Fepradinol	Antiinflammatory	36981-91-6		C <sub>12</sub> H <sub>19</sub> NO <sub>2</sub>
Feprazone	Antiinflammatory	30748-29-9		C <sub>20</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>
Fepromide	Analgesic	54063-41-1		C <sub>23</sub> H <sub>30</sub> N <sub>2</sub> O <sub>5</sub>
Feprosidnine	Unclassified	22293-47-6		C <sub>11</sub> H <sub>13</sub> N <sub>3</sub> O
Ferric Cacodylate	Anthelmintic	75-60-5		C <sub>2</sub> H <sub>7</sub> AsO <sub>2</sub>
Ferric Glycerophosphate	Hemantic	56-81-5		C <sub>3</sub> H <sub>8</sub> O <sub>3</sub>
Fesoterodine	Urologic	286930-02-7	Y	C <sub>26</sub> H <sub>37</sub> NO <sub>3</sub>
Fetoxylate	Muscle Relaxant	54063-45-5		C <sub>36</sub> H <sub>36</sub> N <sub>2</sub> O <sub>3</sub>
Fexicaine	Anesthetic	54063-46-6		C <sub>25</sub> H <sub>34</sub> N <sub>2</sub> O <sub>4</sub>
Fexinidazole	Antiprotozoal	59729-37-2	Y	C <sub>12</sub> H <sub>13</sub> N <sub>3</sub> O <sub>3</sub> S
Fexofenadine	Antihistaminic	83799-24-0	Y	C <sub>32</sub> H <sub>39</sub> NO <sub>4</sub>
Fezatione	Antifungal	15387-18-5		C <sub>17</sub> H <sub>14</sub> N <sub>2</sub> S <sub>2</sub>
Fezolamine Fumarate	Antidepressant	80410-36-2		C <sub>20</sub> H <sub>23</sub> N <sub>3</sub>
Fiacitabine	Antiviral	69123-90-6		C <sub>9</sub> H <sub>11</sub> FIN <sub>3</sub> O <sub>4</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Fialuridine	Antiviral	69123-98-4		C <sub>9</sub> H <sub>10</sub> FIN <sub>2</sub> O <sub>5</sub>
Fibracillin	Antibiotic	51154-48-4		C <sub>26</sub> H <sub>28</sub> ClN <sub>3</sub> O <sub>6</sub> S
Fidarestat	Antidiabetic	136087-85-9		C <sub>12</sub> H <sub>10</sub> FN <sub>3</sub> O <sub>4</sub>
Fidexaban	Anticoagulant	183305-24-0		C <sub>25</sub> H <sub>24</sub> F <sub>2</sub> N <sub>6</sub> O <sub>5</sub>
Fiduxosin	Androgen	208993-54-8		C <sub>30</sub> H <sub>29</sub> N <sub>5</sub> O <sub>4</sub> S
Figopitant	Antiemetic	502422-74-4		C <sub>27</sub> H <sub>31</sub> F <sub>6</sub> N <sub>3</sub> O
Filaminast	Bronchodilator	141184-34-1		C <sub>15</sub> H <sub>20</sub> N <sub>2</sub> O <sub>4</sub>
Flenadol	Analgesic	78168-92-0		C <sub>14</sub> H <sub>19</sub> NO <sub>4</sub>
Filipin	Antifungal	480-49-9		C <sub>35</sub> H <sub>58</sub> O <sub>11</sub>
Finafloxacin	Antibiotic	209342-40-5		C <sub>20</sub> H <sub>19</sub> FN <sub>4</sub> O <sub>4</sub>
Finasteride	Urologic	98319-26-7	Y	C <sub>23</sub> H <sub>36</sub> N <sub>2</sub> O <sub>2</sub>
Fingolimod	Immunomodulator	162359-55-9	Y	C <sub>19</sub> H <sub>33</sub> NO <sub>2</sub>
Finrozole	Antiprotozoal	160146-17-8		C <sub>18</sub> H <sub>15</sub> FN <sub>4</sub> O
Fipamezole	Antihypertensive	150586-58-6		C <sub>14</sub> H <sub>15</sub> FN <sub>2</sub>
Fipexide	Nootropic	34161-24-5		C <sub>20</sub> H <sub>21</sub> ClN <sub>2</sub> O <sub>4</sub>
Firocoxib	Antiinflammatory	189954-96-9		C <sub>17</sub> H <sub>20</sub> O <sub>5</sub> S
Fispemifene	Antineoplastic	341524-89-8		C <sub>26</sub> H <sub>27</sub> ClO <sub>3</sub>
Flamenol	Antiarrhythmic	2174-64-3		C <sub>7</sub> H <sub>8</sub> O <sub>3</sub>
Flavamine	Unclassified	15686-60-9		C <sub>21</sub> H <sub>23</sub> NO <sub>2</sub>
Flavodic Acid	Unclassified	37470-13-6		C <sub>19</sub> H <sub>14</sub> O <sub>8</sub>
Flavodilol Maleate	Antihypertensive	79619-31-1		C <sub>21</sub> H <sub>23</sub> NO <sub>4</sub>
Flavoxate	Antispasmodic	15301-69-6	Y	C <sub>24</sub> H <sub>25</sub> NO <sub>4</sub>
Flazalone	Antiinflammatory	21221-18-1		C <sub>19</sub> H <sub>19</sub> F <sub>2</sub> NO <sub>2</sub>
Flecainide Acetate	Antiarrhythmic	54143-55-4	Y	C <sub>17</sub> H <sub>20</sub> F <sub>6</sub> N <sub>2</sub> O <sub>3</sub>
Flerobutanol	Antidepressant	82101-10-8		C <sub>12</sub> H <sub>18</sub> FNO
Fleroxacin	Antibiotic	79660-72-3		C <sub>17</sub> H <sub>18</sub> F <sub>3</sub> N <sub>3</sub> O <sub>3</sub>
Flesinoxan	Anxiolytic	98206-10-1		C <sub>22</sub> H <sub>26</sub> FN <sub>3</sub> O <sub>4</sub>
Flestolol Sulfate	Antihypertensive	87721-62-8		C <sub>15</sub> H <sub>22</sub> FN <sub>3</sub> O <sub>4</sub>
Fletazepam	Muscle Relaxant	34482-99-0		C <sub>17</sub> H <sub>13</sub> ClF <sub>4</sub> N <sub>2</sub>
Flezelastrine	Bronchodilator	135381-77-0		C <sub>29</sub> H <sub>30</sub> FN <sub>3</sub> O
Flibanserin	Antidepressant	167933-07-5		C <sub>20</sub> H <sub>21</sub> F <sub>3</sub> N <sub>4</sub> O
Flindokalner	Nootropic	187523-35-9		C <sub>16</sub> H <sub>10</sub> ClF <sub>4</sub> NO <sub>2</sub>
Floctafenine	Analgesic	23779-99-9		C <sub>20</sub> H <sub>17</sub> F <sub>3</sub> N <sub>2</sub> O <sub>4</sub>
Flomoxef	Antibiotic	99665-00-6		C <sub>15</sub> H <sub>18</sub> F <sub>2</sub> N <sub>6</sub> O <sub>7</sub> S <sub>2</sub>
Flopropione	Antispasmodic	2295-58-1		C <sub>9</sub> H <sub>10</sub> O <sub>4</sub>
Florantyrone	Choleretic	519-95-9		C <sub>20</sub> H <sub>14</sub> O <sub>3</sub>
Flordipine	Antihypertensive	77590-96-6		C <sub>26</sub> H <sub>33</sub> F <sub>3</sub> N <sub>2</sub> O <sub>5</sub>
Floredil	Vasodilator	53731-36-5		C <sub>16</sub> H <sub>25</sub> NO <sub>4</sub>
Florfenicol	Antibiotic	73231-34-2		C <sub>12</sub> H <sub>14</sub> Cl <sub>2</sub> FN <sub>4</sub> O <sub>4</sub> S
Florifenine	Antiinflammatory	83863-79-0		C <sub>23</sub> H <sub>22</sub> F <sub>3</sub> N <sub>3</sub> O <sub>2</sub>
Flosatidil	Vasodilator	113593-34-3		C <sub>26</sub> H <sub>34</sub> F <sub>3</sub> N <sub>3</sub> O <sub>3</sub> S
Flosequinan	Antihypertensive	76568-02-0		C <sub>11</sub> H <sub>10</sub> FNO <sub>2</sub> S
Flosulide	Antiinflammatory	80937-31-1		C <sub>16</sub> H <sub>13</sub> F <sub>2</sub> NO <sub>4</sub> S
Flotrenizine	Antihistaminic	89224-08-8		C <sub>31</sub> H <sub>38</sub> F <sub>2</sub> N <sub>2</sub> O
Floverine	Analgesic	27318-86-1		C <sub>10</sub> H <sub>14</sub> O <sub>4</sub>
Floxacillin	Antibiotic	5250-39-5	Y	C <sub>19</sub> H <sub>17</sub> ClFN <sub>3</sub> O <sub>5</sub> S
Floxacrine	Nootropic	53966-34-0		C <sub>20</sub> H <sub>13</sub> ClF <sub>3</sub> NO <sub>3</sub>
Floxuridine	Antiviral	50-91-9	Y	C <sub>9</sub> H <sub>11</sub> FN <sub>2</sub> O <sub>5</sub>
Fluacizine	Antidepressant	30223-48-4		C <sub>20</sub> H <sub>21</sub> F <sub>3</sub> N <sub>2</sub> O <sub>5</sub>
Flualamide	Diuretic	5107-49-3		C <sub>17</sub> H <sub>23</sub> F <sub>3</sub> N <sub>2</sub> O <sub>2</sub>
Fluanisone	Antipsychotic	1480-19-9		C <sub>21</sub> H <sub>25</sub> FN <sub>2</sub> O <sub>2</sub>
Fluazacort	Antiinflammatory	19888-56-3		C <sub>25</sub> H <sub>30</sub> FNO <sub>6</sub>
Flubanilate	Nootropic	847-20-1		C <sub>14</sub> H <sub>19</sub> F <sub>3</sub> N <sub>2</sub> O <sub>2</sub>
Flubendazole	Anthelmintic	31430-15-6	Y	C <sub>16</sub> H <sub>12</sub> FN <sub>3</sub> O <sub>3</sub>
Flubepride	Antiprotozoal	56488-61-0		C <sub>20</sub> H <sub>24</sub> FN <sub>3</sub> O <sub>4</sub> S
Flucarbril	Analgesic	2261-94-1		C <sub>11</sub> H <sub>8</sub> F <sub>3</sub> NO
Flucetorex	Anorexic	40256-99-3		C <sub>20</sub> H <sub>21</sub> F <sub>3</sub> N <sub>2</sub> O <sub>3</sub>
Flucindole	Antipsychotic	40594-09-0		C <sub>14</sub> H <sub>16</sub> F <sub>2</sub> N <sub>2</sub>
Fluciprazine	Antipsychotic	54340-64-6		C <sub>21</sub> H <sub>29</sub> FN <sub>2</sub> O <sub>2</sub>
Flucloronide	Glucocorticoid	3693-39-8		C <sub>24</sub> H <sub>29</sub> Cl <sub>2</sub> FO <sub>5</sub>
Fluconazole	Antifungal	86386-73-4	Y	C <sub>13</sub> H <sub>12</sub> F <sub>2</sub> N <sub>6</sub> O
Flucrylate	Dermatologic	23023-91-8		C <sub>7</sub> H <sub>6</sub> F <sub>3</sub> NO <sub>2</sub>
Flucytosine	Antifungal	2022-85-7	Y	C <sub>4</sub> H <sub>4</sub> FN <sub>3</sub> O

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Fludalanine	Antibacterial	35523-45-6		C <sub>3</sub> H <sub>5</sub> DFNO <sub>2</sub>
Fludarabine	Antineoplastic	21679-14-1	Y	C <sub>10</sub> H <sub>12</sub> FN <sub>5</sub> O <sub>4</sub>
Fludiazepam	Anxiolytic	3900-31-0		C <sub>16</sub> H <sub>12</sub> ClFN <sub>2</sub> O
Fludorex	Anorexic	15221-81-5		C <sub>11</sub> H <sub>14</sub> F <sub>3</sub> NO
Fludoxopone	Antiprotozoal	71923-29-0		C <sub>21</sub> H <sub>21</sub> FN <sub>2</sub> O <sub>3</sub>
Fludrocortisone	Steroid	127-31-1	Y	C <sub>21</sub> H <sub>29</sub> FO <sub>5</sub>
Fludrocortisone Acetate	Steroid	514-36-3	Y	C <sub>23</sub> H <sub>31</sub> FO <sub>6</sub>
Flufenamic Acid	Antiinflammatory	530-78-9		C <sub>14</sub> H <sub>10</sub> F <sub>3</sub> NO <sub>2</sub>
Flufenisal	Analgesic	22494-27-5		C <sub>15</sub> H <sub>11</sub> FO <sub>4</sub>
Flufosal	Analgesic	65708-37-4		C <sub>8</sub> H <sub>6</sub> F <sub>3</sub> O <sub>6</sub> P
Flufylline	Bronchodilator	82190-91-8		C <sub>21</sub> H <sub>24</sub> FN <sub>5</sub> O <sub>3</sub>
Fluindarol	Vasodilator	6723-40-6		C <sub>16</sub> H <sub>9</sub> F <sub>3</sub> O <sub>2</sub>
Fluindione	Anticonvulsant	957-56-2		C <sub>15</sub> H <sub>9</sub> FO <sub>2</sub>
Flumazenil	Antidote	78755-81-4		C <sub>15</sub> H <sub>14</sub> FN <sub>3</sub> O <sub>3</sub>
Flumecinol	Hepatoprotectant	56430-99-0		C <sub>16</sub> H <sub>15</sub> F <sub>3</sub> O
Flumedroxone	Analgesic	15687-21-5		C <sub>22</sub> H <sub>29</sub> F <sub>3</sub> O <sub>3</sub>
Flumequine	Antibacterial	42835-25-6		C <sub>14</sub> H <sub>12</sub> FNO <sub>3</sub>
Flumeridone	Antiemetic	75444-64-3		C <sub>22</sub> H <sub>23</sub> ClFN <sub>5</sub> O <sub>2</sub>
Flumethasone	Glucocorticoid	2135-17-3		C <sub>22</sub> H <sub>28</sub> F <sub>2</sub> O <sub>5</sub>
Flumethasone Pivalate	Glucocorticoid	2002-29-1		C <sub>27</sub> H <sub>36</sub> F <sub>2</sub> O <sub>6</sub>
Flumethiazide	Ophthalmic	148-56-1		C <sub>8</sub> H <sub>6</sub> F <sub>3</sub> N <sub>3</sub> O <sub>4</sub> S <sub>2</sub>
Flumethrin	Ectoparasiticide	69770-45-2		C <sub>28</sub> H <sub>22</sub> Cl <sub>2</sub> FNO <sub>3</sub>
Flumetramide	Muscle Relaxant	7125-73-7		C <sub>11</sub> H <sub>10</sub> F <sub>3</sub> NO <sub>2</sub>
Flumexadol	Sedative	30914-89-7		C <sub>11</sub> H <sub>12</sub> F <sub>3</sub> NO
Flumezapine	Antipsychotic	61325-80-2		C <sub>17</sub> H <sub>19</sub> FN <sub>4</sub> S
Fluminorex	Anorexic	720-76-3		C <sub>10</sub> H <sub>9</sub> F <sub>3</sub> N <sub>2</sub> O
Flumizole	Antiinflammatory	36740-73-5		C <sub>18</sub> H <sub>15</sub> F <sub>3</sub> N <sub>2</sub> O <sub>2</sub>
Flumoxonide	Steroid	60135-22-0		C <sub>26</sub> H <sub>34</sub> F <sub>2</sub> O <sub>7</sub>
Flunamine	Antidepressant	50366-32-0		C <sub>15</sub> H <sub>15</sub> F <sub>2</sub> NO
Flunarizine	Vasodilator	52468-60-7	y	C <sub>26</sub> H <sub>26</sub> F <sub>2</sub> N <sub>2</sub>
Flunidazole	Antiprotozoal	4548-15-6		C <sub>11</sub> H <sub>10</sub> FN <sub>3</sub> O <sub>3</sub>
Flunisolide	Glucocorticoid	3385-03-3		C <sub>24</sub> H <sub>31</sub> FO <sub>6</sub>
Flunisolide Acetate	Antiinflammatory	4533-89-5		C <sub>26</sub> H <sub>33</sub> FO <sub>7</sub>
Flunitrazepam	Sedative	1622-62-4	Y	C <sub>16</sub> H <sub>12</sub> FN <sub>3</sub> O <sub>3</sub>
Flunixin	Antiinflammatory	38677-85-9		C <sub>14</sub> H <sub>11</sub> F <sub>3</sub> N <sub>2</sub> O <sub>2</sub>
Flunoprost	Antiulcerative	86348-98-3		C <sub>22</sub> H <sub>29</sub> FO <sub>5</sub>
Flunoxaprofen	Antiinflammatory	66934-18-7		C <sub>16</sub> H <sub>12</sub> FNO <sub>3</sub>
Fluocinolone Acetonide	Antiinflammatory	67-73-2		C <sub>24</sub> H <sub>30</sub> F <sub>2</sub> O <sub>6</sub>
Fluocinonide	Antiinflammatory	356-12-7		C <sub>26</sub> H <sub>32</sub> F <sub>2</sub> O <sub>7</sub>
Fluocortin Butyl	Antiinflammatory	41767-29-7		C <sub>26</sub> H <sub>35</sub> FO <sub>5</sub>
Fluocortolone	Glucocorticoid	152-97-6		C <sub>22</sub> H <sub>29</sub> FO <sub>4</sub>
Fluocortolone Caproate	Glucocorticoid	303-40-2		C <sub>28</sub> H <sub>39</sub> FO <sub>5</sub>
Fluoresone	Anticonvulsant	2924-67-6		C <sub>8</sub> H <sub>9</sub> FO <sub>2</sub> S
Fluorometholone	Glucocorticoid	426-13-1		C <sub>22</sub> H <sub>29</sub> FO <sub>4</sub>
Fluorouracil	Antineoplastic	51-21-8		C <sub>4</sub> H <sub>3</sub> FN <sub>2</sub> O <sub>2</sub>
Fluotracen	Antipsychotic	35764-73-9	Y	C <sub>21</sub> H <sub>24</sub> F <sub>3</sub> N
Fluoxetine	Antidepressant	54910-89-3	Y	C <sub>17</sub> H <sub>18</sub> F <sub>3</sub> NO
Fluoxymesterone	Androgen	76-43-7		C <sub>20</sub> H <sub>29</sub> FO <sub>3</sub>
Fluparoxan	Antidepressant	105182-45-4	Y	C <sub>10</sub> H <sub>10</sub> FNO <sub>2</sub>
Flupentixol	Antipsychotic	2709-56-0	Y	C <sub>23</sub> H <sub>25</sub> F <sub>3</sub> N <sub>2</sub> OS
Fluperamide	Antispasmodic	53179-10-5		C <sub>30</sub> H <sub>32</sub> ClF <sub>3</sub> N <sub>2</sub> O <sub>2</sub>
Fluperlapine	Antipsychotic	67121-76-0		C <sub>19</sub> H <sub>20</sub> FN <sub>3</sub>
Fluperolone Acetate	Glucocorticoid	2119-75-7		C <sub>24</sub> H <sub>31</sub> FO <sub>6</sub>
Fluphenazine Decanoate	Antipsychotic	5002-47-1		C <sub>32</sub> H <sub>44</sub> F <sub>3</sub> N <sub>3</sub> O <sub>2</sub> S
Fluphenazine Enanthate	Antipsychotic	2746-81-8	Y	C <sub>29</sub> H <sub>38</sub> F <sub>3</sub> N <sub>3</sub> O <sub>2</sub> S
Fluphenazine	Antipsychotic	69-23-8		C <sub>22</sub> H <sub>26</sub> F <sub>3</sub> N <sub>3</sub> OS
Flupimazine	Antipsychotic	47682-41-7		C <sub>23</sub> H <sub>27</sub> F <sub>3</sub> N <sub>2</sub> O <sub>2</sub> S
Flupirtine	Analgesic	56995-20-1	Y	C <sub>15</sub> H <sub>17</sub> FN <sub>4</sub> O <sub>2</sub>
Flupranone	Analgesic	21686-10-2		C <sub>20</sub> H <sub>24</sub> FN <sub>3</sub> O <sub>2</sub>
Fluprazine	Antihypertensive	76716-60-4		C <sub>14</sub> H <sub>19</sub> F <sub>3</sub> N <sub>4</sub> O
Fluprednidene	Analgesic	2193-87-5		C <sub>22</sub> H <sub>27</sub> FO <sub>5</sub>
Fluprednisolone	Glucocorticoid	53-34-9	Y	C <sub>21</sub> H <sub>27</sub> FO <sub>5</sub>
Fluprednisolone Valerate	Glucocorticoid	23257-44-5		C <sub>26</sub> H <sub>35</sub> FO <sub>6</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Fluprofen	Antiinflammatory	17692-38-5		C <sub>15</sub> H <sub>13</sub> FO <sub>2</sub>
Fluprofylline	Bronchodilator	85118-43-0		C <sub>22</sub> H <sub>26</sub> FN <sub>5</sub> O <sub>3</sub>
Fluproquazone	Analgesic	40507-23-1		C <sub>18</sub> H <sub>17</sub> FN <sub>2</sub> O
Fluprostenol	Prostaglandin	40666-16-8		C <sub>23</sub> H <sub>29</sub> F <sub>3</sub> O <sub>6</sub>
Fluquazone	Antiinflammatory	37554-40-8		C <sub>16</sub> H <sub>10</sub> ClF <sub>3</sub> N <sub>2</sub> O
Fluradoline	Analgesic	71316-84-2		C <sub>17</sub> H <sub>16</sub> FNOS
Flurandrenolide	Glucocorticoid	1524-88-5		C <sub>24</sub> H <sub>33</sub> FO <sub>6</sub>
Flurantel	Anthelminthic	30533-89-2		C <sub>19</sub> H <sub>12</sub> F <sub>6</sub> N <sub>2</sub> O <sub>7</sub>
Flurazepam	Anticonvulsant	17617-23-1	Y	C <sub>21</sub> H <sub>23</sub> ClFN <sub>3</sub> O
Flurbiprofen	Antiinflammatory	5104-49-4	Y	C <sub>15</sub> H <sub>13</sub> FO <sub>2</sub>
Fluretofen	Antiinflammatory	56917-29-4		C <sub>14</sub> H <sub>9</sub> F
Flurithromycin	Antibiotic	82664-20-8		C <sub>37</sub> H <sub>66</sub> FNO <sub>13</sub>
Flurocitabine	Antineoplastic	37717-21-8		C <sub>9</sub> H <sub>10</sub> FN <sub>5</sub> O <sub>4</sub>
Flurofamide	Antibiotic	70788-28-2		C <sub>7</sub> H <sub>9</sub> FN <sub>3</sub> O <sub>2</sub> P
Flurogestone Acetate	Progestogen	2529-45-5		C <sub>23</sub> H <sub>31</sub> FO <sub>5</sub>
Flurothyl	Nootropic	333-36-8		C <sub>4</sub> H <sub>4</sub> F <sub>6</sub> O
Fluroxene	Anesthetic	406-90-6		C <sub>4</sub> H <sub>5</sub> F <sub>3</sub> O
Flusoxolol	Antihypertensive	84057-96-5		C <sub>22</sub> H <sub>30</sub> FNO <sub>4</sub>
Fluspiperone	Antipsychotic	54965-22-9		C <sub>23</sub> H <sub>25</sub> F <sub>2</sub> N <sub>3</sub> O <sub>2</sub>
Fluspirilene	Antipsychotic	1841-19-6	Y	C <sub>29</sub> H <sub>31</sub> F <sub>2</sub> N <sub>3</sub> O
Flutamide	Antineoplastic	13311-84-7	Y	C <sub>11</sub> H <sub>11</sub> F <sub>3</sub> N <sub>2</sub> O <sub>3</sub>
Flutazolam	Anxiolytic	27060-91-9		C <sub>19</sub> H <sub>18</sub> ClFN <sub>2</sub> O <sub>3</sub>
Flutemazepam	Anxiolytic	52391-89-6		C <sub>16</sub> H <sub>12</sub> ClFN <sub>2</sub> O <sub>2</sub> S
Flutiazin	Antiinflammatory	7220-56-6		C <sub>14</sub> H <sub>8</sub> F <sub>3</sub> NO <sub>2</sub> S
Fluticasone Propionate	Glucocorticoid	80474-14-2		C <sub>25</sub> H <sub>31</sub> F <sub>3</sub> O <sub>5</sub> S
Flutizenol	Antiarrhythmic	10202-40-1		C <sub>20</sub> H <sub>24</sub> F <sub>3</sub> N <sub>3</sub> OS <sub>2</sub>
Flutomidate	Sedative	84962-75-4		C <sub>14</sub> H <sub>15</sub> FN <sub>2</sub> O <sub>2</sub>
Flutonidine	Antihypertensive	28125-87-3		C <sub>10</sub> H <sub>12</sub> FN <sub>3</sub>
Flutoprazepam	Anxiolytic	25967-29-7		C <sub>19</sub> H <sub>16</sub> ClFN <sub>2</sub> O
Flutrimazole	Antifungal	119006-77-8		C <sub>22</sub> H <sub>16</sub> F <sub>2</sub> N <sub>2</sub>
Flutroline	Antipsychotic	70801-02-4		C <sub>27</sub> H <sub>25</sub> F <sub>3</sub> N <sub>2</sub> O
Flutropium Bromide	Bronchodilator	63516-07-4		C <sub>24</sub> H <sub>29</sub> BrFNO <sub>3</sub>
Fluvastatin	Antihyperlipidemic	93957-54-1	Y	C <sub>24</sub> H <sub>26</sub> FNO <sub>4</sub>
Fluvoxamine	Antidepressant	54739-18-3	Y	C <sub>15</sub> H <sub>12</sub> F <sub>3</sub> N <sub>2</sub> O <sub>2</sub>
Fluzinamide	Anticonvulsant	76263-13-3		C <sub>12</sub> H <sub>13</sub> F <sub>3</sub> N <sub>2</sub> O <sub>2</sub>
Fluzoperine	Antitussive	52867-77-3		C <sub>15</sub> H <sub>19</sub> FN <sub>2</sub> O <sub>2</sub>
Fodipir	Antitussive	118248-91-2		C <sub>22</sub> H <sub>32</sub> N <sub>4</sub> O <sub>14</sub> P <sub>2</sub>
Folescutol	Capillary Protectant	15687-22-6		C <sub>14</sub> H <sub>15</sub> NO <sub>5</sub>
Fomepizole	Antidote	7554-65-6	Y	C <sub>4</sub> H <sub>6</sub> N <sub>2</sub>
Fomidacillin	Antibiotic	98048-07-8		C <sub>24</sub> H <sub>28</sub> N <sub>6</sub> O <sub>10</sub> S
Fominoben	Antitussive	18053-31-1		C <sub>21</sub> H <sub>24</sub> ClN <sub>3</sub> O <sub>3</sub>
Fomocaine	Anesthetic	17692-39-6		C <sub>20</sub> H <sub>25</sub> NO <sub>2</sub>
Fonazine Mesylate	Antimigraine	7456-24-8		C <sub>19</sub> H <sub>25</sub> N <sub>3</sub> O <sub>2</sub> S <sub>2</sub>
Fopirtoline	Analgesic	22514-23-4		C <sub>11</sub> H <sub>15</sub> ClN <sub>2</sub> OS
Forasartan	Antihypertensive	145216-43-9		C <sub>23</sub> H <sub>28</sub> N <sub>8</sub>
Forfenimex	Immunomodulator	71522-58-2		C <sub>9</sub> H <sub>11</sub> NO <sub>4</sub>
Formebolone	Steroid	2454-11-7		C <sub>21</sub> H <sub>28</sub> O <sub>4</sub>
Formestane	Antineoplastic	566-48-3		C <sub>19</sub> H <sub>26</sub> O <sub>3</sub>
Formetorex	Anorexic	22148-75-0		C <sub>10</sub> H <sub>13</sub> NO
Forminitrazole	Unclassified	500-08-3		C <sub>4</sub> H <sub>3</sub> N <sub>3</sub> O <sub>3</sub> S
Formocortal	Glucocorticoid	2825-60-7		C <sub>29</sub> H <sub>38</sub> ClFO <sub>8</sub>
Formoterol	Bronchodilator	73573-87-2	Y	C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> O <sub>4</sub>
Forodesine	Antineoplastic	209799-67-7		C <sub>11</sub> H <sub>14</sub> N <sub>4</sub> O <sub>4</sub>
Foropafant	Antithrombotic	136468-36-5		C <sub>28</sub> H <sub>40</sub> N <sub>4</sub> S
Fosamprenavir	Antiviral	226700-79-4	Y	C <sub>25</sub> H <sub>36</sub> N <sub>3</sub> O <sub>9</sub> PS
Fosarilate	Antiviral	73514-87-1		C <sub>17</sub> H <sub>28</sub> ClO <sub>5</sub> P
Fosazepam	Sedative	35322-07-7		C <sub>18</sub> H <sub>18</sub> ClN <sub>2</sub> O <sub>2</sub> P
Foscarnet	Antiviral	4428-95-9		CH <sub>3</sub> O <sub>5</sub> P
Foscolic Acid	Unclassified	2398-95-0		C <sub>6</sub> H <sub>11</sub> O <sub>8</sub> P
Fosenazide	Unclassified	16543-10-5		C <sub>14</sub> H <sub>15</sub> N <sub>2</sub> O <sub>2</sub> P
Fosfluconazole	Antifungal	194798-83-9		C <sub>13</sub> H <sub>13</sub> F <sub>2</sub> N <sub>6</sub> O <sub>4</sub> P
Fosfluridine Tidoxil	Antiviral	174638-15-4		C <sub>34</sub> H <sub>62</sub> FN <sub>2</sub> O <sub>10</sub> PS
Fosfomycin	Antibiotic	23155-02-4	Y	C <sub>3</sub> H <sub>7</sub> O <sub>4</sub> P

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Fosfonet Sodium	Antiviral	4408-78-0		C <sub>2</sub> H <sub>5</sub> O <sub>5</sub> P
Fosfosol	Analgesic	6064-83-1		C <sub>7</sub> H <sub>7</sub> O <sub>6</sub> P
Fosfructose Trisodium	Cardiotonic	488-69-7		C <sub>6</sub> H <sub>14</sub> O <sub>12</sub> P <sub>2</sub>
Fosinopril	Antihypertensive	98048-97-6		C <sub>30</sub> H <sub>46</sub> NO <sub>7</sub> P
Fosinoprilat	Antihypertensive	95399-71-6		C <sub>23</sub> H <sub>34</sub> NO <sub>5</sub> P
Fosmenic Acid	Unclassified	13237-70-2		C <sub>7</sub> H <sub>13</sub> O <sub>3</sub> P
Fosmidomycin	Antibiotic	66508-53-0		C <sub>4</sub> H <sub>10</sub> NO <sub>5</sub> P
Fosopamine	Cardiotonic	103878-96-2		C <sub>9</sub> H <sub>14</sub> NO <sub>5</sub> P
Fosphenytoin	Anticonvulsant	93390-81-9		C <sub>16</sub> H <sub>15</sub> N <sub>2</sub> O <sub>6</sub> P
Fospirate	Anthelminthic	5598-52-7		C <sub>7</sub> H <sub>7</sub> Cl <sub>3</sub> NO <sub>4</sub> P
Fospropofol Disodium	Sedative	258516-89-1		C <sub>13</sub> H <sub>21</sub> O <sub>5</sub> P
Fosquidone	Antineoplastic	114517-02-1		C <sub>28</sub> H <sub>22</sub> NO <sub>6</sub> P
Fostedil	Vasodilator	75889-62-2		C <sub>18</sub> H <sub>20</sub> NO <sub>3</sub> PS
Fostriecin Sodium	Antineoplastic	87810-56-8		C <sub>19</sub> H <sub>27</sub> O <sub>9</sub> P
Fosveset	Antitussive	193901-91-6		C <sub>33</sub> H <sub>44</sub> N <sub>3</sub> O <sub>14</sub> P
Fotemustine	Antineoplastic	92118-27-9		C <sub>9</sub> H <sub>19</sub> ClN <sub>3</sub> O <sub>5</sub> P
Fozivudine Tidoxil	Antiviral	141790-23-0		C <sub>35</sub> H <sub>64</sub> N <sub>5</sub> O <sub>8</sub> PS
Frabuprofen	Antiinflammatory	98207-14-8		C <sub>26</sub> H <sub>33</sub> F <sub>3</sub> N <sub>2</sub> O <sub>2</sub>
Fradafiban	Antithrombotic	148396-36-5		C <sub>20</sub> H <sub>21</sub> N <sub>3</sub> O <sub>4</sub>
Frakefamide	Ant ulcerative	188196-22-7		C <sub>30</sub> H <sub>34</sub> FN <sub>5</sub> O <sub>5</sub>
Framycetin	Antibiotic	119-04-0		C <sub>23</sub> H <sub>46</sub> N <sub>6</sub> O <sub>13</sub>
Frentizole	Immunomodulator	26130-02-9		C <sub>15</sub> H <sub>13</sub> N <sub>3</sub> O <sub>2</sub> S
Freselestat	Antidiabetic	208848-19-5		C <sub>23</sub> H <sub>28</sub> N <sub>6</sub> O <sub>4</sub>
Fronepidil	Antihypertensive	79700-63-3		C <sub>21</sub> H <sub>31</sub> NO <sub>2</sub>
fropenem	Antibiotic	106560-14-9		C <sub>12</sub> H <sub>15</sub> NO <sub>5</sub> S
Frovatriptan	Antimigraine	158747-02-5	Y	C <sub>14</sub> H <sub>17</sub> N <sub>3</sub> O
Froxiprost	Bronchodilator	62559-74-4		C <sub>24</sub> H <sub>29</sub> F <sub>3</sub> O <sub>6</sub>
Ftaxilide	Antidiabetic	19368-18-4		C <sub>16</sub> H <sub>15</sub> NO <sub>3</sub>
Ftivazide	Antibacterial	149-17-7		C <sub>14</sub> H <sub>13</sub> N <sub>3</sub> O <sub>3</sub>
Ftormetazine	Antipsychotic	33414-30-1		C <sub>21</sub> H <sub>22</sub> F <sub>3</sub> N <sub>3</sub> OS
Ftorpropazine	Antidepressant	33414-36-7		C <sub>22</sub> H <sub>24</sub> F <sub>3</sub> N <sub>3</sub> O <sub>2</sub> S
Fubrogonium Iodide	Unclassified	3690-58-2		C <sub>14</sub> H <sub>23</sub> BrNO <sub>3</sub> I
Fudosteine	Mucolytic	13189-98-5	Y	C <sub>6</sub> H <sub>13</sub> NO <sub>5</sub> S
Fulvestrant	Antineoplastic	129453-61-8		C <sub>32</sub> H <sub>47</sub> F <sub>5</sub> O <sub>3</sub> S
Fumagillin	Antineoplastic	23110-15-8	Y	C <sub>26</sub> H <sub>34</sub> O <sub>7</sub>
Fumoxicillin	Antibacterial	78186-33-1		C <sub>21</sub> H <sub>21</sub> N <sub>3</sub> O <sub>6</sub> S
Fuprazole	Ant ulcerative	60248-23-9		C <sub>28</sub> H <sub>30</sub> N <sub>4</sub> O <sub>2</sub>
Furacrinic Acid	Unclassified	23580-33-8		C <sub>13</sub> H <sub>14</sub> O <sub>4</sub>
Furafylline	Bronchodilator	80288-49-9		C <sub>12</sub> H <sub>12</sub> N <sub>4</sub> O <sub>3</sub>
Furalazine	Antibiotic	556-12-7		C <sub>9</sub> H <sub>7</sub> N <sub>5</sub> O <sub>3</sub>
Furaltadone	Antibiotic	139-91-3		C <sub>13</sub> H <sub>16</sub> N <sub>4</sub> O <sub>6</sub>
Furaprofen	Antiinflammatory	67700-30-5		C <sub>17</sub> H <sub>14</sub> O <sub>3</sub>
Furazabol	Steroid	1239-29-8		C <sub>20</sub> H <sub>30</sub> N <sub>2</sub> O <sub>2</sub>
Furazolium Chloride	Antibacterial	3878-26-0		C <sub>9</sub> H <sub>8</sub> ClN <sub>3</sub> O <sub>3</sub> S
Furbucillin	Antibiotic	54340-65-7		C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> O <sub>7</sub> S
Furciprofen	Antiinflammatory	58012-63-8		C <sub>15</sub> H <sub>11</sub> ClO <sub>3</sub>
Furegrelate Sodium	Antihypertensive	85666-24-6		C <sub>15</sub> H <sub>11</sub> NO <sub>3</sub>
Furethidine	Antihypertensive	2385-81-1		C <sub>21</sub> H <sub>31</sub> NO <sub>4</sub>
Furfenorex	Anorexic	3776-93-0		C <sub>15</sub> H <sub>19</sub> NO
Furfuryltrimethyl Ammonium Iodide	Unclassified	7618-86-2		C <sub>8</sub> H <sub>14</sub> INO
Furidarone	Cardiotonic	4662-17-3		C <sub>13</sub> H <sub>10</sub> I <sub>2</sub> O <sub>3</sub>
Furmethoxadone	Unclassified	6281-26-1		C <sub>9</sub> H <sub>9</sub> N <sub>3</sub> O <sub>5</sub>
Furnidipine	Antihypertensive	138661-03-7		C <sub>21</sub> H <sub>24</sub> N <sub>2</sub> O <sub>7</sub>
Furobufen	Antiinflammatory	38873-55-1		C <sub>16</sub> H <sub>12</sub> O <sub>4</sub>
Furodazole	Anthelminthic	56119-96-1		C <sub>15</sub> H <sub>11</sub> N <sub>3</sub> O <sub>2</sub>
Furofenac	Antiinflammatory	56983-13-2		C <sub>12</sub> H <sub>14</sub> O <sub>3</sub>
Furomazine	Analgesic	28532-90-3		C <sub>24</sub> H <sub>27</sub> ClN <sub>2</sub> O <sub>5</sub> S
Furomine	Antianginal	142996-66-5		C <sub>20</sub> H <sub>32</sub> N <sub>2</sub> O <sub>4</sub>
Furosemide	Diuretic	54-31-9	Y	C <sub>12</sub> H <sub>11</sub> ClN <sub>2</sub> O <sub>5</sub> S
Furostilbestrol	Antineoplastic	549-40-6		C <sub>28</sub> H <sub>24</sub> O <sub>6</sub>
Furterene	Diuretic	7761-75-3		C <sub>10</sub> H <sub>9</sub> N <sub>7</sub> O
Fusidic Acid	Antibacterial	6990-06-3	Y	C <sub>31</sub> H <sub>48</sub> O <sub>6</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Fuzlocillin	Antibiotic	66327-51-3		C <sub>25</sub> H <sub>26</sub> N <sub>6</sub> O <sub>8</sub> S
Gabapentin	Anticonvulsant	60142-96-3	Y	C <sub>9</sub> H <sub>17</sub> NO <sub>2</sub>
Gabexate	Anticoagulant	39492-01-8		C <sub>16</sub> H <sub>23</sub> N <sub>3</sub> O <sub>4</sub>
Gaboxadol	Anticonvulsant	64603-91-4		C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>
Gacyclidine	Anticonvulsant	68134-81-6		C <sub>16</sub> H <sub>25</sub> NS
Galamustine	Antineoplastic	105618-02-8		C <sub>10</sub> H <sub>19</sub> Cl <sub>2</sub> NO <sub>5</sub>
Galantamine	Nootropic	357-70-0	Y	C <sub>17</sub> H <sub>21</sub> NO <sub>3</sub>
Galarubicin	Antineoplastic	195612-80-7		C <sub>30</sub> H <sub>32</sub> FNO <sub>13</sub>
Galdanetron	Antiemetic	116684-92-5		C <sub>18</sub> H <sub>19</sub> N <sub>3</sub> O
Gallamine Triethiodide	Neuromuscular Blocking Agent	65-29-2		C <sub>30</sub> H <sub>60</sub> I <sub>3</sub> N <sub>3</sub> O <sub>3</sub>
Gallopamil	Antianginal	16662-47-8	Y	C <sub>28</sub> H <sub>40</sub> N <sub>2</sub> O <sub>5</sub>
Galocitabine	Antineoplastic	124012-42-6		C <sub>19</sub> H <sub>22</sub> FN <sub>3</sub> O <sub>8</sub>
Galosemide	Diuretic	52157-91-2		C <sub>15</sub> H <sub>14</sub> F <sub>3</sub> N <sub>3</sub> O <sub>5</sub> S
Gamfexine	Antidepressant	7273-99-6		C <sub>17</sub> H <sub>27</sub> N
Gamma-Aminobutyric Acid	Antihypertensive	56-12-2		C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub>
Gamolenic Acid	Dermatologic	506-26-3	Y	C <sub>18</sub> H <sub>30</sub> O <sub>2</sub>
Ganaxolone	Anticonvulsant	38398-32-2	Y	C <sub>22</sub> H <sub>36</sub> O <sub>2</sub>
Ganciclovir	Antiviral	82410-32-0	Y	C <sub>9</sub> H <sub>13</sub> N <sub>5</sub> O <sub>4</sub>
Gangliefene	Vasodilator	299-61-6		C <sub>20</sub> H <sub>33</sub> NO <sub>3</sub>
Ganstigmine	Neuromuscular Blocking Agent	457075-21-7		C <sub>22</sub> H <sub>27</sub> N <sub>3</sub> O <sub>3</sub>
Gantofiban	Antithrombotic	183547-57-1		C <sub>21</sub> H <sub>29</sub> N <sub>5</sub> O <sub>6</sub>
Gapicomine	Analgesic	1539-39-5		C <sub>12</sub> H <sub>13</sub> N <sub>3</sub>
Gapromidine	Analgesic	106686-40-2		C <sub>14</sub> H <sub>21</sub> N <sub>7</sub>
Garenoxacin Mesylate	Antibacterial	194804-75-6		C <sub>23</sub> H <sub>20</sub> F <sub>2</sub> N <sub>2</sub> O <sub>4</sub>
Gatifloxacin	Antibiotic	112811-59-3		C <sub>19</sub> H <sub>22</sub> FN <sub>3</sub> O <sub>4</sub>
Gavestinel	Nootropic	153436-22-7		C <sub>18</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>3</sub>
Gedocarnil	Anxiolytic	109623-97-4		C <sub>23</sub> H <sub>21</sub> ClN <sub>2</sub> O <sub>4</sub>
Gefarnate	Antilucerative	51-77-4		C <sub>27</sub> H <sub>44</sub> O <sub>2</sub>
Gefitinib	Antineoplastic	184475-35-2	Y	C <sub>22</sub> H <sub>24</sub> ClFN <sub>4</sub> O <sub>3</sub>
Gemazocine	Analgesic	54063-47-7		C <sub>20</sub> H <sub>29</sub> NO
Gemcabene Calcium	Antihyperlipidemic	183293-82-5		C <sub>16</sub> H <sub>30</sub> O <sub>5</sub>
Gemcadiol	Antihyperlipidemic	35449-36-6		C <sub>14</sub> H <sub>30</sub> O <sub>2</sub>
Gemcitabine	Antineoplastic	95058-81-4		C <sub>9</sub> H <sub>11</sub> F <sub>2</sub> N <sub>3</sub> O <sub>4</sub>
Gemprost	Prostaglandin	64318-79-2		C <sub>23</sub> H <sub>38</sub> O <sub>5</sub>
Gemfibrozil	Antihyperlipidemic	25812-30-0	Y	C <sub>15</sub> H <sub>22</sub> O <sub>3</sub>
Gemifloxacin	Antibiotic	175463-14-6	Y	C <sub>18</sub> H <sub>20</sub> FN <sub>3</sub> O <sub>4</sub>
Gemopatrilat	Antihypertensive	160135-92-2		C <sub>19</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub> S
Gepefrine	Antihypotensive	18840-47-6		C <sub>9</sub> H <sub>13</sub> NO
Gepirone	Anxiolytic	83928-76-1	Y	C <sub>19</sub> H <sub>29</sub> N <sub>5</sub> O <sub>2</sub>
Geroquinol	Antibiotic	10457-66-6		C <sub>16</sub> H <sub>22</sub> O <sub>2</sub>
Gestaclone	Progestogen	19291-69-1		C <sub>23</sub> H <sub>27</sub> ClO <sub>2</sub>
Gestadienol	Unclassified	14340-01-3		C <sub>20</sub> H <sub>26</sub> O <sub>3</sub>
Gestodene	Progestogen	60282-87-3		C <sub>21</sub> H <sub>26</sub> O <sub>2</sub>
Gestonorone Caproate	Progestogen	1253-28-7		C <sub>26</sub> H <sub>38</sub> O <sub>4</sub>
Gestrinone	Progestogen	16320-04-0	Y	C <sub>21</sub> H <sub>24</sub> O <sub>2</sub>
Gevotroline	Capillary Protectant	107266-06-8		C <sub>19</sub> H <sub>20</sub> FN <sub>3</sub>
Gimatecan	Antineoplastic	292618-32-7		C <sub>25</sub> H <sub>25</sub> N <sub>3</sub> O <sub>5</sub>
Gimeracil	Antineoplastic	103766-25-2		C <sub>5</sub> H <sub>4</sub> ClNO <sub>2</sub>
Giparmen	Unclassified	67268-43-3		C <sub>13</sub> H <sub>10</sub> O <sub>3</sub>
Giracodazole	Antineoplastic	110883-46-0		C <sub>6</sub> H <sub>11</sub> ClN <sub>4</sub> O
Girisopam	Anxiolytic	82230-53-3		C <sub>18</sub> H <sub>17</sub> ClN <sub>2</sub> O <sub>2</sub>
Gitaloxin	Cardiotonic	3261-53-8		C <sub>42</sub> H <sub>64</sub> O <sub>15</sub>
Gitoformate	Cardiotonic	10176-39-3		C <sub>46</sub> H <sub>64</sub> O <sub>19</sub>
Glafenine	Analgesic	3820-67-5		C <sub>19</sub> H <sub>17</sub> ClN <sub>2</sub> O <sub>4</sub>
Glaucarubin	Antiamebic	1448-23-3		C <sub>25</sub> H <sub>36</sub> O <sub>10</sub>
Glaziovine	Antilucerative	6808-72-6		C <sub>18</sub> H <sub>19</sub> NO <sub>3</sub>
Glemanserine	Anxiolytic	107703-78-6		C <sub>20</sub> H <sub>25</sub> NO
Glenvastatin	Antihyperlipidemic	122254-45-9		C <sub>27</sub> H <sub>26</sub> FNO <sub>3</sub>
Gliamilide	Antidiabetic	51876-98-3		C <sub>23</sub> H <sub>33</sub> N <sub>5</sub> O <sub>5</sub> S
Glibornuride	Antidiabetic	26944-48-9	Y	C <sub>18</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub> S
Glibutimine	Antilucerative	25859-76-1		C <sub>21</sub> H <sub>30</sub> N <sub>4</sub> O <sub>3</sub> S

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Glicaramide	Antidiabetic	36980-34-4		C <sub>30</sub> H <sub>42</sub> N <sub>6</sub> O <sub>5</sub> S
Glicetanile Sodium	Antidiabetic	24455-58-1		C <sub>23</sub> H <sub>25</sub> ClN <sub>4</sub> O <sub>4</sub> S
Gliclazide	Antidiabetic	21187-98-4		C <sub>15</sub> H <sub>21</sub> N <sub>3</sub> O <sub>3</sub> S
Gliflumide	Antidiabetic	35273-88-2		C <sub>25</sub> H <sub>29</sub> FN <sub>4</sub> O <sub>4</sub> S
Glimepiride	Antidiabetic	93479-97-1	Y	C <sub>24</sub> H <sub>34</sub> N <sub>4</sub> O <sub>5</sub> S
Glipalamide	Antidiabetic	37598-94-0		C <sub>12</sub> H <sub>15</sub> N <sub>3</sub> O <sub>3</sub> S
Glipizide	Antidiabetic	29094-61-9	Y	C <sub>21</sub> H <sub>27</sub> N <sub>5</sub> O <sub>4</sub> S
Gliquidone	Antidiabetic	33342-05-1		C <sub>27</sub> H <sub>33</sub> N <sub>3</sub> O <sub>6</sub> S
Glisamuride	Antidiabetic	74680-07-2		C <sub>23</sub> H <sub>31</sub> N <sub>5</sub> O <sub>4</sub> S
Glisentide	Antidiabetic	32797-92-5		C <sub>22</sub> H <sub>27</sub> N <sub>3</sub> O <sub>5</sub> S
Glisolamide	Antidiabetic	24477-37-0		C <sub>20</sub> H <sub>26</sub> N <sub>4</sub> O <sub>5</sub> S
Glisoxepide	Antidiabetic	25046-79-1		C <sub>20</sub> H <sub>27</sub> N <sub>5</sub> O <sub>5</sub> S
Gloxazone	Antibiotic	2507-91-7		C <sub>8</sub> H <sub>16</sub> N <sub>6</sub> O <sub>5</sub> S
Gloximonam	Antibacterial	90850-05-8		C <sub>18</sub> H <sub>25</sub> N <sub>5</sub> O <sub>8</sub> S
Glucalox	Unclassified	18673-08-0		C <sub>3</sub> H <sub>7</sub> AlO <sub>4</sub>
Glucametacin	Antiinflammatory	52443-21-7		C <sub>25</sub> H <sub>27</sub> ClN <sub>2</sub> O <sub>8</sub>
Gluconolactone	Antidote	90-80-2		C <sub>6</sub> H <sub>10</sub> O <sub>6</sub>
Glucosamine	Antirheumatic	3416-24-8	Y	C <sub>6</sub> H <sub>13</sub> NO <sub>5</sub>
Glucosulfamide	Antibiotic	500-74-3		C <sub>13</sub> H <sub>22</sub> N <sub>2</sub> O <sub>11</sub> S <sub>2</sub>
Glucosulfone	Antibiotic	551-89-3		C <sub>24</sub> H <sub>36</sub> N <sub>2</sub> O <sub>18</sub> S <sub>3</sub>
Glucurrolactone	Unclassified	32449-92-6		C <sub>6</sub> H <sub>8</sub> O <sub>6</sub>
Glucuronamide	Antibiotic	3789-97-7		C <sub>6</sub> H <sub>11</sub> NO <sub>6</sub>
Glufosfamide	Antineoplastic	132682-98-5		C <sub>10</sub> H <sub>21</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>7</sub> P
Glunicate	Antihyperlipidemic	80763-86-6		C <sub>36</sub> H <sub>28</sub> N <sub>6</sub> O <sub>10</sub>
Glutamic Acid	Anticonvulsant	56-86-0		C <sub>5</sub> H <sub>9</sub> NO <sub>4</sub>
Glutaurine	Anticonvulsant	56488-60-9		C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> O <sub>6</sub> S
Glutethimide	Sedative	77-21-4		C <sub>13</sub> H <sub>15</sub> NO <sub>2</sub>
Glyburide	Antidiabetic	10238-21-8	Y	C <sub>23</sub> H <sub>28</sub> ClN <sub>3</sub> O <sub>5</sub> S
Glybuthiazol	Antidiabetic	535-65-9		C <sub>12</sub> H <sub>16</sub> N <sub>4</sub> O <sub>2</sub> S <sub>2</sub>
Glybuzole	Antidiabetic	1492-02-0		C <sub>12</sub> H <sub>15</sub> N <sub>3</sub> O <sub>2</sub> S <sub>2</sub>
Glycopyramide	Antiarrhythmic	631-27-6		C <sub>11</sub> H <sub>14</sub> ClN <sub>3</sub> O <sub>3</sub> S
Glycobiarsol	Antiamebic	775514-86-8		C <sub>8</sub> H <sub>9</sub> AsBiNO <sub>6</sub>
Glycocyamine	Cardiotonic	352-97-6		C <sub>3</sub> H <sub>7</sub> N <sub>3</sub> O <sub>2</sub>
Glycopyrrolate	Antispasmodic	596-51-0	Y	C <sub>19</sub> H <sub>28</sub> BrN <sub>3</sub> O <sub>3</sub>
Glycyclamide	Antitussive	664-95-9		C <sub>14</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> S
Glycyrrhizin	Antiinflammatory	1405-86-3		C <sub>42</sub> H <sub>62</sub> O <sub>16</sub>
Glyhexamide	Antidiabetic	451-71-8		C <sub>16</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub> S
Glymidine Sodium	Antidiabetic	339-44-6		C <sub>13</sub> H <sub>15</sub> N <sub>3</sub> O <sub>4</sub> S
Glyoctamide	Antidiabetic	1038-59-1		C <sub>16</sub> H <sub>24</sub> N <sub>2</sub> O <sub>3</sub> S
Glyparamide	Antidiabetic	5581-42-0		C <sub>15</sub> H <sub>16</sub> ClN <sub>3</sub> O <sub>3</sub> S
Glypinamide	Unclassified	1228-19-9		C <sub>13</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>3</sub> S
Glysobuzole	Antidiabetic	3567-08-6		C <sub>13</sub> H <sub>17</sub> N <sub>3</sub> O <sub>3</sub> S <sub>2</sub>
Goralatide	Antihypertensive	120081-14-3		C <sub>20</sub> H <sub>33</sub> N <sub>5</sub> O <sub>9</sub>
Goxalapladi	Antihyperlipidemic	412950-27-7		C <sub>40</sub> H <sub>39</sub> F <sub>5</sub> N <sub>4</sub> O <sub>3</sub>
Granisetron	Antiemetic	109889-09-0	Y	C <sub>18</sub> H <sub>21</sub> D <sub>3</sub> N <sub>4</sub> O
Grepafloxacin	Antibiotic	119914-60-2	Y	C <sub>19</sub> H <sub>22</sub> FN <sub>3</sub> O <sub>3</sub>
Griseofulvin	Antifungal	126-07-8	Y	C <sub>17</sub> H <sub>17</sub> ClO <sub>6</sub>
Guabenxan	Antihypertensive	19889-45-3	Y	C <sub>10</sub> H <sub>13</sub> N <sub>3</sub> O <sub>2</sub>
Guacetisal	Analgesic	55482-89-8		C <sub>16</sub> H <sub>14</sub> O <sub>5</sub>
Guafecainol	Antiarrhythmic	36199-78-7		C <sub>16</sub> H <sub>27</sub> NO <sub>4</sub>
Guaiacol	Expectorant	90-05-1		C <sub>7</sub> H <sub>8</sub> O <sub>2</sub>
Guaiacol Carbonate	Expectorant	553-17-3		C <sub>15</sub> H <sub>14</sub> O <sub>5</sub>
Guaiactamine	Expectorant	15687-23-7		C <sub>13</sub> H <sub>21</sub> NO <sub>2</sub>
Guaiapate	Antitussive	852-42-6		C <sub>18</sub> H <sub>29</sub> NO <sub>4</sub>
Guaietolin	Expectorant	63834-83-3		C <sub>11</sub> H <sub>16</sub> O <sub>4</sub>
Guaiifenesin	Expectorant	93-14-1	Y	C <sub>10</sub> H <sub>14</sub> O <sub>4</sub>
Guaimesal	Expectorant	81674-79-5		C <sub>16</sub> H <sub>14</sub> O <sub>5</sub>
Guaiasteine	Cardiotonic	103181-72-2		C <sub>15</sub> H <sub>19</sub> NO <sub>4</sub> S <sub>2</sub>
Guamecycline	Antibiotic	16545-11-2		C <sub>29</sub> H <sub>38</sub> N <sub>8</sub> O <sub>8</sub>
Guanabenz	Antihypertensive	5051-62-7		C <sub>8</sub> H <sub>8</sub> Cl <sub>2</sub> N <sub>4</sub>
Guanaciline Sulfate	Antihypertensive	1463-28-1		C <sub>9</sub> H <sub>18</sub> N <sub>4</sub>
Guanadrel	Antihypertensive	40580-59-4	Y	C <sub>10</sub> H <sub>19</sub> N <sub>3</sub> O <sub>2</sub>
Guanazodine	Antihypertensive	32059-15-7		C <sub>9</sub> H <sub>20</sub> N <sub>4</sub>



Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Guanclifone	Unclassified	55926-23-3		C <sub>9</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>4</sub>
Guancydine	Antihypertensive	1113-10-6		C <sub>7</sub> H <sub>14</sub> N <sub>4</sub>
Guanethidine	Antihypertensive	55-65-2	Y	C <sub>10</sub> H <sub>22</sub> N <sub>4</sub>
Guanfacine	Antihypertensive	29110-47-2	Y	C <sub>9</sub> H <sub>9</sub> Cl <sub>2</sub> N <sub>3</sub> O
Guanidine	Cholinergic	113-00-8		CH <sub>5</sub> N <sub>3</sub>
Guanisoquin Sulfate	Antihypertensive	154-73-4		C <sub>10</sub> H <sub>12</sub> BrN <sub>3</sub>
Guanoclor Sulfate	Antihypertensive	5001-32-1		C <sub>9</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>4</sub> O
Guanoctine	Antihypertensive	3658-25-1		C <sub>9</sub> H <sub>21</sub> N <sub>3</sub>
Guanoxabenz	Antihypertensive	24047-25-4		C <sub>8</sub> H <sub>8</sub> Cl <sub>2</sub> N <sub>4</sub> O
Guanoxan	Antihypertensive	2165-19-7		C <sub>10</sub> H <sub>13</sub> N <sub>3</sub> O <sub>2</sub>
Guanoxyfen Sulfate	Antihypertensive	13050-83-4		C <sub>10</sub> H <sub>15</sub> N <sub>3</sub> O
Gusperimus Trihydrochloride	Immunosuppressant	98629-43-7		C <sub>17</sub> H <sub>37</sub> N <sub>7</sub> O <sub>3</sub>
Halazepam	Sedative	23092-17-3	Y	C <sub>17</sub> H <sub>12</sub> ClF <sub>3</sub> N <sub>2</sub> O
Halcinonide	Antiinflammatory	3093-35-4		C <sub>24</sub> H <sub>32</sub> ClFO <sub>5</sub>
Halobetasol Propionate	Antiinflammatory	66852-54-8		C <sub>25</sub> H <sub>31</sub> ClF <sub>2</sub> O <sub>5</sub>
Halocortolone	Glucocorticoid	24320-27-2		C <sub>22</sub> H <sub>27</sub> ClF <sub>2</sub> O <sub>3</sub>
Halofantrine	Antimalarial	69756-53-2	Y	C <sub>26</sub> H <sub>30</sub> Cl <sub>2</sub> F <sub>3</sub> NO
Halofenate	Uricosuric	26718-25-2		C <sub>19</sub> H <sub>17</sub> ClF <sub>3</sub> NO <sub>4</sub>
Halofuginone	Antiprotozoal	55837-20-2		C <sub>16</sub> H <sub>17</sub> BrClN <sub>3</sub> O <sub>3</sub>
Halometasone	Antiinflammatory	50629-82-8		C <sub>22</sub> H <sub>27</sub> ClF <sub>2</sub> O <sub>5</sub>
Halonamine	Antibiotic	50583-06-7		C <sub>15</sub> H <sub>15</sub> ClFNO
Halopemide	Antipsychotic	59831-65-1		C <sub>21</sub> H <sub>22</sub> ClFN <sub>4</sub> O <sub>2</sub>
Halopenium Chloride	Unclassified	7008-13-1		C <sub>22</sub> H <sub>30</sub> BrCl <sub>2</sub> NO
Haloperidol	Antispasmodic	52-86-8	Y	C <sub>21</sub> H <sub>23</sub> ClFNO <sub>2</sub>
Haloperidol Decanoate	Antipsychotic	74050-97-8		C <sub>31</sub> H <sub>41</sub> ClFNO <sub>3</sub>
Halopredone Acetate	Antiinflammatory	57781-14-3		C <sub>25</sub> H <sub>29</sub> BrF <sub>2</sub> O <sub>7</sub>
Haloprogestrone	Progestogen	3538-57-6		C <sub>21</sub> H <sub>28</sub> BrFO <sub>2</sub>
Haloprogin	Antibacterial	777-11-7		C <sub>9</sub> H <sub>4</sub> Cl <sub>3</sub> IO
Halothane	Anesthetic	151-67-7		C <sub>2</sub> HBrClF <sub>3</sub>
Haloxazolam	Sedative	59128-97-1		C <sub>17</sub> H <sub>14</sub> BrFN <sub>2</sub> O <sub>2</sub>
Haloxon	Anthelmintic	321-55-1		C <sub>14</sub> H <sub>14</sub> Cl <sub>3</sub> O <sub>6</sub> P
Hepronicate	Vasodilator	7237-81-2		C <sub>28</sub> H <sub>31</sub> N <sub>3</sub> O <sub>6</sub>
Heptabarbital	Sedative	509-86-4		C <sub>13</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>
Heptaminol	Antihypotensive	372-66-7		C <sub>8</sub> H <sub>19</sub> NO
Heptaverine	Antispasmodic	54063-48-8		C <sub>18</sub> H <sub>25</sub> N
Heptolamide	Antidepressant	1034-82-8		C <sub>15</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub> S
Hepzidine	Antidepressant	1096-72-6		C <sub>21</sub> H <sub>25</sub> NO
Hetacillin	Antibiotic	3511-16-8		C <sub>19</sub> H <sub>23</sub> N <sub>3</sub> O <sub>4</sub> S
Heteronium Bromide	Mydriatic	7247-57-6		C <sub>18</sub> H <sub>22</sub> BrNO <sub>3</sub> S
Hexacyclonate Sodium	Nootropic	7491-42-1		C <sub>9</sub> H <sub>16</sub> O <sub>3</sub>
Hexacyprone	Mydriatic	892-01-3		C <sub>16</sub> H <sub>20</sub> O <sub>3</sub>
Hexadiline	Vasodilator	3626-67-3		C <sub>19</sub> H <sub>33</sub> N
Hexafluorenium	Muscle Relaxant	4844-10-4		C <sub>36</sub> H <sub>42</sub> Br <sub>2</sub> N <sub>2</sub>
Hexamethonium Bromide	Antihypertensive	55-97-0		C <sub>12</sub> H <sub>30</sub> Br <sub>2</sub> N <sub>2</sub>
Hexamidine	Antitumor	125-33-7		C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Hexapradol	Unclassified	15599-37-8		C <sub>19</sub> H <sub>25</sub> NO
Hexapropfen	Antiinflammatory	24645-20-3		C <sub>15</sub> H <sub>20</sub> O <sub>2</sub>
Hexapropymate	Sedative	358-52-1		C <sub>10</sub> H <sub>15</sub> NO <sub>2</sub>
Hexasonium Iodide	Antispasmodic	25330-82-9		C <sub>18</sub> H <sub>27</sub> IO <sub>2</sub> S
Hexazole	Unclassified	4671-03-8		C <sub>10</sub> H <sub>17</sub> N <sub>3</sub>
Hexcarbacholine Bromide	Muscle Relaxant	306-41-2		C <sub>20</sub> H <sub>26</sub> N <sub>4</sub> O <sub>2</sub>
Hexedine	Antibacterial	5980-31-4		C <sub>22</sub> H <sub>45</sub> N <sub>3</sub>
Hexestrol	Estrogen	84-16-2		C <sub>18</sub> H <sub>22</sub> O <sub>2</sub>
Hexobarbital	Sedative	56-29-1		C <sub>12</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>
Hexobendine	Vasodilator	54-03-5		C <sub>30</sub> H <sub>44</sub> N <sub>2</sub> O <sub>10</sub>
Hexoprenaline	Bronchodilator	3215-70-1		C <sub>22</sub> H <sub>32</sub> N <sub>2</sub> O <sub>6</sub>
Hexylcaine	Anesthetic	532-77-4		C <sub>16</sub> H <sub>23</sub> NO <sub>2</sub>
Hexylresorcinol	Anthelmintic	136-77-6		C <sub>12</sub> H <sub>18</sub> O <sub>2</sub>
Histamine	Antineoplastic	51-45-6		C <sub>5</sub> H <sub>9</sub> N <sub>3</sub>
Histapyrrodine	Antihistaminic	493-80-1		C <sub>19</sub> H <sub>24</sub> N <sub>2</sub>
Homarylamine	Muscle Relaxant	451-77-4		C <sub>10</sub> H <sub>13</sub> NO <sub>2</sub>
Homatropine Hydrobromide	Mydriatic	87-00-3		C <sub>16</sub> H <sub>21</sub> NO <sub>3</sub>
Homatropine Methylbromide	Mydriatic	31610-86-3	Y	C <sub>17</sub> H <sub>24</sub> BrNO <sub>3</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Homidium Bromide	Anthelmintic	1239-45-8		C <sub>21</sub> H <sub>20</sub> BrN <sub>3</sub>
Homochlorcyclizine	Antihistaminic	848-53-3		C <sub>19</sub> H <sub>23</sub> ClN <sub>2</sub>
Homofenazine	Sedative	3833-99-6		C <sub>23</sub> H <sub>28</sub> F <sub>3</sub> N <sub>3</sub> OS
Homopipramol	Antidepressant	35142-68-8		C <sub>24</sub> H <sub>31</sub> N <sub>3</sub> O
Homosalate	Dermatologic	118-56-9		C <sub>16</sub> H <sub>22</sub> O <sub>3</sub>
Homprenorphine	Analgesic	16549-56-7		C <sub>28</sub> H <sub>37</sub> NO <sub>4</sub>
Hopantenic Acid	Nootropic	18679-90-8		C <sub>10</sub> H <sub>19</sub> NO <sub>5</sub>
Hoquizil	Bronchodilator	21560-59-8		C <sub>19</sub> H <sub>26</sub> N <sub>4</sub> O <sub>5</sub>
Hycanthon	Anthelmintic	3105-97-3		C <sub>20</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub> S
Hydracarbazine	Diuretic	3614-47-9		C <sub>5</sub> H <sub>7</sub> N <sub>5</sub> O
Hydralazine	Antihypertensive	86-54-4	Y	C <sub>8</sub> H <sub>8</sub> N <sub>4</sub>
Hydrastine	Cardiotonic	118-08-1		C <sub>21</sub> H <sub>21</sub> NO <sub>6</sub>
Hydrastinine	Cardiotonic	6592-85-4		C <sub>11</sub> H <sub>13</sub> NO <sub>3</sub>
Hydrobentizide	Diuretic	13957-38-5		C <sub>15</sub> H <sub>16</sub> ClN <sub>3</sub> O <sub>4</sub> S <sub>3</sub>
Hydrochlorothiazide	Diuretic	58-93-5	Y	C <sub>7</sub> H <sub>8</sub> ClN <sub>3</sub> O <sub>4</sub> S <sub>2</sub>
Hydrocodone	Antitussive	125-29-1	Y	C <sub>18</sub> H <sub>21</sub> NO <sub>3</sub>
Hydrocortamate	Glucocorticoid	76-47-1		C <sub>27</sub> H <sub>41</sub> NO <sub>6</sub>
Hydrocortisone	Glucocorticoid	50-23-7	Y	C <sub>21</sub> H <sub>30</sub> O <sub>5</sub>
Hydrocortisone Aceponate	Glucocorticoid	74050-20-7		C <sub>26</sub> H <sub>36</sub> O <sub>7</sub>
Hydrocortisone Acetate	Glucocorticoid	50-03-3		C <sub>23</sub> H <sub>32</sub> O <sub>6</sub>
Hydrocortisone Buteptrate	Glucocorticoid	72590-77-3		C <sub>28</sub> H <sub>40</sub> O <sub>7</sub>
Hydrocortisone Butyrate	Glucocorticoid	13609-67-1		C <sub>25</sub> H <sub>36</sub> O <sub>6</sub>
Hydrocortisone Cypionate	Glucocorticoid	508-99-6		C <sub>29</sub> H <sub>42</sub> O <sub>6</sub>
Hydrocortisone Hemisuccinate	Glucocorticoid	2203-97-6		C <sub>25</sub> H <sub>34</sub> O <sub>8</sub>
Hydrocortisone Sodium Phosphate	Glucocorticoid	3863-59-0		C <sub>21</sub> H <sub>31</sub> O <sub>8</sub> P
Hydrocortisone Tebutate	Glucocorticoid	508-96-3		C <sub>27</sub> H <sub>40</sub> O <sub>6</sub>
Hydrocortisone Valerate	Glucocorticoid	57524-89-7		C <sub>26</sub> H <sub>38</sub> O <sub>6</sub>
Hydrocotamine	Hemostatic	550-10-7		C <sub>12</sub> H <sub>15</sub> NO <sub>3</sub>
Hydroflumethiazide	Antihypertensive	135-09-1	Y	C <sub>8</sub> H <sub>8</sub> F <sub>3</sub> N <sub>3</sub> O <sub>4</sub> S <sub>2</sub>
Hydromadinone	Progestogen	16469-74-2		C <sub>21</sub> H <sub>29</sub> ClO <sub>3</sub>
Hydromorfinol	Analgesic	2183-56-4		C <sub>17</sub> H <sub>21</sub> NO <sub>4</sub>
Hydromorphone	Analgesic	466-99-9	Y	C <sub>17</sub> H <sub>19</sub> NO <sub>3</sub>
Hydroxindasate	Unclassified	7008-14-2		C <sub>21</sub> H <sub>24</sub> N <sub>2</sub> O <sub>3</sub>
Hydroxindasol	Unclassified	7008-15-3		C <sub>19</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>
Hydroxyamphetamine	Adrenergic	103-86-6		C <sub>9</sub> H <sub>13</sub> NO
Hydroxychloroquine	Antimalarial	118-42-3	Y	C <sub>18</sub> H <sub>26</sub> ClN <sub>3</sub> O
Hydroxydione Sodium Succinate	Anesthetic	80-96-6		C <sub>25</sub> H <sub>36</sub> O <sub>6</sub>
Hydroxyhexamide	Antidiabetic	3168-01-2		C <sub>15</sub> H <sub>22</sub> N <sub>2</sub> O <sub>4</sub> S
Hydroxypethidine	Analgesic	468-56-4		C <sub>15</sub> H <sub>21</sub> NO <sub>3</sub>
Hydroxyphenamate	Anxiolytic	50-19-1		C <sub>11</sub> H <sub>15</sub> NO <sub>3</sub>
Hydroxyprocaine	Analgesic	487-53-6		C <sub>13</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub>
Hydroxyprogesterone	Progestogen	68-96-2		C <sub>21</sub> H <sub>30</sub> O <sub>3</sub>
Hydroxyprogesterone Caproate	Progestogen	630-56-8		C <sub>27</sub> H <sub>40</sub> O <sub>4</sub>
Hydroxypyridine Tartrate	Analgesic	7008-17-5		C <sub>9</sub> H <sub>9</sub> NO <sub>6</sub>
Hydroxystenozole	Unclassified	19120-01-5		C <sub>21</sub> H <sub>30</sub> N <sub>2</sub> O
Hydroxystilbamidine	Antiprotozoal	495-99-8		C <sub>16</sub> H <sub>16</sub> N <sub>4</sub> O
Hydroxytetracaine	Anesthetic	490-98-2		C <sub>15</sub> H <sub>24</sub> N <sub>2</sub> O <sub>3</sub>
Hydroxytoluic Acid	Antiinflammatory	83-40-9		C <sub>8</sub> H <sub>8</sub> O <sub>3</sub>
Hydroxyurea	Antineoplastic	127-07-1	Y	CH <sub>4</sub> N <sub>2</sub> O <sub>2</sub>
Hydroxyzine	Anxiolytic	68-88-2	Y	C <sub>21</sub> H <sub>27</sub> ClN <sub>2</sub> O <sub>2</sub>
Hydroxyzine Pamoate	Anxiolytic	130-85-8		C <sub>23</sub> H <sub>16</sub> O <sub>6</sub>
Hymecromone	Choleretic	90-33-5		C <sub>10</sub> H <sub>8</sub> O <sub>3</sub>
Hyoscyamine	Antispasmodic	101-31-5		C <sub>17</sub> H <sub>23</sub> NO <sub>3</sub>
Hypericin	Antidepressant	548-04-9		C <sub>30</sub> H <sub>16</sub> O <sub>8</sub>
Ibacinabine	Antiviral	611-53-0		C <sub>9</sub> H <sub>12</sub> IN <sub>3</sub> O <sub>4</sub>
Ibafloxacin	Antibacterial	91618-36-9		C <sub>15</sub> H <sub>14</sub> FNO <sub>3</sub>
Ibandronate	Bone Resorption Inhibitor	114084-78-5		C <sub>9</sub> H <sub>23</sub> NO <sub>7</sub> P <sub>2</sub>
Ibazocine	Analgesic	57653-28-8		C <sub>20</sub> H <sub>29</sub> NO
Ibopamine	Cardiotonic	66195-31-1	Y	C <sub>17</sub> H <sub>25</sub> NO <sub>4</sub>
Ibrolipim	Antiobesity	133208-93-2		C <sub>19</sub> H <sub>20</sub> BrN <sub>2</sub> O <sub>4</sub> P
Ibrotamide	Sedative	466-14-8		C <sub>7</sub> H <sub>14</sub> BrNO
Ibudilast	Vasodilator	50847-11-5	Y	C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O
Ibufenac	Analgesic	1553-60-2		C <sub>12</sub> H <sub>16</sub> O <sub>2</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Ibuprofen	Antiinflammatory	15687-27-1	Y	C <sub>13</sub> H <sub>18</sub> O <sub>2</sub>
Ibuprofen Piconol	Antiinflammatory	64622-45-3		C <sub>19</sub> H <sub>22</sub> NO <sub>2</sub>
Ibuproxam	Antiinflammatory	53648-05-8		C <sub>13</sub> H <sub>19</sub> NO <sub>2</sub>
Ibutamoren Mesylate	Pituitary	159634-47-6		C <sub>27</sub> H <sub>36</sub> N <sub>4</sub> O <sub>5</sub> S
Ibuterol	Bronchodilator	53034-85-8		C <sub>20</sub> H <sub>31</sub> NO <sub>5</sub>
Ibutilide	Antiarrhythmic	122647-31-8		C <sub>20</sub> H <sub>36</sub> N <sub>2</sub> O <sub>3</sub> S
Ibuproverine	Antispasmodic	31221-85-9		C <sub>18</sub> H <sub>26</sub> O <sub>3</sub>
Iclaprim	Antibacterial	192314-93-5		C <sub>19</sub> H <sub>22</sub> N <sub>4</sub> O <sub>3</sub>
Iclazepam	Anxiolytic	57916-70-8		C <sub>21</sub> H <sub>21</sub> ClN <sub>2</sub> O <sub>2</sub>
Icodulinum	Unclassified	138511-81-6		C <sub>10</sub> H <sub>10</sub> N <sub>2</sub> OS
Icofungipen	Antifungal	198022-65-0		C <sub>7</sub> H <sub>11</sub> NO <sub>2</sub>
Icometasone Enbutate	Steroid	103466-73-5		C <sub>28</sub> H <sub>37</sub> ClO <sub>7</sub>
Icomucret	Unclassified	54845-95-3		C <sub>20</sub> H <sub>32</sub> O <sub>3</sub>
Icopezil Maleate	Nootropic	145508-78-7		C <sub>23</sub> H <sub>25</sub> N <sub>3</sub> O <sub>2</sub>
Icosapent	Antihyperlipidemic	10417-94-4	Y	C <sub>20</sub> H <sub>30</sub> O <sub>2</sub>
Icospiramide	Antiinflammatory	79449-99-3		C <sub>28</sub> H <sub>31</sub> F <sub>2</sub> N <sub>5</sub> O <sub>2</sub>
Icotidine	Antihistaminic	71351-79-6		C <sub>21</sub> H <sub>25</sub> N <sub>5</sub> O <sub>2</sub>
Icrocaptide	Antiinflammatory	169543-49-1		C <sub>21</sub> H <sub>40</sub> N <sub>8</sub> O <sub>5</sub>
Idarubicin	Antineoplastic	58957-92-9	Y	C <sub>26</sub> H <sub>27</sub> NO <sub>9</sub>
Idaverine	Antispasmodic	100927-13-7		C <sub>24</sub> H <sub>39</sub> N <sub>3</sub> O <sub>3</sub>
Idazoxan	Antiparkinsonian	79944-58-4		C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>
Idebenone	Nootropic	58186-27-9	Y	C <sub>19</sub> H <sub>30</sub> O <sub>5</sub>
Idenast	Bronchodilator	108674-88-0		C <sub>28</sub> H <sub>31</sub> FN <sub>4</sub> O <sub>2</sub>
Idoxifene	Antineoplastic	116057-75-1		C <sub>28</sub> H <sub>30</sub> INO
Idoxuridine	Antiviral	54-42-2		C <sub>9</sub> H <sub>11</sub> IN <sub>2</sub> O <sub>5</sub>
Idralfidine	Sedative	95668-38-5		C <sub>11</sub> H <sub>14</sub> N <sub>4</sub> O
Idramantone	Unclassified	20098-14-0		C <sub>10</sub> H <sub>14</sub> O <sub>2</sub>
Idrapril	Antihypertensive	127420-24-0		C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> O <sub>5</sub>
Idremcinal	Gastroprokinetic	110480-13-2		C <sub>39</sub> H <sub>69</sub> NO <sub>12</sub>
Idrocilamide	Muscle Relaxant	6961-46-2		C <sub>11</sub> H <sub>13</sub> NO <sub>2</sub>
Idronoxil	Antineoplastic	81267-65-4	Y	C <sub>15</sub> H <sub>12</sub> O <sub>3</sub>
Idropranolol	Antihypertensive	27581-02-8		C <sub>16</sub> H <sub>23</sub> NO <sub>2</sub>
Ifenprodil	Vasodilator	23210-56-2	Y	C <sub>21</sub> H <sub>27</sub> NO <sub>2</sub>
Iferanserlin	Antihypertensive	58754-46-4		C <sub>23</sub> H <sub>28</sub> N <sub>2</sub> O
Ifetroban	Antithrombotic	143443-90-7		C <sub>25</sub> H <sub>32</sub> N <sub>2</sub> O <sub>5</sub>
Ifosfamide	Antineoplastic	3778-73-2		C <sub>7</sub> H <sub>15</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub> P
Ifoxetine	Antidepressant	66208-11-5		C <sub>13</sub> H <sub>19</sub> NO <sub>2</sub>
Iganidipine	Vasodilator	119687-33-1		C <sub>28</sub> H <sub>38</sub> N <sub>4</sub> O <sub>6</sub>
Igmesine	Antidepressant	140850-73-3		C <sub>23</sub> H <sub>29</sub> N
Iguratimod	Immunomodulator	123663-49-0	Y	C <sub>17</sub> H <sub>14</sub> N <sub>2</sub> O <sub>6</sub> S
Ilaprazole	Antiulcerative	172152-36-2	Y	C <sub>19</sub> H <sub>18</sub> N <sub>4</sub> O <sub>2</sub> S
Ilepcimide	Anticonvulsant	82857-82-7		C <sub>15</sub> H <sub>17</sub> NO <sub>3</sub>
Iliparicil	Antithrombotic	137214-72-3		C <sub>16</sub> H <sub>18</sub> O <sub>6</sub> S
Ilmofosine	Antineoplastic	83519-04-4		C <sub>26</sub> H <sub>56</sub> NO <sub>5</sub> PS
Ilomastat	Ophthalmic	142880-36-2		C <sub>20</sub> H <sub>28</sub> N <sub>4</sub> O <sub>4</sub>
Ilonidap	Antiinflammatory	135202-79-8		C <sub>14</sub> H <sub>8</sub> ClFN <sub>2</sub> O <sub>3</sub> S
Iloperidone	Antipsychotic	133454-47-4	Y	C <sub>24</sub> H <sub>27</sub> FN <sub>2</sub> O <sub>4</sub>
Iloprost	Antithrombotic	78919-13-8	Y	C <sub>22</sub> H <sub>32</sub> O <sub>4</sub>
Imafen	Antidepressant	59198-18-4		C <sub>11</sub> H <sub>13</sub> N <sub>3</sub>
Imanixil	Antihypertensive	75689-93-9		C <sub>17</sub> H <sub>17</sub> F <sub>3</sub> N <sub>6</sub> O <sub>2</sub>
Imatinib	Antineoplastic	152459-95-5	Y	C <sub>29</sub> H <sub>31</sub> N <sub>7</sub> O
Imazodan	Cardiotonic	84243-58-3		C <sub>13</sub> H <sub>12</sub> N <sub>4</sub> O
Imcarbofos	Anthelminthic	66608-32-0		C <sub>17</sub> H <sub>30</sub> N <sub>4</sub> O <sub>7</sub> P <sub>2</sub> S <sub>2</sub>
Imexon	Immunomodulator	59643-91-3		C <sub>4</sub> H <sub>5</sub> N <sub>3</sub> O
Imiclopazine	Antipsychotic	7224-08-0		C <sub>25</sub> H <sub>32</sub> ClN <sub>5</sub> OS
Imidafenacin	Antidepressant	170105-16-5	Y	C <sub>20</sub> H <sub>21</sub> N <sub>3</sub> O
Imidapril	Antihypertensive	89371-37-9	Y	C <sub>20</sub> H <sub>27</sub> N <sub>3</sub> O <sub>6</sub>
Imidaprilat	Antihypertensive	89371-44-8		C <sub>18</sub> H <sub>23</sub> N <sub>3</sub> O <sub>6</sub>
Imidazole Salicylate	Antiinflammatory	288-32-4		C <sub>3</sub> H <sub>4</sub> N <sub>2</sub>
Imidocarb	Antiprotozoal	27885-92-3		C <sub>19</sub> H <sub>20</sub> N <sub>6</sub> O
Imidoline	Antipsychotic	7303-78-8		C <sub>13</sub> H <sub>18</sub> ClN <sub>3</sub> O
Imiglitazar	Antidiabetic	250601-04-8		C <sub>28</sub> H <sub>26</sub> N <sub>2</sub> O <sub>5</sub>
Imiloxan	Antidepressant	81167-16-0		C <sub>14</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Iminophenimide	Unclassified	7008-18-6		C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Imipenem	Antibacterial	64221-86-9		C <sub>12</sub> H <sub>17</sub> N <sub>3</sub> O <sub>4</sub> S
Imipramine	Antidepressant	50-49-7	Y	C <sub>19</sub> H <sub>24</sub> N <sub>2</sub>
Imipraminoxide	Antidepressant	6829-98-7		C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> O
Imiquimod	Antiviral	99011-02-6		C <sub>14</sub> H <sub>16</sub> N <sub>4</sub>
Imirestat	Antidiabetic	89391-50-4		C <sub>15</sub> H <sub>8</sub> F <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Imitrodast	Antiinflammatory	114686-12-3		C <sub>13</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> S
Imolamine	Antianginal	318-23-0		C <sub>14</sub> H <sub>20</sub> N <sub>4</sub> O
Imoxiterol	Bronchodilator	88578-07-8		C <sub>20</sub> H <sub>25</sub> N <sub>3</sub> O <sub>3</sub>
Impacarzine	Anthelminthic	41340-39-0		C <sub>28</sub> H <sub>55</sub> N <sub>5</sub> O <sub>2</sub>
Implitapide	Antihyperlipidemic	177469-96-4		C <sub>35</sub> H <sub>37</sub> N <sub>3</sub> O <sub>2</sub>
Improsulfan	Antineoplastic	13425-98-4		C <sub>8</sub> H <sub>19</sub> NO <sub>6</sub> S <sub>2</sub>
Imuracetam	Nootropic	67542-41-0		C <sub>11</sub> H <sub>18</sub> N <sub>4</sub> O <sub>3</sub>
Inaperisone	Muscle Relaxant	99323-21-4		C <sub>16</sub> H <sub>23</sub> NO
Incadronic Acid	Antineoplastic	124351-85-5		C <sub>8</sub> H <sub>19</sub> NO <sub>6</sub> P <sub>2</sub>
Incyclinide	Dermatologic	15866-90-7	Y	C <sub>19</sub> H <sub>17</sub> NO <sub>7</sub>
Indacaterol	Bronchodilator	312753-06-3		C <sub>24</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub>
Indacrinone	Antihypertensive	56049-88-8		C <sub>18</sub> H <sub>14</sub> Cl <sub>2</sub> O <sub>4</sub>
Indalpine	Antidepressant	63758-79-2		C <sub>15</sub> H <sub>20</sub> N <sub>2</sub>
Indanazoline	Decongestant	40507-78-6		C <sub>12</sub> H <sub>15</sub> N <sub>3</sub>
Indanidine	Antihypotensive	85392-79-6		C <sub>11</sub> H <sub>13</sub> N <sub>5</sub>
Indanorex	Anorexic	16112-96-2		C <sub>12</sub> H <sub>17</sub> NO
Indapamide	Antihypertensive	26807-65-8	Y	C <sub>16</sub> H <sub>16</sub> ClN <sub>3</sub> O <sub>3</sub> S
Indatraline	Antipsychotic	86939-10-8		C <sub>16</sub> H <sub>15</sub> Cl <sub>2</sub> N
Indecainide	Antiarrhythmic	74517-78-5		C <sub>20</sub> H <sub>24</sub> N <sub>2</sub> O
Indeloxazine	Antidepressant	60929-23-9	Y	C <sub>14</sub> H <sub>17</sub> NO <sub>2</sub>
Indenolol	Antiarrhythmic	60607-68-3	Y	C <sub>15</sub> H <sub>21</sub> NO <sub>2</sub>
Indibulin	Antineoplastic	204205-90-3	Y	C <sub>22</sub> H <sub>16</sub> ClN <sub>3</sub> O <sub>2</sub>
Indinavir	Antiviral	150378-17-9	Y	C <sub>36</sub> H <sub>47</sub> N <sub>5</sub> O <sub>4</sub>
Indiplon	Sedative	325715-02-4		C <sub>20</sub> H <sub>16</sub> N <sub>4</sub> O <sub>2</sub> S
Indisetron	Antiemetic	141549-75-9	Y	C <sub>17</sub> H <sub>23</sub> N <sub>5</sub> O
Indisulam	Antineoplastic	165668-41-7		C <sub>14</sub> H <sub>12</sub> ClN <sub>3</sub> O <sub>4</sub> S <sub>2</sub>
Indobufen	Antithrombotic	63610-08-2		C <sub>18</sub> H <sub>17</sub> NO <sub>3</sub>
Indocate	Estrogen	31386-25-1		C <sub>22</sub> H <sub>26</sub> N <sub>2</sub> O <sub>2</sub>
Indolapril	Antihypertensive	80876-01-3		C <sub>24</sub> H <sub>34</sub> N <sub>2</sub> O <sub>5</sub>
Indolidan	Cardiotonic	100643-96-7		C <sub>14</sub> H <sub>15</sub> N <sub>3</sub> O <sub>2</sub>
Indomethacin	Antiinflammatory	53-86-1	Y	C <sub>19</sub> H <sub>16</sub> ClNO <sub>4</sub>
Indopanolol	Antianginal	69907-17-1		C <sub>20</sub> H <sub>23</sub> ClN <sub>2</sub> O <sub>3</sub>
Indopine	Urologic	3569-26-4		C <sub>23</sub> H <sub>28</sub> N <sub>2</sub>
Indoprofen	Analgesic	31842-01-0		C <sub>17</sub> H <sub>15</sub> NO <sub>3</sub>
Indoramim	Antihypertensive	26844-12-2		C <sub>22</sub> H <sub>25</sub> N <sub>3</sub> O
Indorelate	Antihypertensive	73758-06-2		C <sub>13</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>
Indoxole	Antiinflammatory	5034-76-4		C <sub>22</sub> H <sub>19</sub> NO <sub>2</sub>
Indriline	Nootropic	7395-90-6		C <sub>19</sub> H <sub>21</sub> N
Inecalcitol	Bone Resorption Inhibitor	163217-09-2	Y	C <sub>26</sub> H <sub>40</sub> O <sub>3</sub>
Ingliforib	Antidiabetic	186392-65-4		C <sub>23</sub> H <sub>24</sub> ClN <sub>3</sub> O <sub>5</sub>
Inicarone	Anticoagulant	39178-37-5		C <sub>17</sub> H <sub>15</sub> NO <sub>2</sub>
Inocoterone Acetate	Dermatologic	83646-86-0		C <sub>18</sub> H <sub>26</sub> O <sub>3</sub>
Inogatran	Antithrombotic	155415-08-0		C <sub>21</sub> H <sub>38</sub> N <sub>6</sub> O <sub>4</sub>
Inosine Pranobex	Antiviral	58-63-9	Y	C <sub>10</sub> H <sub>12</sub> N <sub>4</sub> O <sub>5</sub>
Inositol Niacinate	Vasodilator	6556-11-2		C <sub>42</sub> H <sub>30</sub> N <sub>6</sub> O <sub>12</sub>
Inproquone	Antiamoebic	436-40-8		C <sub>16</sub> H <sub>22</sub> N <sub>2</sub> O <sub>4</sub>
Intermedine	Antineoplastic	10285-06-0		C <sub>15</sub> H <sub>25</sub> NO <sub>5</sub>
Intoplicine	Antiarrhythmic	125974-72-3		C <sub>21</sub> H <sub>24</sub> N <sub>4</sub> O
Intrazole	Antiinflammatory	15992-13-9		C <sub>17</sub> H <sub>12</sub> ClN <sub>5</sub> O
Intriptyline	Antidepressant	27466-27-9		C <sub>21</sub> H <sub>19</sub> N
Iobutoic Acid	Choleretic	13445-12-0		C <sub>15</sub> H <sub>16</sub> I <sub>3</sub> NO <sub>5</sub>
Iodetryl	Unclassified	7008-02-8		C <sub>20</sub> H <sub>38</sub> I <sub>2</sub> O <sub>2</sub>
Iodobenzoic Acid	Unclassified	1321-07-9		C <sub>7</sub> H <sub>5</sub> IO <sub>2</sub>
Iodocystine	Unclassified	1320-92-9		C <sub>6</sub> H <sub>11</sub> IN <sub>2</sub> O <sub>4</sub> S <sub>2</sub>
Iodoform	Antibacterial	75-47-8		CHI <sub>3</sub>
Iodophthalein Sodium	Laxative	386-17-4		C <sub>20</sub> H <sub>10</sub> I <sub>4</sub> O <sub>4</sub>
Iodoquinol	Antiamoebic	83-73-8		C <sub>9</sub> H <sub>5</sub> I <sub>2</sub> NO

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Iodothiouracil	Antineoplastic	5984-97-4		C <sub>4</sub> H <sub>3</sub> IN <sub>2</sub> OS
Iosimide	Antiinflammatory	79211-10-2		C <sub>21</sub> H <sub>30</sub> I <sub>3</sub> N <sub>3</sub> O <sub>9</sub>
Ipamorelin	Cardiotonic	170851-70-4		C <sub>38</sub> H <sub>49</sub> N <sub>9</sub> O <sub>5</sub>
Ipazilide Fumarate	Antiarrhythmic	115436-73-2		C <sub>24</sub> H <sub>30</sub> N <sub>4</sub> O
Ipenoxazone	Antidepressant	104454-71-9		C <sub>22</sub> H <sub>34</sub> N <sub>2</sub> O <sub>2</sub>
Ipidacrine	Nootropic	62732-44-9		C <sub>12</sub> H <sub>16</sub> N <sub>2</sub>
Ipragratine	Unclassified	22150-28-3		C <sub>20</sub> H <sub>29</sub> NO <sub>3</sub>
Ipramidil	Vasodilator	83656-38-6		C <sub>10</sub> H <sub>16</sub> N <sub>4</sub> O <sub>4</sub>
Ipratropium	Bronchodilator	60205-81-4		C <sub>20</sub> H <sub>30</sub> NO <sub>3</sub>
Ipravacaine	Analgesic	166181-63-1		C <sub>18</sub> H <sub>26</sub> N <sub>2</sub> O
Iprazochrome	Hemostatic	7248-21-7		C <sub>12</sub> H <sub>16</sub> N <sub>4</sub> O <sub>3</sub>
Ipriflavone	Steroid	35212-22-7		C <sub>18</sub> H <sub>16</sub> O <sub>3</sub>
Iprindole	Antidepressant	5560-72-5		C <sub>19</sub> H <sub>28</sub> N <sub>2</sub>
Iproclozide	Antidepressant	3544-35-2		C <sub>11</sub> H <sub>15</sub> ClN <sub>2</sub> O <sub>2</sub>
Iprocrolol	Unclassified	37855-80-4		C <sub>18</sub> H <sub>21</sub> NO <sub>6</sub>
Iproheptine	Antihistaminic	13946-02-6		C <sub>11</sub> H <sub>25</sub> N
Iproniazid	Antidepressant	54-92-2		C <sub>9</sub> H <sub>13</sub> N <sub>3</sub> O
Ipronidazole	Antiprotozoal	14885-29-1		C <sub>7</sub> H <sub>11</sub> N <sub>3</sub> O <sub>2</sub>
Iprotiazem	Antihypertensive	105118-13-6		C <sub>37</sub> H <sub>49</sub> N <sub>3</sub> O <sub>5</sub> S
Iproxamine	Vasodilator	52403-19-7		C <sub>18</sub> H <sub>29</sub> NO <sub>4</sub>
Iprozilamine	Unclassified	55477-19-5		C <sub>13</sub> H <sub>22</sub> ClN <sub>5</sub> S
Ipsalazide	Antiinflammatory	623571-82-4		C <sub>16</sub> H <sub>13</sub> N <sub>3</sub> O <sub>6</sub>
Ipsapirone	Anxiolytic	95847-70-4		C <sub>19</sub> H <sub>23</sub> N <sub>5</sub> O <sub>3</sub> S
Iquindamine	Analgesic	55299-11-1		C <sub>15</sub> H <sub>23</sub> N <sub>3</sub>
Iralukast	Bronchodilator	151581-24-7		C <sub>38</sub> H <sub>37</sub> F <sub>3</sub> O <sub>8</sub> S
Irampanel	Nootropic	206260-33-5		C <sub>18</sub> H <sub>19</sub> N <sub>3</sub> O <sub>2</sub>
Irbesartan	Antihypertensive	138402-11-6	Y	C <sub>25</sub> H <sub>28</sub> N <sub>6</sub> O
Irindalone	Antihypertensive	96478-43-2		C <sub>24</sub> H <sub>29</sub> FN <sub>4</sub> O
Irinotecan	Antineoplastic	97682-44-5		C <sub>33</sub> H <sub>38</sub> N <sub>4</sub> O <sub>6</sub>
Irloxacin	Antibiotic	91524-15-1		C <sub>16</sub> H <sub>13</sub> FN <sub>2</sub> O <sub>3</sub>
Irofulven	Antineoplastic	158440-71-2		C <sub>15</sub> H <sub>18</sub> O <sub>3</sub>
Irolapride	Antiemetic	64779-98-2		C <sub>19</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub>
Iroxanadine	Antihistaminic	276690-58-5		C <sub>14</sub> H <sub>20</sub> N <sub>4</sub> O
Irsogladine	Anticulcerative	57381-26-7	Y	C <sub>9</sub> H <sub>7</sub> Cl <sub>2</sub> N <sub>5</sub>
Irtamazole	Uricosuric	129369-64-8		C <sub>18</sub> H <sub>16</sub> N <sub>4</sub>
Isaglidole	Antidiabetic	110605-64-6		C <sub>11</sub> H <sub>13</sub> FN <sub>4</sub>
Isalmadol	Analgesic	269079-62-1		C <sub>22</sub> H <sub>27</sub> NO <sub>4</sub>
Isalsteine	Mucolytic	116818-99-6		C <sub>14</sub> H <sub>15</sub> NO <sub>6</sub> S
Isamfazon	Antiinflammatory	55902-02-8		C <sub>22</sub> H <sub>23</sub> N <sub>3</sub> O <sub>2</sub>
Isamoltan	Antidepressant	55050-95-8		C <sub>16</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>
Isamoxole	Bronchodilator	57067-46-6		C <sub>12</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>
Isatoribine	Immunomodulator	122970-40-5		C <sub>10</sub> H <sub>12</sub> N <sub>4</sub> O <sub>6</sub> S
Isaxonine	Nootropic	4214-72-6		C <sub>7</sub> H <sub>11</sub> N <sub>3</sub>
Isbogrel	Antithrombotic	89667-40-3		C <sub>18</sub> H <sub>19</sub> NO <sub>2</sub>
Isbufylline	Bronchodilator	90162-60-0		C <sub>11</sub> H <sub>16</sub> N <sub>4</sub> O <sub>2</sub>
Isepamicin	Antibacterial	58152-03-7		C <sub>22</sub> H <sub>43</sub> N <sub>5</sub> O <sub>12</sub>
Isoaminile	Antitussive	77-51-0		C <sub>16</sub> H <sub>24</sub> N <sub>2</sub>
Isobromindione	Anticoagulant	1470-35-5		C <sub>15</sub> H <sub>9</sub> BrO <sub>2</sub>
Isobucaine	Analgesic	14055-89-1		C <sub>15</sub> H <sub>23</sub> NO <sub>2</sub>
Isobutamben	Anesthetic	94-14-4		C <sub>11</sub> H <sub>15</sub> NO <sub>2</sub>
Isocarboxazid	Antidepressant	59-63-2		C <sub>12</sub> H <sub>13</sub> N <sub>3</sub> O <sub>2</sub>
Isoconazole	Antibacterial	27523-40-6		C <sub>18</sub> H <sub>14</sub> Cl <sub>4</sub> N <sub>2</sub> O
Isocromil	Antihistaminic	57009-15-1		C <sub>19</sub> H <sub>16</sub> O <sub>5</sub>
Isocyclamine	Unclassified	105-23-7		C <sub>8</sub> H <sub>17</sub> N
Isoetharine	Bronchodilator	530-08-5		C <sub>13</sub> H <sub>21</sub> NO <sub>3</sub>
Isofezolac	Antiinflammatory	50270-33-2		C <sub>23</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>
Isoflupredone Acetate	Antiinflammatory	338-98-7		C <sub>23</sub> H <sub>29</sub> FO <sub>6</sub>
Isoflurane	Anesthetic	26675-46-7		C <sub>3</sub> H <sub>2</sub> ClF <sub>5</sub> O
Isoflurophate	Cholinergic	55-91-4		C <sub>6</sub> H <sub>14</sub> FO <sub>3</sub> P
Isomazole	Cardiotonic	86315-52-8		C <sub>14</sub> H <sub>13</sub> N <sub>3</sub> O <sub>2</sub> S
Isometamidium Chloride	Anthelminthic	34301-55-8		C <sub>28</sub> H <sub>26</sub> ClN <sub>7</sub>
Isomethadone	Analgesic	466-40-0		C <sub>21</sub> H <sub>27</sub> NO

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Isometheptene	Antimigraine	503-01-5		C <sub>9</sub> H <sub>19</sub> N
Isomolpan	Antipsychotic	107320-86-5		C <sub>15</sub> H <sub>21</sub> NO <sub>2</sub>
Isomylamine	Muscle Relaxant	28815-27-2		C <sub>18</sub> H <sub>35</sub> NO <sub>2</sub>
Isoniazid	Antibiotic	54-85-3	Y	C <sub>6</sub> H <sub>7</sub> N <sub>3</sub> O
Isonixin	Analgesic	57021-61-1		C <sub>14</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Isoprazone	Analgesic	56463-68-4		C <sub>15</sub> H <sub>18</sub> N <sub>2</sub> O
Isoprednidene	Glucocorticoid	17332-61-5		C <sub>22</sub> H <sub>28</sub> O <sub>5</sub>
Isoprofen	Antiinflammatory	57144-56-6		C <sub>15</sub> H <sub>20</sub> O <sub>2</sub>
Isopropamide	Antispasmodic	7492-32-2		C <sub>23</sub> H <sub>33</sub> N <sub>2</sub> O
Isopropicillin	Antibiotic	4780-24-9		C <sub>18</sub> H <sub>22</sub> N <sub>2</sub> O <sub>5</sub> S
Isoproterenol	Bronchodilator	7683-59-2		C <sub>11</sub> H <sub>17</sub> NO <sub>3</sub>
Isosorbide	Antianginal	652-67-5		C <sub>6</sub> H <sub>10</sub> O <sub>4</sub>
Isosorbide Dinitrate	Antianginal	87-33-2	Y	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O <sub>8</sub>
Isosorbide Mononitrate	Vasodilator	16051-77-7		C <sub>6</sub> H <sub>9</sub> NO <sub>6</sub>
Isospaglumic Acid	Nootropic	3106-85-2		C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> O <sub>8</sub>
Isosulpride	Antipsychotic	42792-26-7		C <sub>15</sub> H <sub>23</sub> N <sub>3</sub> O <sub>4</sub> S
Isothipendyl	Antihistaminic	482-15-5		C <sub>16</sub> H <sub>19</sub> N <sub>3</sub> S
Isotiquimide	Antiulcerative	56717-18-1		C <sub>11</sub> H <sub>14</sub> N <sub>2</sub> S
Isotretinoin	Dermatologic	4759-48-2	Y	C <sub>20</sub> H <sub>28</sub> O <sub>2</sub>
Isotretinoin Anisatil	Dermatologic	127471-94-7		C <sub>29</sub> H <sub>36</sub> O <sub>4</sub>
Isovaleramide	Anxiolytic	541-46-8		C <sub>5</sub> H <sub>11</sub> NO
Isoxaprolol	Ophthalmic	75949-60-9		C <sub>19</sub> H <sub>26</sub> N <sub>2</sub> O <sub>3</sub>
Isoxepac	Antiinflammatory	55453-87-7		C <sub>16</sub> H <sub>12</sub> O <sub>4</sub>
Isoxicam	Antiinflammatory	34552-84-6		C <sub>14</sub> H <sub>13</sub> N <sub>3</sub> O <sub>5</sub> S
Isosuprine	Vasodilator	395-28-8		C <sub>18</sub> H <sub>23</sub> NO <sub>3</sub>
Ispinesib Mesylate	Antineoplastic	336113-53-2		C <sub>30</sub> H <sub>33</sub> ClN <sub>4</sub> O <sub>2</sub>
Ispronidine	Analgesic	252870-53-4	Y	C <sub>14</sub> H <sub>22</sub> N <sub>2</sub> O
Isradipine	Antihypertensive	75695-93-1	Y	C <sub>19</sub> H <sub>21</sub> N <sub>3</sub> O <sub>5</sub>
Israpafant	Antithrombotic	117279-73-9		C <sub>28</sub> H <sub>29</sub> ClN <sub>4</sub> S
Istaroxime	Antiviral	203737-93-3		C <sub>21</sub> H <sub>32</sub> N <sub>2</sub> O <sub>3</sub>
Istradefylline	Antiparkinsonian	155270-99-8	Y	C <sub>20</sub> H <sub>24</sub> N <sub>4</sub> O <sub>4</sub>
Itameline	Antipsychotic	145071-44-9	Y	C <sub>14</sub> H <sub>15</sub> ClN <sub>2</sub> O <sub>3</sub>
Itanoxone	Analgesic	58182-63-1		C <sub>17</sub> H <sub>13</sub> ClO <sub>3</sub>
Itasetron	Antidepressant	123258-84-4		C <sub>16</sub> H <sub>20</sub> N <sub>4</sub> O <sub>2</sub>
Itazigrel	Anticoagulant	70529-35-0		C <sub>18</sub> H <sub>14</sub> F <sub>3</sub> NO <sub>2</sub> S
Itopride	Gastroprokinetic	122898-67-3		C <sub>20</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub>
Itraconazole	Antifungal	84625-61-6	Y	C <sub>35</sub> H <sub>38</sub> Cl <sub>2</sub> N <sub>8</sub> O <sub>4</sub>
Itriglumide	Gastroprokinetic	201605-51-8		C <sub>33</sub> H <sub>38</sub> N <sub>2</sub> O <sub>4</sub>
Itrocainide	Antiarrhythmic	90828-99-2		C <sub>23</sub> H <sub>27</sub> N <sub>3</sub> O
Itrocinonide	Steroid	106033-96-9		C <sub>29</sub> H <sub>38</sub> F <sub>2</sub> O <sub>9</sub>
Ivabradine	Antihypotensive	155974-00-8	Y	C <sub>27</sub> H <sub>36</sub> N <sub>2</sub> O <sub>5</sub>
Ivarimod	Antiarrhythmic	53003-81-9		C <sub>30</sub> H <sub>44</sub> N <sub>2</sub> O <sub>5</sub>
Ivoqualine	Anxiolytic	72714-75-1		C <sub>20</sub> H <sub>26</sub> N <sub>2</sub> O
Ixabepilone	Antineoplastic	219989-84-1		C <sub>27</sub> H <sub>42</sub> N <sub>2</sub> O <sub>5</sub> S
Izonsteride	Antineoplastic	176975-26-1		C <sub>24</sub> H <sub>26</sub> N <sub>2</sub> O <sub>5</sub> S <sub>2</sub>
Josamycin	Antibiotic	16846-24-5	Y	C <sub>42</sub> H <sub>69</sub> NO <sub>15</sub>
Kainic Acid	Anthelminthic	487-79-6		C <sub>10</sub> H <sub>15</sub> NO <sub>4</sub>
Kalafungin	Antifungal	11048-15-0		C <sub>16</sub> H <sub>12</sub> O <sub>6</sub>
Kanamycin Sulfate	Antibiotic	59-01-8		C <sub>18</sub> H <sub>36</sub> N <sub>4</sub> O <sub>11</sub>
Kebuzone	Antirheumatic	853-34-9		C <sub>19</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>
Keracyanin	Unclassified	28338-59-2		C <sub>27</sub> H <sub>31</sub> ClO <sub>15</sub>
Ketamine	Anesthetic	6740-88-1		C <sub>13</sub> H <sub>16</sub> CINO
Ketanserin	Antihypertensive	74050-98-9		C <sub>22</sub> H <sub>22</sub> FN <sub>3</sub> O <sub>3</sub>
Ketazocine	Analgesic	36292-69-0		C <sub>18</sub> H <sub>23</sub> NO <sub>2</sub>
Ketazolam	Anxiolytic	27223-35-4	Y	C <sub>20</sub> H <sub>17</sub> ClN <sub>2</sub> O <sub>3</sub>
Kethoxal	Antiviral	27762-78-3		C <sub>6</sub> H <sub>12</sub> O <sub>4</sub>
Ketipramine Fumarate	Antidepressant	796-29-2		C <sub>19</sub> H <sub>22</sub> N <sub>2</sub> O
Ketobemidone	Analgesic	469-79-4		C <sub>15</sub> H <sub>21</sub> NO <sub>2</sub>
Ketocaine	Analgesic	1092-46-2		C <sub>18</sub> H <sub>29</sub> NO <sub>2</sub>
Ketocainol	Antiarrhythmic	7488-92-8		C <sub>18</sub> H <sub>31</sub> NO <sub>2</sub>
Ketoconazole	Antifungal	65277-42-1	Y	C <sub>26</sub> H <sub>28</sub> Cl <sub>2</sub> N <sub>4</sub> O <sub>4</sub>
Ketoprofen	Antiinflammatory	22071-15-4	Y	C <sub>16</sub> H <sub>14</sub> O <sub>3</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Ketorfanol	Analgesic	79798-39-3		C <sub>20</sub> H <sub>25</sub> NO <sub>2</sub>
Ketorolac	Analgesic	74103-06-3	Y	C <sub>15</sub> H <sub>13</sub> NO <sub>3</sub>
Ketotifen	Antihistaminic	34580-13-7	Y	C <sub>19</sub> H <sub>19</sub> NOS
Ketotrexate	Antineoplastic	52196-22-2		C <sub>21</sub> H <sub>27</sub> N <sub>7</sub> O <sub>6</sub>
Khellin	Vasodilator	82-02-0		C <sub>14</sub> H <sub>12</sub> O <sub>5</sub>
Khelloside	Antihyperlipidemic	17226-75-4		C <sub>19</sub> H <sub>20</sub> O <sub>10</sub>
Kitasamycin	Antibacterial	1392-21-8		C <sub>35</sub> H <sub>59</sub> NO <sub>13</sub>
Labetalol	Antihypertensive	36894-69-6	Y	C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> O <sub>3</sub>
Lachesine Chloride	Unclassified	1164-38-1		C <sub>20</sub> H <sub>26</sub> ClNO <sub>3</sub>
Lacidipine	Antihypertensive	103890-78-4	Y	C <sub>26</sub> H <sub>33</sub> NO <sub>6</sub>
Lacosamide	Antiprotozoal	175481-36-4	Y	C <sub>13</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>
Lactitol	Laxative	585-86-4		C <sub>12</sub> H <sub>24</sub> O <sub>11</sub>
Lactulose	Laxative	4618-18-2	Y	C <sub>12</sub> H <sub>22</sub> O <sub>11</sub>
Ladirubicin	Antineoplastic	171047-47-5		C <sub>29</sub> H <sub>31</sub> NO <sub>11</sub> S
Ladostigil Tartrate	Nootropic	209394-27-4		C <sub>16</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>
Laflunimus	Immunomodulator	147076-36-6		C <sub>15</sub> H <sub>13</sub> F <sub>3</sub> N <sub>2</sub> O <sub>2</sub>
Lafutidine	Antiulcerative	118288-08-7	Y	C <sub>22</sub> H <sub>29</sub> N <sub>3</sub> O <sub>4</sub> S
Lagatide	Unclassified	157476-77-2		C <sub>33</sub> H <sub>58</sub> N <sub>10</sub> O <sub>9</sub>
Laidlomycin Propionate Potassium	Antibiotic	78734-47-1		C <sub>40</sub> H <sub>66</sub> O <sub>13</sub>
Lamifiban	Antithrombotic	144412-49-7		C <sub>24</sub> H <sub>28</sub> N <sub>4</sub> O <sub>6</sub>
Lamivudine	Antiviral	134678-17-4	Y	C <sub>8</sub> H <sub>11</sub> N <sub>3</sub> O <sub>3</sub> S
Lamotrigine	Anticonvulsant	84057-84-1	Y	C <sub>9</sub> H <sub>7</sub> Cl <sub>2</sub> N <sub>5</sub>
Lamtidine	Antiulcerative	73278-54-3		C <sub>18</sub> H <sub>28</sub> N <sub>6</sub> O
Lanatoside C	Cardiotonic	17575-22-3		C <sub>49</sub> H <sub>76</sub> O <sub>20</sub>
Landirolol	Antihypertensive	133242-30-5		C <sub>25</sub> H <sub>39</sub> N <sub>3</sub> O <sub>8</sub>
Lanepitant	Antiemetic	170566-84-4		C <sub>33</sub> H <sub>45</sub> N <sub>5</sub> O <sub>3</sub>
Lanicemine	Nootropic	153322-05-5		C <sub>13</sub> H <sub>14</sub> N <sub>2</sub>
Laniquidar	Antineoplastic	197509-46-9		C <sub>37</sub> H <sub>36</sub> N <sub>4</sub> O <sub>3</sub>
Lanoconazole	Antifungal	101530-10-3		C <sub>14</sub> H <sub>10</sub> ClN <sub>3</sub> S <sub>2</sub>
Lanperisone	Muscle Relaxant	116287-14-0		C <sub>15</sub> H <sub>18</sub> F <sub>3</sub> NO
Lanproston	Prostaglandin	105674-77-9		C <sub>24</sub> H <sub>31</sub> ClO <sub>7</sub>
Lansoprazole	Antiulcerative	103577-45-3	Y	C <sub>16</sub> H <sub>14</sub> F <sub>3</sub> N <sub>3</sub> O <sub>2</sub> S
Lantanoprost	Prostaglandin	1402923-77-6		C <sub>30</sub> H <sub>47</sub> BO <sub>5</sub>
Lapatinib Ditosylate	Antineoplastic	231277-92-2	Y	C <sub>29</sub> H <sub>26</sub> ClFN <sub>4</sub> O <sub>4</sub> S
Lapisteride	Antineoplastic	142139-60-4		C <sub>29</sub> H <sub>40</sub> N <sub>2</sub> O <sub>3</sub>
Laprafylline	Bronchodilator	90749-32-9		C <sub>29</sub> H <sub>36</sub> N <sub>6</sub> O <sub>2</sub>
Laquinimod	Nootropic	248281-84-7	Y	C <sub>19</sub> H <sub>17</sub> ClN <sub>2</sub> O <sub>3</sub>
Lasalocid	Antibiotic	25999-31-9		C <sub>34</sub> H <sub>54</sub> O <sub>8</sub>
Lasinavir	Antiviral	175385-62-3		C <sub>35</sub> H <sub>53</sub> N <sub>3</sub> O <sub>9</sub>
Lasofixifene	Antineoplastic	180916-16-9		C <sub>28</sub> H <sub>31</sub> NO <sub>2</sub>
Latanoprost	Antiglaucoma	130209-82-4		C <sub>26</sub> H <sub>40</sub> O <sub>5</sub>
Latidectin	Antiprotozoal	926308-28-3		C <sub>46</sub> H <sub>61</sub> NO <sub>11</sub>
Laurcetium Bromide	Unclassified	1794-75-8		C <sub>18</sub> H <sub>38</sub> BrNO <sub>2</sub>
Laureth 10s	Contraceptive	13081-34-0		C <sub>16</sub> H <sub>34</sub> O <sub>2</sub> S
Laurixamine	Sedative	7617-74-5		C <sub>15</sub> H <sub>33</sub> NO
Lauroguadine	Antiprotozoal	135-43-3		C <sub>20</sub> H <sub>36</sub> N <sub>6</sub> O
Lavoltidine Succinate	Antiulcerative	76956-02-0		C <sub>19</sub> H <sub>29</sub> N <sub>5</sub> O <sub>2</sub>
Lazabemide	Antiparkinsonian	103878-84-8		C <sub>8</sub> H <sub>10</sub> ClN <sub>3</sub> O
Lecimibide	Antihyperlipidemic	130804-35-2		C <sub>34</sub> H <sub>40</sub> F <sub>2</sub> N <sub>4</sub> OS
Leco Zotan	Nootropic	434283-16-6		C <sub>28</sub> H <sub>29</sub> N <sub>5</sub> O <sub>3</sub>
Ledazerol	Antihypertensive	434283-16-6		C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>
Ledoxantrone Trihydrochloride	Antineoplastic	113457-05-9		C <sub>21</sub> H <sub>27</sub> N <sub>5</sub> OS
Lefetamine	Analgesic	7262-75-1		C <sub>16</sub> H <sub>19</sub> N
Leflunomide	Antirheumatic	75706-12-6	Y	C <sub>12</sub> H <sub>19</sub> F <sub>3</sub> N <sub>2</sub> O <sub>2</sub>
Leiopyrrole	Unclassified	5633-16-9		C <sub>23</sub> H <sub>28</sub> N <sub>2</sub> O
Lemidosul	Unclassified	88041-40-1		C <sub>12</sub> H <sub>19</sub> NO <sub>3</sub> S
Lemildipine	Antiarrhythmic	94739-29-4		C <sub>20</sub> H <sub>22</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>6</sub>
Leminoprazole	Antiulcerative	104340-86-5		C <sub>19</sub> H <sub>23</sub> N <sub>3</sub> OS
Lemuteporfin	Antineoplastic	215808-49-4		C <sub>44</sub> H <sub>48</sub> N <sub>4</sub> O <sub>10</sub>
Lenalidomide	Immunomodulator	191732-72-6	Y	C <sub>13</sub> H <sub>13</sub> N <sub>3</sub> O <sub>3</sub>
Lenampicillin	Antibacterial	86273-18-9		C <sub>21</sub> H <sub>23</sub> N <sub>3</sub> O <sub>7</sub> S
Lenapenem	Antibacterial	149951-16-6		C <sub>18</sub> H <sub>29</sub> N <sub>3</sub> O <sub>5</sub> S
Leniquinsin	Antihypertensive	10351-50-5		C <sub>20</sub> H <sub>20</sub> N <sub>2</sub> O <sub>4</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Lenperone	Antipsychotic	24678-13-5		C <sub>22</sub> H <sub>23</sub> F <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Leptacline	Antihypertensive	5005-72-1		C <sub>12</sub> H <sub>23</sub> N
Lercanidipine	Antihypertensive	100427-26-7	Y	C <sub>36</sub> H <sub>41</sub> N <sub>3</sub> O <sub>6</sub>
Lergotrile	Pituitary	36945-03-6		C <sub>17</sub> H <sub>18</sub> ClN <sub>3</sub>
Lerisetron	Antiemetic	143257-98-1		C <sub>18</sub> H <sub>20</sub> N <sub>4</sub>
Lesopitron	Anxiolytic	132449-46-8		C <sub>15</sub> H <sub>21</sub> ClN <sub>6</sub>
Lestaurtinib	Antineoplastic	111358-88-4		C <sub>26</sub> H <sub>21</sub> N <sub>3</sub> O <sub>4</sub>
Leteprenim	Nootropic	138117-50-7		C <sub>15</sub> H <sub>13</sub> N <sub>5</sub> O <sub>4</sub>
Lethane Ethyl Thiocyanate)	Anesthetic	112-56-1		C <sub>9</sub> H <sub>17</sub> NO <sub>2</sub> S
Letimide	Analgesic	26513-90-6		C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>
Letosteine	Mucolytic	53943-88-7	Y	C <sub>10</sub> H <sub>17</sub> NO <sub>4</sub> S <sub>2</sub>
Letrazuril	Antibacterial	103337-74-2		C <sub>17</sub> H <sub>9</sub> Cl <sub>2</sub> FN <sub>4</sub> O <sub>2</sub>
Letrozole	Antineoplastic	112809-51-5	Y	C <sub>17</sub> H <sub>11</sub> N <sub>5</sub>
Leucinocaine	Analgesic	92-23-9		C <sub>17</sub> H <sub>28</sub> N <sub>2</sub> O <sub>2</sub>
Leucocianidol	Capillary Protectant	480-17-1		C <sub>15</sub> H <sub>14</sub> O <sub>7</sub>
Leucovorin	Antidote	58-05-9		C <sub>20</sub> H <sub>23</sub> N <sub>7</sub> O <sub>7</sub>
Leurubicin	Antineoplastic	70774-25-3		C <sub>33</sub> H <sub>40</sub> N <sub>2</sub> O <sub>12</sub>
Levalbuterol	Bronchodilator	34391-04-3		C <sub>13</sub> H <sub>21</sub> NO <sub>3</sub>
Levallorphan	Antidote	152-02-3		C <sub>19</sub> H <sub>25</sub> NO
Levamphetamine Succinate	Anorexic	156-34-3		C <sub>9</sub> H <sub>13</sub> N
Levamisole	Anthelmintic	14769-73-4		C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> S
Levcromakalim	Antihypertensive	94535-50-9		C <sub>16</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>
Levcycloserine	Antibacterial	339-72-0		C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>
Levobutamine Lactobionate	Cardiotonic	61661-06-1		C <sub>18</sub> H <sub>23</sub> NO <sub>3</sub>
Levobutamine Lactobionate	Cardiotonic	96-82-2		C <sub>12</sub> H <sub>22</sub> O <sub>12</sub>
Levemopamil	Antiarrhythmic	101238-51-1		C <sub>23</sub> H <sub>30</sub> N <sub>2</sub>
Levetiracetam	Anticonvulsant	102767-28-2	Y	C <sub>8</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Levisoprenaline	Bronchodilator	51-31-0		C <sub>11</sub> H <sub>17</sub> NO <sub>3</sub>
Levlofedidine	Antihypertensive	81447-78-1		C <sub>11</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>2</sub> O
Levmetamfetamine	Decongestant	33817-09-3		C <sub>10</sub> H <sub>15</sub> N
Levobetaxolol	Antihypertensive	93221-48-8		C <sub>18</sub> H <sub>29</sub> NO <sub>3</sub>
Levobunolol	Antiglaucoma	47141-42-4		C <sub>17</sub> H <sub>25</sub> NO <sub>3</sub>
Levobupivacaine	Anesthetic	27262-47-1		C <sub>18</sub> H <sub>28</sub> N <sub>2</sub> O
Levocabastine	Antihistaminic	79516-68-0		C <sub>26</sub> H <sub>29</sub> FN <sub>2</sub> O <sub>2</sub>
Levocetirizine	Antihistaminic	130018-77-8	Y	C <sub>21</sub> H <sub>25</sub> ClN <sub>2</sub> O <sub>3</sub>
Levodopa	Antiparkinsonian	59-92-7	Y	C <sub>9</sub> H <sub>11</sub> NO <sub>4</sub>
Levodropropizine	Antitussive	99291-25-5	Y	C <sub>13</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>
Levofacetoperane	Anorexic	24558-01-8		C <sub>14</sub> H <sub>19</sub> NO <sub>2</sub>
Levofenfluramine	Anorexic	37577-24-5		C <sub>12</sub> H <sub>16</sub> F <sub>3</sub> N
Levofloxacin	Antibiotic	100986-85-4	Y	C <sub>18</sub> H <sub>20</sub> FN <sub>3</sub> O <sub>4</sub>
Levofuraltadone	Antibacterial	3795-88-8		C <sub>13</sub> H <sub>16</sub> N <sub>4</sub> O <sub>6</sub>
Levolansoprazole	Antilulcerative	138530-95-7		C <sub>16</sub> H <sub>14</sub> F <sub>3</sub> N <sub>3</sub> O <sub>2</sub> S
Levoleucovorin Calcium	Antidote	68538-85-2	Y	C <sub>20</sub> H <sub>23</sub> N <sub>7</sub> O <sub>7</sub>
Levomenol	Antiarrhythmic	23089-26-1		C <sub>15</sub> H <sub>26</sub> O
Levomenthol	Dermatologic	2216-51-5		C <sub>10</sub> H <sub>20</sub> O
Levomepromazine	Analgesic	60-99-1		C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> OS
Levomethadone	Analgesic	125-58-6		C <sub>21</sub> H <sub>27</sub> NO
Levomethadyl Acetate	Analgesic	1477-40-3		C <sub>23</sub> H <sub>31</sub> NO <sub>2</sub>
Levomethorphan	Antitussive	125-70-2		C <sub>18</sub> H <sub>25</sub> NO
Levometiomeprazine	Analgesic	1759-09-7		C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> S <sub>2</sub>
Levomoprolol	Antihypertensive	77164-20-6		C <sub>13</sub> H <sub>21</sub> NO <sub>3</sub>
Levomoramide	Analgesic	5666-11-5		C <sub>25</sub> H <sub>32</sub> N <sub>2</sub> O <sub>2</sub>
Levonantradol	Analgesic	71048-87-8		C <sub>27</sub> H <sub>35</sub> NO <sub>4</sub>
Levonordefrin	Antihypertensive	829-74-3		C <sub>9</sub> H <sub>13</sub> NO <sub>3</sub>
Levonorgestrel	Progestogen	797-63-7	Y	C <sub>21</sub> H <sub>28</sub> O <sub>2</sub>
Levophenacilmorphan	Analgesic	10061-32-2		C <sub>24</sub> H <sub>27</sub> NO <sub>2</sub>
Levopropoxyphene	Antitussive	2338-37-6		C <sub>22</sub> H <sub>29</sub> NO <sub>2</sub>
Levopropylcillin	Antibacterial	3736-12-7		C <sub>18</sub> H <sub>22</sub> N <sub>2</sub> O <sub>5</sub> S
Levopropylhexedrine	Adrenergic	6192-97-8		C <sub>10</sub> H <sub>21</sub> N
Levoprotiline	Antidepressant	76496-68-9		C <sub>20</sub> H <sub>23</sub> NO
Levormeloxifene	Estrogen	78994-23-7		C <sub>30</sub> H <sub>35</sub> NO <sub>3</sub>
Levorphanol	Analgesic	77-07-6	Y	C <sub>17</sub> H <sub>23</sub> NO
Levosalbutamol	Bronchodilator	34391-04-3	Y	C <sub>13</sub> H <sub>21</sub> NO <sub>3</sub>



Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Levosemotiadil	Antiarrhythmic	116476-16-5		C <sub>29</sub> H <sub>32</sub> N <sub>2</sub> O <sub>6</sub> S
Levosimendan	Cardiotonic	141505-33-1		C <sub>14</sub> H <sub>12</sub> N <sub>6</sub> O
Levosulpiride	Antidepressant	23672-07-3	Y	C <sub>15</sub> H <sub>23</sub> N <sub>3</sub> O <sub>4</sub> S
Levotofisopam	Anxiolytic	82059-51-6		C <sub>22</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub>
Levoxadrol	Anesthetic	4792-18-1		C <sub>20</sub> H <sub>23</sub> NO <sub>2</sub>
Lexacalcitol	Dermatologic	131875-08-6		C <sub>29</sub> H <sub>48</sub> O <sub>4</sub>
Lexipafant	Anticoagulant	139133-26-9		C <sub>23</sub> H <sub>30</sub> N <sub>4</sub> O <sub>4</sub> S
Lexithromycin	Antibacterial	53066-26-5		C <sub>38</sub> H <sub>70</sub> N <sub>2</sub> O <sub>13</sub>
Lexofenac	Antiinflammatory	41387-02-4		C <sub>14</sub> H <sub>14</sub> O <sub>3</sub>
Liarozole	Antineoplastic	115575-11-6		C <sub>17</sub> H <sub>13</sub> ClN <sub>4</sub>
Libecillide	Unclassified	27826-45-5		C <sub>23</sub> H <sub>32</sub> N <sub>4</sub> O <sub>7</sub> S
Libenzapril	Antihypertensive	109214-55-3		C <sub>18</sub> H <sub>25</sub> N <sub>3</sub> O <sub>5</sub>
Licarbazepine	Anticonvulsant	29331-92-8		C <sub>15</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Licofelone	Antiinflammatory	156897-06-2		C <sub>23</sub> H <sub>22</sub> ClNO <sub>2</sub>
Licostinel	Antipsychotic	153504-81-5		C <sub>8</sub> H <sub>3</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>4</sub>
Lidadronic Acid	Bone Resorption Inhibitor	63132-38-7		C <sub>5</sub> H <sub>16</sub> N <sub>2</sub> O <sub>6</sub> P <sub>2</sub>
Lidamide	Antidiarrheal	66871-56-5		C <sub>11</sub> H <sub>16</sub> N <sub>4</sub> O
Lidanserin	Anxiolytic	73725-85-6		C <sub>26</sub> H <sub>31</sub> FN <sub>2</sub> O <sub>4</sub>
Lidocaine	Anesthetic	137-58-6		C <sub>14</sub> H <sub>22</sub> N <sub>2</sub> O
Lidoflazine	Vasodilator	3416-26-0		C <sub>30</sub> H <sub>35</sub> F <sub>2</sub> N <sub>3</sub> O
Lidorestat	Antidiabetic	245116-90-9		C <sub>18</sub> H <sub>11</sub> F <sub>3</sub> N <sub>2</sub> O <sub>2</sub> S
Lifarizine	Anticoagulant	119514-66-8		C <sub>29</sub> H <sub>32</sub> N <sub>4</sub>
Lifibrate	Antihyperlipidemic	22204-91-7		C <sub>20</sub> H <sub>21</sub> Cl <sub>2</sub> NO <sub>4</sub>
Lifibrol	Antihyperlipidemic	96609-16-4		C <sub>21</sub> H <sub>26</sub> O <sub>4</sub>
Lilopristone	Abortifacient	97747-88-1		C <sub>29</sub> H <sub>37</sub> NO <sub>3</sub>
Limaprost	Prostaglandin	74397-12-9	Y	C <sub>22</sub> H <sub>36</sub> O <sub>5</sub>
Limazocic	Hepatoprotectant	128620-82-6		C <sub>8</sub> H <sub>13</sub> NO <sub>3</sub> S <sub>2</sub>
Linaprazan	Antiulcerative	248919-64-4		C <sub>21</sub> H <sub>26</sub> F <sub>4</sub> O <sub>2</sub>
Linarotene	Dermatologic	127304-28-3		C <sub>23</sub> H <sub>30</sub> N <sub>2</sub> O <sub>2</sub> S
Lincomycin	Antibiotic	154-21-2		C <sub>18</sub> H <sub>34</sub> N <sub>2</sub> O <sub>6</sub> S
Lindane	Dermatologic	58-89-9		C <sub>6</sub> H <sub>6</sub> Cl <sub>6</sub>
Linetastine	Antihistaminic	159776-68-8		C <sub>35</sub> H <sub>40</sub> N <sub>2</sub> O <sub>6</sub>
Linezolid	Antibiotic	165800-03-3	Y	C <sub>16</sub> H <sub>20</sub> FN <sub>3</sub> O <sub>4</sub>
Linogiride	Antidiabetic	75358-37-1		C <sub>16</sub> H <sub>22</sub> N <sub>4</sub> O
Linopirdine	Nootropic	105431-72-9		C <sub>26</sub> H <sub>21</sub> N <sub>3</sub> O
Linotroban	Antithrombotic	120824-08-0		C <sub>14</sub> H <sub>15</sub> NO <sub>5</sub> S <sub>2</sub>
Linsidomine	Antianginal	33876-97-0	Y	C <sub>6</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub>
Lintitript	Gastroprokinetic	136381-85-6		C <sub>20</sub> H <sub>14</sub> ClN <sub>3</sub> O <sub>5</sub> S
Lintopride	Antipsychotic	107429-63-0		C <sub>14</sub> H <sub>19</sub> ClN <sub>4</sub> O <sub>2</sub>
Liothyronine	Thyroid	6893-02-3	Y	C <sub>15</sub> H <sub>12</sub> I <sub>3</sub> NO <sub>4</sub>
Lipoic Acid, Alpha	Antidote	1200-22-2		C <sub>8</sub> H <sub>14</sub> O <sub>2</sub> S <sub>2</sub>
Liranaftate	Antifungal	88678-31-3		C <sub>18</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub> S
Lirequinil	Sedative	143943-73-1		C <sub>26</sub> H <sub>25</sub> ClN <sub>2</sub> O <sub>3</sub>
Lirexapride	Antipsychotic	145414-12-6		C <sub>24</sub> H <sub>36</sub> ClN <sub>3</sub> O <sub>2</sub>
Lirimilast	Antiinflammatory	329306-27-6		C <sub>17</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>6</sub> S
Lioldine	Mydriatic	105102-20-3		C <sub>20</sub> H <sub>20</sub> F <sub>2</sub> N <sub>4</sub>
Lisadimate	Dermatologic	136-44-7		C <sub>10</sub> H <sub>13</sub> NO <sub>4</sub>
Lisdexamfetamine Dimesylate	Nootropic	608137-32-2	Y	C <sub>15</sub> H <sub>25</sub> N <sub>3</sub> O
Lisinopril	Antihypertensive	76547-98-3	Y	C <sub>21</sub> H <sub>31</sub> N <sub>3</sub> O <sub>5</sub>
Lisofylline	Immunomodulator	100324-81-0		C <sub>13</sub> H <sub>20</sub> N <sub>4</sub> O <sub>3</sub>
Lisuride	Antimigraine	18016-80-3	Y	C <sub>20</sub> H <sub>26</sub> N <sub>4</sub> O
Lithium Carbonate	Sedative	463-79-6	Y	CH <sub>2</sub> O <sub>3</sub>
Litomeglvir	Antiviral	321915-31-5		C <sub>25</sub> H <sub>30</sub> N <sub>4</sub> O <sub>5</sub> S
Litoxetine	Antidepressant	86811-09-8		C <sub>16</sub> H <sub>19</sub> NO
Litracen	Antidepressant	5118-30-9		C <sub>20</sub> H <sub>23</sub> N
Lixazinone Sulfate	Cardiotonic	94192-59-3		C <sub>21</sub> H <sub>28</sub> N <sub>4</sub> O <sub>3</sub>
Lixivaptan	Plasma Volume Expander	168079-32-1	Y	C <sub>27</sub> H <sub>21</sub> ClFN <sub>3</sub> O <sub>2</sub>
Lobeline	Respiratory Stimulant	90-69-7		C <sub>22</sub> H <sub>27</sub> NO <sub>2</sub>
Lobendazole	Anthelmintic	6306-71-4		C <sub>10</sub> H <sub>11</sub> N <sub>3</sub> O <sub>2</sub>
Lobenzarit	Antirheumatic	63329-53-3	Y	C <sub>14</sub> H <sub>10</sub> ClNO <sub>4</sub>
Lobucavir	Antiviral	127759-89-1		C <sub>11</sub> H <sub>15</sub> N <sub>5</sub> O <sub>3</sub>
Lobuprofen	Analgesic	98207-12-6		C <sub>25</sub> H <sub>33</sub> ClN <sub>2</sub> O <sub>2</sub>
Locicortolone Dicibate	Glucocorticoid	78467-68-2		C <sub>36</sub> H <sub>50</sub> Cl <sub>2</sub> O <sub>5</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Lodaxaprine	Antineoplastic	93181-81-8		C <sub>15</sub> H <sub>16</sub> ClN <sub>3</sub> O
Lodazecar	Antihyperlipidemic	87646-83-1		C <sub>22</sub> H <sub>24</sub> BrClN <sub>4</sub> O <sub>4</sub>
Lodelaben	Antirheumatic	111149-90-7		C <sub>25</sub> H <sub>41</sub> ClO <sub>3</sub>
Lodenosine	Antiviral	110143-10-7		C <sub>10</sub> H <sub>12</sub> FN <sub>5</sub> O <sub>2</sub>
Lodinixil	Antihypertensive	86627-50-1		C <sub>14</sub> H <sub>17</sub> ClN <sub>4</sub>
Lodiperone	Adrenergic	72444-63-4		C <sub>21</sub> H <sub>20</sub> Cl <sub>2</sub> FN <sub>3</sub> O <sub>2</sub>
Lodoxamide	Antihistaminic	53882-12-5		C <sub>11</sub> H <sub>6</sub> ClN <sub>3</sub> O <sub>6</sub>
Lofemizole	Antiinflammatory	65571-68-8		C <sub>10</sub> H <sub>9</sub> ClN <sub>2</sub>
Lofendazam	Anxiolytic	29176-29-2		C <sub>15</sub> H <sub>13</sub> ClN <sub>2</sub> O
Lofentanil Oxalate	Analgesic	61380-40-3		C <sub>25</sub> H <sub>32</sub> N <sub>2</sub> O <sub>3</sub>
Lofepamine	Antidepressant	23047-25-8	Y	C <sub>26</sub> H <sub>27</sub> ClN <sub>2</sub> O
Lofexidine	Antihypertensive	31036-80-3	Y	C <sub>11</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>2</sub> O
Loflucarban	Antifungal	790-69-2		C <sub>13</sub> H <sub>9</sub> Cl <sub>2</sub> FN <sub>2</sub> S
Lombazole	Antibacterial	60628-98-0		C <sub>22</sub> H <sub>17</sub> ClN <sub>2</sub>
Lomefloxacin	Antibiotic	98079-51-7		C <sub>17</sub> H <sub>19</sub> F <sub>2</sub> N <sub>3</sub> O <sub>3</sub>
Lomeguatrib	Antineoplastic	192441-08-0		C <sub>10</sub> H <sub>8</sub> BrN <sub>5</sub> OS
Lomerizine	Antimigraine	101477-55-8	Y	C <sub>27</sub> H <sub>30</sub> F <sub>2</sub> N <sub>2</sub> O <sub>3</sub>
Lometraline	Antipsychotic	34910-85-5		C <sub>13</sub> H <sub>18</sub> ClNO
Lometrexol Sodium	Antineoplastic	106400-81-1		C <sub>21</sub> H <sub>25</sub> N <sub>5</sub> O <sub>6</sub>
Lomevactone	Antidote	81478-25-3		C <sub>18</sub> H <sub>17</sub> ClO <sub>2</sub>
Lomifylline	Bronchodilator	10226-54-7		C <sub>13</sub> H <sub>18</sub> N <sub>4</sub> O <sub>3</sub>
Lomofungin	Antifungal	26786-84-5		C <sub>15</sub> H <sub>10</sub> N <sub>2</sub> O <sub>6</sub>
Lomustine	Antineoplastic	13010-47-4	Y	C <sub>9</sub> H <sub>16</sub> ClN <sub>3</sub> O <sub>2</sub>
Lonafarnib	Antineoplastic	193275-84-2		C <sub>27</sub> H <sub>31</sub> Br <sub>2</sub> ClN <sub>4</sub> O <sub>2</sub>
Lonapalene	Dermatologic	91431-42-4		C <sub>16</sub> H <sub>15</sub> ClO <sub>6</sub>
Lonaprofen	Analgesic	41791-49-5		C <sub>14</sub> H <sub>13</sub> ClO <sub>3</sub>
Lonazolac	Antiinflammatory	53808-88-1		C <sub>17</sub> H <sub>13</sub> ClN <sub>2</sub> O <sub>2</sub>
Lonidamine	Antineoplastic	50264-69-2	Y	C <sub>15</sub> H <sub>10</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Loperamide	Antidiarrheal	53179-11-6	Y	C <sub>29</sub> H <sub>33</sub> ClN <sub>2</sub> O <sub>2</sub>
Loperamide Oxide	Antidiarrheal	106900-12-3		C <sub>29</sub> H <sub>33</sub> ClN <sub>2</sub> O <sub>3</sub>
Lopinavir	Antiviral	192725-17-0	Y	C <sub>37</sub> H <sub>48</sub> N <sub>4</sub> O <sub>5</sub>
Lopirazepam	Sedative	42863-81-0		C <sub>14</sub> H <sub>9</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>2</sub>
Loprazolam	Sedative	61197-73-7		C <sub>23</sub> H <sub>21</sub> ClN <sub>6</sub> O <sub>3</sub>
Loprodolol	Muscle Relaxant	2209-86-1		C <sub>5</sub> H <sub>10</sub> Cl <sub>2</sub> O <sub>2</sub>
Loracarbef	Antibiotic	76470-66-1	Y	C <sub>16</sub> H <sub>16</sub> ClN <sub>3</sub> O <sub>4</sub>
Lorajmine	Antiarrhythmic	47562-08-3		C <sub>22</sub> H <sub>27</sub> ClN <sub>2</sub> O <sub>3</sub>
Lorapride	Antipsychotic	68677-06-5		C <sub>14</sub> H <sub>22</sub> ClN <sub>3</sub> O <sub>3</sub> S
Loratadine	Antihistaminic	79794-75-5	Y	C <sub>22</sub> H <sub>23</sub> ClN <sub>2</sub> O <sub>2</sub>
Lorazepam	Anxiolytic	846-49-1	Y	C <sub>15</sub> H <sub>10</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Lorbamate	Muscle Relaxant	24353-88-6		C <sub>12</sub> H <sub>22</sub> N <sub>2</sub> O <sub>4</sub>
Lorcainide	Antiarrhythmic	59729-31-6		C <sub>22</sub> H <sub>27</sub> ClN <sub>2</sub> O
Lorcinaldol	Analgesic	104719-71-3		C <sub>17</sub> H <sub>19</sub> ClN <sub>4</sub>
Loreclezole	Anticonvulsant	117857-45-1		C <sub>10</sub> H <sub>6</sub> Cl <sub>3</sub> N <sub>3</sub>
Lormetazepam	Sedative	848-75-9	Y	C <sub>16</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Lornoxicam	Analgesic	70374-39-9	Y	C <sub>13</sub> H <sub>10</sub> ClN <sub>3</sub> O <sub>4</sub> S <sub>2</sub>
Lorpiprazole	Antipsychotic	108785-69-9		C <sub>21</sub> H <sub>26</sub> F <sub>3</sub> N <sub>5</sub>
Lortalamine	Antidepressant	70384-91-7		C <sub>15</sub> H <sub>17</sub> ClN <sub>2</sub> O <sub>2</sub>
Lorzafone	Sedative	59179-95-2		C <sub>18</sub> H <sub>17</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>3</sub>
Losartan	Antihypertensive	114798-26-4	Y	C <sub>22</sub> H <sub>23</sub> ClN <sub>6</sub> O
Losigamone	Anticonvulsant	112856-44-7		C <sub>12</sub> H <sub>11</sub> ClO <sub>4</sub>
Losindole	Antidepressant	69175-77-5		C <sub>19</sub> H <sub>20</sub> ClN
Losmipifen	Analgesic	74168-08-4		C <sub>17</sub> H <sub>15</sub> ClO <sub>4</sub>
Losoxantrone	Antineoplastic	88303-60-0		C <sub>22</sub> H <sub>27</sub> N <sub>5</sub> O <sub>4</sub>
Losulazine	Antihypertensive	72141-57-2		C <sub>27</sub> H <sub>22</sub> F <sub>4</sub> N <sub>4</sub> O <sub>3</sub> S
Loteprednol Etabonate	Antiinflammatory	82034-46-6		C <sub>24</sub> H <sub>31</sub> ClO <sub>7</sub>
Lotifazole	Antiinflammatory	71119-10-3		C <sub>12</sub> H <sub>9</sub> Cl <sub>3</sub> N <sub>2</sub> O <sub>2</sub> S
Lotrafiban	Antithrombotic	171049-14-2		C <sub>23</sub> H <sub>32</sub> N <sub>4</sub> O <sub>4</sub>
Lotrifen	Abortifacient	66535-86-2		C <sub>16</sub> H <sub>10</sub> ClN <sub>3</sub>
Lotucaine	Anesthetic	42373-58-0		C <sub>18</sub> H <sub>29</sub> NO <sub>2</sub>
Lovastatin	Antihyperlipidemic	75330-75-5	Y	C <sub>24</sub> H <sub>36</sub> O <sub>5</sub>
Loviride	Antiviral	147362-57-0		C <sub>17</sub> H <sub>16</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Loxanast	Unclassified	69915-62-4		C <sub>14</sub> H <sub>26</sub> O <sub>2</sub>
Loxapine	Anxiolytic	1977-10-2	Y	C <sub>18</sub> H <sub>18</sub> ClN <sub>3</sub> O

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Loxiglumide	Gastroprokinetic	107097-80-3		C <sub>21</sub> H <sub>30</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>5</sub>
Loxoprofen	Antiinflammatory	68767-14-6	Y	C <sub>15</sub> H <sub>18</sub> O <sub>3</sub>
Lozilurea	Ant ulcerative	71475-35-9		C <sub>10</sub> H <sub>13</sub> ClN <sub>2</sub> O
Lubazodone	Antidepressant	161178-07-0		C <sub>14</sub> H <sub>18</sub> FNO <sub>2</sub>
Lubeluzole	Nootropic	144665-07-6		C <sub>22</sub> H <sub>25</sub> F <sub>2</sub> N <sub>3</sub> O <sub>2</sub> S
Lubiprostone	Laxative	333963-40-9	Y	C <sub>20</sub> H <sub>32</sub> F <sub>2</sub> O <sub>5</sub>
Lucanthone	Anthelminthic	479-50-5		C <sub>20</sub> H <sub>24</sub> N <sub>2</sub> OS
Lucartamide	Antimigraine	76743-10-7		C <sub>12</sub> H <sub>16</sub> N <sub>2</sub> S <sub>2</sub>
Lucimycin	Antibiotic	13058-67-8		C <sub>36</sub> H <sub>53</sub> NO <sub>13</sub>
Lufenuron	Ectoparasiticide	103055-07-8		C <sub>17</sub> H <sub>18</sub> Cl <sub>2</sub> F <sub>8</sub> N <sub>2</sub> O <sub>3</sub>
Lufironil	Dermatologic	128075-79-6		C <sub>13</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub>
Lufuradom	Unclassified	94006-14-1		C <sub>22</sub> H <sub>20</sub> FN <sub>3</sub> O <sub>2</sub>
Luliconazole	Antifungal	187164-19-8		C <sub>14</sub> H <sub>9</sub> Cl <sub>2</sub> N <sub>3</sub> S <sub>2</sub>
Lumefantrine	Antimalarial	82186-77-4		C <sub>30</sub> H <sub>32</sub> Cl <sub>3</sub> NO
Lumiracoxib	Antirheumatic	220991-20-8	Y	C <sub>15</sub> H <sub>13</sub> ClFNO <sub>2</sub>
Lupitidine	Antihistaminic	83903-06-4		C <sub>21</sub> H <sub>27</sub> N <sub>5</sub> O <sub>2</sub> S
Luprostiol	Prostaglandin	67110-79-6		C <sub>21</sub> H <sub>29</sub> ClO <sub>6</sub> S
Lurasidone	Antipsychotic	367514-87-2	Y	C <sub>28</sub> H <sub>36</sub> N <sub>4</sub> O <sub>2</sub> S
Lurosetron Mesylate	Antiemetic	128486-54-4		C <sub>17</sub> H <sub>17</sub> FN <sub>4</sub> O
Lurtotecan Dihydrochloride	Antineoplastic	149882-10-0		C <sub>28</sub> H <sub>30</sub> N <sub>4</sub> O <sub>6</sub>
Lusaperidone	Antipsychotic	214548-46-6		C <sub>22</sub> H <sub>21</sub> N <sub>3</sub> O <sub>2</sub>
Luxabendazole	Anthelminthic	90509-02-7		C <sub>15</sub> H <sub>12</sub> FN <sub>3</sub> O <sub>5</sub> S
Lycetamine	Antibacterial	60209-20-3		C <sub>22</sub> H <sub>47</sub> N <sub>3</sub> O
Lydimycin	Antifungal	10118-85-1		C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub> S
Lymecycline	Antibiotic	992-21-2		C <sub>29</sub> H <sub>38</sub> N <sub>4</sub> O <sub>10</sub>
Lynestrenol	Progestogen	52-76-6		C <sub>20</sub> H <sub>28</sub> O
Lysergide	Antidepressant	50-37-3		C <sub>20</sub> H <sub>25</sub> N <sub>3</sub> O
Mabuprofen	Analgesic	82821-47-4		C <sub>15</sub> H <sub>23</sub> NO <sub>2</sub>
Mabuterol	Bronchodilator	56341-08-3		C <sub>13</sub> H <sub>18</sub> ClF <sub>3</sub> N <sub>2</sub> O
Maduramicin	Antibacterial	79356-08-4		C <sub>47</sub> H <sub>80</sub> O <sub>17</sub>
Mafenide	Antibiotic	138-39-6		C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> S
Mafopezazine	Antipsychotic	80428-29-1		C <sub>22</sub> H <sub>28</sub> FN <sub>3</sub> O <sub>3</sub>
Mafofamide	Antineoplastic	88859-04-5		C <sub>9</sub> H <sub>19</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>5</sub> PS <sub>2</sub>
Malathion	Ectoparasiticide	121-75-5		C <sub>10</sub> H <sub>19</sub> O <sub>6</sub> PS <sub>2</sub>
Maleylsulfathiazole	Antibiotic	515-57-1		C <sub>13</sub> H <sub>11</sub> N <sub>3</sub> O <sub>5</sub> S <sub>2</sub>
Malotilate	Hepatic Protectant	59937-28-9		C <sub>12</sub> H <sub>16</sub> O <sub>4</sub> S <sub>2</sub>
Mandelic Acid	Dermatologic	90-64-2		C <sub>8</sub> H <sub>8</sub> O <sub>3</sub>
Manidipine 6300	Vasodilator	89226-50-6		C <sub>33</sub> H <sub>38</sub> N <sub>4</sub> O <sub>6</sub>
Manifaxine	Antidepressant	135306-39-7		C <sub>12</sub> H <sub>15</sub> F <sub>2</sub> NO <sub>2</sub>
Manitimus	Immunomodulator	202057-76-9		C <sub>15</sub> H <sub>11</sub> F <sub>3</sub> N <sub>2</sub> O <sub>2</sub>
Mannitol	Diuretic	69-65-8		C <sub>6</sub> H <sub>14</sub> O <sub>6</sub>
Mannitol Hexantrate	Vasodilator	15825-70-4		C <sub>6</sub> H <sub>8</sub> N <sub>6</sub> O <sub>18</sub>
Mannomustine	Antineoplastic	576-68-1		C <sub>10</sub> H <sub>22</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>4</sub>
Mannosulfan	Antineoplastic	7518-35-6		C <sub>10</sub> H <sub>22</sub> O <sub>14</sub> S <sub>4</sub>
Manozodil	Unclassified	77528-67-7		C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> S
Mantabegron	Antidiabetic	36144-08-8		C <sub>19</sub> H <sub>27</sub> NO <sub>2</sub>
Mapinastine	Antihistaminic	140945-32-0		C <sub>23</sub> H <sub>34</sub> N <sub>6</sub> O
Maprotiline	Antidepressant	10262-69-8	Y	C <sub>20</sub> H <sub>23</sub> N
Maraviroc	Antiviral	376348-65-1	Y	C <sub>29</sub> H <sub>41</sub> F <sub>2</sub> N <sub>5</sub> O
Marbofloxacin	Antibiotic	115550-35-1		C <sub>17</sub> H <sub>19</sub> FN <sub>4</sub> O <sub>4</sub>
Maribavir	Antiviral	176161-24-3	Y	C <sub>15</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub> Cl <sub>2</sub>
Marimastat	Antineoplastic	154039-60-8		C <sub>15</sub> H <sub>29</sub> N <sub>3</sub> O <sub>5</sub>
Mariptiline	Antidepressant	60070-14-6		C <sub>18</sub> H <sub>18</sub> N <sub>2</sub> O
Maropitant Citrate	Antiemetic	147116-67-4		C <sub>32</sub> H <sub>40</sub> N <sub>2</sub> O
Maroxepin	Antidepressant	65509-24-2		C <sub>19</sub> H <sub>19</sub> NO
Masoprocol	Antineoplastic	27686-84-6		C <sub>18</sub> H <sub>22</sub> O <sub>4</sub>
Mavacoxib	Antiinflammatory	170569-88-7		C <sub>16</sub> H <sub>11</sub> F <sub>4</sub> N <sub>3</sub> O <sub>2</sub> S
Maxacalcitol	Dermatologic	103909-75-7		C <sub>26</sub> H <sub>42</sub> O <sub>4</sub>
Maytansine	Antineoplastic	35846-53-8		C <sub>34</sub> H <sub>46</sub> ClN <sub>3</sub> O <sub>10</sub>
Mazapertine Succinate	Antipsychotic	134208-17-6		C <sub>26</sub> H <sub>35</sub> N <sub>3</sub> O <sub>2</sub>
Mazaticol	Antiparkinsonian	42024-98-6		C <sub>21</sub> H <sub>27</sub> NO <sub>3</sub> S <sub>2</sub>
Mazindol	Anorexic	22232-71-9	Y	C <sub>16</sub> H <sub>13</sub> ClN <sub>2</sub> O
Mazipredone	Antiinflammatory	13085-08-0		C <sub>26</sub> H <sub>38</sub> N <sub>2</sub> O <sub>4</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Mazokalim	Antihypertensive	164178-54-5		C <sub>23</sub> H <sub>28</sub> N <sub>6</sub> O <sub>6</sub>
Mebanazine	Antipsychotic	65-64-5		C <sub>8</sub> H <sub>12</sub> N <sub>2</sub>
Mebendazole	Anthelminthic	31431-39-7	Y	C <sub>16</sub> H <sub>13</sub> N <sub>3</sub> O <sub>3</sub>
Mebezoside	Capillary Protectant	55902-93-7		C <sub>28</sub> H <sub>32</sub> O <sub>6</sub>
Mebeverine	Antispasmodic	3625-06-7	Y	C <sub>25</sub> H <sub>35</sub> NO <sub>5</sub>
Mebezonium Iodide	Antitussive	7681-78-9		C <sub>19</sub> H <sub>40</sub> I <sub>2</sub> N <sub>2</sub>
Mebhydrolin	Antihistaminic	524-81-2		C <sub>19</sub> H <sub>20</sub> N <sub>2</sub>
Mebiquine	Antidiarrheal	23910-07-8		C <sub>10</sub> H <sub>10</sub> BiNO <sub>3</sub>
Mebolazine	Antianginal	3625-07-8		C <sub>42</sub> H <sub>68</sub> N <sub>2</sub> O <sub>2</sub>
Mebutamate	Antihypertensive	64-55-1		C <sub>10</sub> H <sub>20</sub> N <sub>2</sub> O <sub>4</sub>
Mebutizide	Diuretic	3568-00-1		C <sub>13</sub> H <sub>20</sub> ClN <sub>3</sub> O <sub>4</sub> S <sub>2</sub>
Mecamylamine	Antihypertensive	60-40-2		C <sub>11</sub> H <sub>21</sub> N
Mecarbonate	Antihypertensive	15574-49-9		C <sub>13</sub> H <sub>15</sub> NO <sub>3</sub>
Mechlorethamine	Antineoplastic	51-75-2		C <sub>5</sub> H <sub>11</sub> Cl <sub>2</sub> N
Meciadanol	Antiulcerative	65350-86-9		C <sub>16</sub> H <sub>16</sub> O <sub>6</sub>
Mecinarone	Vasodilator	26225-59-2		C <sub>24</sub> H <sub>27</sub> NO <sub>6</sub>
Meclinetant	Antineoplastic	146362-70-1		C <sub>32</sub> H <sub>31</sub> ClN <sub>4</sub> O <sub>5</sub>
Meclizine	Antiemetic	569-65-3	Y	C <sub>25</sub> H <sub>27</sub> ClN <sub>2</sub>
Meclocycline	Antibacterial	2013-58-3		C <sub>22</sub> H <sub>21</sub> ClN <sub>2</sub> O <sub>8</sub>
Meclofenamic Acid	Antiinflammatory	644-62-2		C <sub>14</sub> H <sub>11</sub> Cl <sub>2</sub> NO <sub>2</sub>
Meclofenoxate	Nootropic	51-68-3		C <sub>12</sub> H <sub>16</sub> ClNO <sub>3</sub>
Meclonazepam	Sedative	58662-84-3		C <sub>16</sub> H <sub>12</sub> ClN <sub>3</sub> O <sub>3</sub>
Mecloqualone	Sedative	340-57-8		C <sub>15</sub> H <sub>11</sub> ClN <sub>2</sub> O
Mecloralurea	Anxiolytic	1954-79-6		C <sub>4</sub> H <sub>7</sub> Cl <sub>3</sub> N <sub>2</sub> O <sub>2</sub>
Meclorison DIBUTYRATE	Antiinflammatory	10549-91-4		C <sub>30</sub> H <sub>40</sub> Cl <sub>2</sub> O <sub>6</sub>
Meclozamine	Sedative	5668-06-4		C <sub>19</sub> H <sub>24</sub> ClNO
Mecrylate	Dermatologic	137-05-3		C <sub>5</sub> H <sub>5</sub> NO <sub>2</sub>
Mecysteine	Mucolytic	2485-62-3		C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub> S
Medazepam	Sedative	2898-12-6	Y	C <sub>16</sub> H <sub>15</sub> ClN <sub>2</sub>
Medazomide	Antitussive	300-22-1		C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub>
Medetomidine	Analgesic	86347-14-0		C <sub>13</sub> H <sub>16</sub> N <sub>2</sub>
Medibazine	Vasodilator	53-31-6		C <sub>25</sub> H <sub>26</sub> N <sub>2</sub> O <sub>2</sub>
Medifoxamine	Antidepressant	32359-34-5		C <sub>16</sub> H <sub>19</sub> NO <sub>2</sub>
Medorinone	Cardiotonic	88296-61-1		C <sub>9</sub> H <sub>8</sub> N <sub>2</sub> O
Medorubicin	Antineoplastic	64314-52-9		C <sub>26</sub> H <sub>27</sub> NO <sub>10</sub>
Medrogestone	Progestogen	977-79-7		C <sub>23</sub> H <sub>32</sub> O <sub>2</sub>
Medroxalol	Antihypertensive	56290-94-9		C <sub>20</sub> H <sub>24</sub> N <sub>2</sub> O <sub>5</sub>
Medroxyprogesterone Acetate	Progestogen	71-58-9	Y	C <sub>24</sub> H <sub>34</sub> O <sub>4</sub>
Medrylamine	Antihistaminic	524-99-2		C <sub>18</sub> H <sub>23</sub> NO <sub>2</sub>
Medryson	Glucocorticoid	2668-66-8		C <sub>22</sub> H <sub>32</sub> O <sub>3</sub>
Mefeclozazine	Unclassified	1243-33-0		C <sub>20</sub> H <sub>25</sub> ClN <sub>2</sub> O <sub>2</sub>
Mefenamic Acid	Antiinflammatory	61-68-7	Y	C <sub>15</sub> H <sub>15</sub> NO <sub>2</sub>
Mefenidil	Vasodilator	58261-91-9		C <sub>12</sub> H <sub>11</sub> N <sub>3</sub>
Mefenidramium Metilsulfate	Unclassified	4858-60-0		C <sub>19</sub> H <sub>27</sub> NO <sub>5</sub> S
Mefenorex	Anorexic	17243-57-1		C <sub>12</sub> H <sub>18</sub> ClN
Mefeserpine	Antihypertensive	3735-85-1		C <sub>32</sub> H <sub>38</sub> N <sub>2</sub> O <sub>8</sub>
Mefexamide	Nootropic	1227-61-8		C <sub>15</sub> H <sub>24</sub> N <sub>2</sub> O <sub>3</sub>
Mefloquine	Antimalarial	53230-10-7	Y	C <sub>17</sub> H <sub>16</sub> F <sub>6</sub> N <sub>2</sub> O
Mefruside	Diuretic	7195-27-9		C <sub>13</sub> H <sub>19</sub> ClN <sub>2</sub> O <sub>5</sub> S <sub>2</sub>
Megalomicin Potassium Phosphate	Antibacterial	28022-11-9		C <sub>44</sub> H <sub>80</sub> N <sub>2</sub> O <sub>15</sub>
Megestrol Acetate	Progestogen	595-33-5	Y	C <sub>24</sub> H <sub>32</sub> O <sub>4</sub>
Meglitinide	Antidiabetic	54870-28-9		C <sub>17</sub> H <sub>16</sub> ClNO <sub>4</sub>
Meglucycline	Antibiotic	31770-79-3		C <sub>29</sub> H <sub>37</sub> N <sub>3</sub> O <sub>13</sub>
Meglumine	Antiprotozoal	6284-40-8	Y	C <sub>7</sub> H <sub>17</sub> NO <sub>5</sub>
Meglumine Metrizoate	Antiprotozoal	1949-45-7		C <sub>12</sub> H <sub>11</sub> I <sub>3</sub> N <sub>2</sub> O <sub>4</sub>
Meglutol	Antihyperlipidemic	503-49-1		C <sub>6</sub> H <sub>10</sub> O <sub>5</sub>
Meladrazine	Anorexic	13957-36-3		C <sub>11</sub> H <sub>23</sub> N <sub>7</sub>
Melagatran	Antithrombotic	159776-70-2		C <sub>22</sub> H <sub>31</sub> N <sub>5</sub> O <sub>4</sub>
Melarsomine	Antiprotozoal	128470-15-5		C <sub>13</sub> H <sub>21</sub> AsN <sub>8</sub> S <sub>2</sub>
Melarsonyl Potassium	Antiprotozoal	37526-80-0		C <sub>13</sub> H <sub>13</sub> AsN <sub>6</sub> O <sub>4</sub> S <sub>2</sub>
Melarsoprol	Antiprotozoal	494-79-1		C <sub>12</sub> H <sub>15</sub> AsN <sub>6</sub> OS <sub>2</sub>
Meldonium	Antiarrhythmic	76144-81-5	Y	C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Melengestrol Acetate	Antineoplastic	2919-66-6		C <sub>25</sub> H <sub>32</sub> O <sub>4</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Meletimide	Antihypertensive	14745-50-7		C <sub>24</sub> H <sub>28</sub> N <sub>2</sub> O <sub>2</sub>
Melevodopa	Antiparkinsonian	7101-51-1		C <sub>10</sub> H <sub>13</sub> NO <sub>4</sub>
Melinamide	Antihyperlipidemic	14417-88-0		C <sub>26</sub> H <sub>41</sub> NO
Melitracen	Antidepressant	5118-29-6		C <sub>21</sub> H <sub>25</sub> N
Melizame	Unclassified	26921-72-2		C <sub>7</sub> H <sub>6</sub> N <sub>4</sub> O <sub>2</sub>
Meloxicam	Antiinflammatory	71125-38-7	Y	C <sub>14</sub> H <sub>13</sub> N <sub>3</sub> O <sub>4</sub> S <sub>2</sub>
Melperone	Antipsychotic	3575-80-2		C <sub>16</sub> H <sub>22</sub> FNO
Melphalan	Antineoplastic	148-82-3	Y	C <sub>13</sub> H <sub>18</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Melquinast	Bronchodilator	87611-28-7		C <sub>15</sub> H <sub>16</sub> N <sub>4</sub> O <sub>3</sub>
Meluadrine	Antihistamine	134865-33-1		C <sub>12</sub> H <sub>18</sub> ClNO <sub>2</sub>
Memantine	Antiparkinsonian	19982-08-2	Y	C <sub>12</sub> H <sub>21</sub> N
Memotine	Antiviral	18429-69-1		C <sub>17</sub> H <sub>17</sub> NO <sub>2</sub>
Menabitan	Analgesic	83784-21-8		C <sub>37</sub> H <sub>56</sub> N <sub>2</sub> O <sub>3</sub>
Menbutone	Choleric	3562-99-0		C <sub>13</sub> H <sub>14</sub> O <sub>4</sub>
Menfegol	Contraceptive	57821-32-6		C <sub>18</sub> H <sub>28</sub> O <sub>2</sub>
Menglytate	Unclassified	579-94-2		C <sub>14</sub> H <sub>26</sub> O <sub>3</sub>
Menitrazepam	Sedative	28781-64-8		C <sub>16</sub> H <sub>17</sub> N <sub>3</sub> O <sub>3</sub>
Menoctone	Antimalarial	14561-42-3		C <sub>24</sub> H <sub>32</sub> O <sub>3</sub>
Menogaril	Antineoplastic	71628-96-1		C <sub>28</sub> H <sub>31</sub> NO <sub>10</sub>
Menthyl Salicylate	Dermatologic	89-46-3		C <sub>17</sub> H <sub>24</sub> O <sub>3</sub>
Meobentine Sulfate	Antiarrhythmic	46464-11-3		C <sub>11</sub> H <sub>17</sub> N <sub>3</sub> O
Meparfynol	Sedative	77-75-8		C <sub>6</sub> H <sub>10</sub> O
Mepazine Acetate	Antipsychotic	60-89-9		C <sub>19</sub> H <sub>22</sub> N <sub>2</sub> S
Mepenzolate	Antispasmodic	25990-43-6	Y	C <sub>21</sub> H <sub>26</sub> NO <sub>3</sub> +
Meperidine	Analgesic	57-42-1	Y	C <sub>15</sub> H <sub>21</sub> NO <sub>2</sub>
Mephenesin	Muscle Relaxant	59-47-2		C <sub>10</sub> H <sub>14</sub> O <sub>3</sub>
Mephenesin Carbamate	Muscle Relaxant	533-06-2		C <sub>11</sub> H <sub>15</sub> NO <sub>4</sub>
Mephenoxalone	Muscle Relaxant	70-07-5		C <sub>11</sub> H <sub>13</sub> NO <sub>4</sub>
Mephentermine	Antihypotensive	100-92-5		C <sub>11</sub> H <sub>17</sub> N
Mephenytoin	Anticonvulsant	50-12-4	Y	C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Mephobarbital	Anticonvulsant	115-38-8	Y	C <sub>13</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>
Mepindolol	Antianginal	23694-81-7	Y	C <sub>15</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>
Mepiperphenidol Bromide	Diuretic	520-20-7		C <sub>19</sub> H <sub>32</sub> BrNO
Mepiprazole	Sedative	20326-12-9		C <sub>16</sub> H <sub>21</sub> ClN <sub>4</sub>
Mepiroxol	Antiinflammatory	6968-72-5		C <sub>6</sub> H <sub>7</sub> NO <sub>2</sub>
Mepitiostane	Oxytocic	21362-69-6		C <sub>25</sub> H <sub>40</sub> O <sub>2</sub> S
Mepivacaine	Anesthetic	96-88-8		C <sub>15</sub> H <sub>22</sub> N <sub>2</sub> O
Mepixanox	Respiratory Stimulant	17854-59-0		C <sub>20</sub> H <sub>21</sub> NO <sub>3</sub>
Mepramidil	Antihypotensive	23891-60-3		C <sub>28</sub> H <sub>33</sub> NO <sub>5</sub>
Meprednisone	Glucocorticoid	1247-42-3		C <sub>22</sub> H <sub>28</sub> O <sub>5</sub>
Meproamate	Sedative	57-53-4		C <sub>9</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub>
Meprochol	Steroid	590-31-8		C <sub>7</sub> H <sub>16</sub> NO.Br
Meproscillarín	Cardiotonic	33396-37-1		C <sub>31</sub> H <sub>44</sub> O <sub>8</sub>
Meprotixol	Antitussive	4295-63-0		C <sub>19</sub> H <sub>23</sub> NO <sub>2</sub> S
Meprylcaine	Anesthetic	495-70-5		C <sub>14</sub> H <sub>21</sub> NO <sub>2</sub>
Meptazinol	Analgesic	54340-58-8	Y	C <sub>15</sub> H <sub>23</sub> NO
Mequidox	Antibacterial	16915-79-0		C <sub>10</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub>
Mequinol	Dermatologic	150-76-5		C <sub>7</sub> H <sub>8</sub> O <sub>2</sub>
Mequitamium Iodide	Antihistaminic	101396-42-3		C <sub>21</sub> H <sub>25</sub> N <sub>2</sub> SI
Mequitazine	Antihistaminic	29216-28-2	Y	C <sub>20</sub> H <sub>22</sub> N <sub>2</sub> S
Meradimate	Dermatologic	134-09-8		C <sub>17</sub> H <sub>25</sub> NO <sub>2</sub>
Merafloxacin	Antibiotic	91188-00-0		C <sub>19</sub> H <sub>23</sub> F <sub>2</sub> N <sub>3</sub> O <sub>3</sub>
Meragidone Sodium	Antipsychotic	792128-03-1		C <sub>10</sub> H <sub>13</sub> HgNO <sub>5</sub>
Merbromin	Antibacterial	55728-51-3		C <sub>20</sub> H <sub>10</sub> B <sub>2</sub> HgO <sub>6</sub>
Mercaptopurine	Antineoplastic	50-44-2	Y	C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> S
Mercurobutol	Antifungal	498-73-7		C <sub>10</sub> H <sub>13</sub> ClHgO
Mergocriptine	Antimigraine	81968-16-3		C <sub>33</sub> H <sub>43</sub> N <sub>5</sub> O <sub>5</sub>
Meribendan	Cardiotonic	119322-27-9		C <sub>15</sub> H <sub>14</sub> N <sub>6</sub> O
Merimepodib	Antiviral	198821-22-6		C <sub>23</sub> H <sub>24</sub> N <sub>4</sub> O <sub>6</sub>
Meropenem	Antibacterial	96036-03-2		C <sub>17</sub> H <sub>25</sub> N <sub>3</sub> O <sub>5</sub> S
Mesabolone	Steroid	7483-09-2		C <sub>26</sub> H <sub>40</sub> O <sub>3</sub>
Mesalamine	Antiinflammatory	89-57-6	Y	C <sub>7</sub> H <sub>7</sub> NO <sub>3</sub>
Meseclazone	Antiinflammatory	29053-27-8		C <sub>11</sub> H <sub>10</sub> ClNO <sub>3</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Mesna	Mucolytic	3375-50-6		C <sub>2</sub> H <sub>6</sub> O <sub>3</sub> S <sub>2</sub>
Mesocarb	Nootropic	34262-84-5		C <sub>18</sub> H <sub>18</sub> N <sub>4</sub> O <sub>2</sub>
Mesoridazine	Antipsychotic	5588-33-0		C <sub>21</sub> H <sub>26</sub> N <sub>2</sub> O <sub>5</sub> S <sub>2</sub>
Mespirenone	Pituitary	87952-98-5		C <sub>25</sub> H <sub>30</sub> O <sub>4</sub> S
Mestanolone	Androgen	521-11-9		C <sub>20</sub> H <sub>32</sub> O <sub>2</sub>
Mesterolone	Androgen	1424-00-6	Y	C <sub>20</sub> H <sub>32</sub> O <sub>2</sub>
Mestilbol	Estrogen	7773-60-6		C <sub>19</sub> H <sub>22</sub> O <sub>2</sub>
Mestranol	Estrogen	72-33-3		C <sub>21</sub> H <sub>26</sub> O <sub>2</sub>
Mesudipine	Antianginal	62658-88-2		C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> O <sub>4</sub> S
Mesulegine	Antidepressant	64795-35-3		C <sub>18</sub> H <sub>26</sub> N <sub>4</sub> O <sub>2</sub> S
Mesulfamide	Antibiotic	122-89-4		C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> O <sub>5</sub> S <sub>2</sub>
Mesulfen	Ectoparasiticide	135-58-0		C <sub>14</sub> H <sub>12</sub> S <sub>2</sub>
Mesuprine	Vasodilator	7541-30-2		C <sub>19</sub> H <sub>26</sub> N <sub>2</sub> O <sub>5</sub> S
Metabutethamine	Anesthetic	4439-25-2		C <sub>13</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>
Metabutoxycaine	Anesthetic	3624-87-1		C <sub>17</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub>
Metacetamol	Analgesic	621-42-1		C <sub>8</sub> H <sub>9</sub> NO <sub>2</sub>
Metaclazepam	Anxiolytic	84031-17-4		C <sub>18</sub> H <sub>18</sub> BrClN <sub>2</sub> O
Metaglycodol	Sedative	13980-94-4		C <sub>11</sub> H <sub>15</sub> ClO <sub>2</sub>
Metahexamide	Antidiabetic	565-33-3		C <sub>14</sub> H <sub>21</sub> N <sub>3</sub> O <sub>3</sub> S
Metahomomenthol	Unclassified	17162-28-6		C <sub>15</sub> H <sub>28</sub> O <sub>3</sub>
Metalol	Antihypertensive	7701-65-7		C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub> S
Metamelfalan	Antineoplastic	1088-80-8		C <sub>13</sub> H <sub>18</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Metamfazon	Antiinflammatory	54063-49-9		C <sub>11</sub> H <sub>11</sub> N <sub>5</sub> O
Metamfepramone	Anorexic	15351-09-4		C <sub>11</sub> H <sub>15</sub> NO
Metampicillin	Antibiotic	6489-97-0		C <sub>17</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub> S
Metanixin	Antiinflammatory	4394-04-1		C <sub>14</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Metapramine	Antidepressant	21730-16-5		C <sub>16</sub> H <sub>18</sub> N <sub>2</sub>
Metaproterenol	Bronchodilator	586-06-1		C <sub>11</sub> H <sub>17</sub> NO <sub>3</sub>
Metaterol	Bronchodilator	3571-71-9		C <sub>11</sub> H <sub>17</sub> NO <sub>2</sub>
Metaxalone	Muscle Relaxant	1665-48-1	Y	C <sub>12</sub> H <sub>15</sub> NO <sub>3</sub>
Metazamide	Antibacterial	14058-90-3		C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>
Metazide	Antibacterial	1707-15-9		C <sub>13</sub> H <sub>14</sub> N <sub>6</sub> O <sub>2</sub>
Metazocine	Analgesic	3734-52-9		C <sub>15</sub> H <sub>21</sub> NO
Metbufen	Antiinflammatory	63472-04-8		C <sub>17</sub> H <sub>16</sub> O <sub>3</sub>
Metcaraphen	Mydriatic	561-79-5		C <sub>20</sub> H <sub>31</sub> NO <sub>2</sub>
Meteneprost	Oxytocic	61263-35-2		C <sub>23</sub> H <sub>38</sub> O <sub>4</sub>
Metergoline	Pituitary	17692-51-2	Y	C <sub>25</sub> H <sub>29</sub> N <sub>3</sub> O <sub>2</sub>
Metergotamine	Analgesic	22336-84-1		C <sub>34</sub> H <sub>37</sub> N <sub>5</sub> O <sub>5</sub>
Metesculetol	Unclassified	52814-39-8		C <sub>12</sub> H <sub>10</sub> O <sub>6</sub>
Metesind Glucuronate	Antineoplastic	138384-68-6		C <sub>23</sub> H <sub>24</sub> N <sub>4</sub> O <sub>3</sub> S
Metethoheptazine	Analgesic	509-84-2		C <sub>17</sub> H <sub>25</sub> NO <sub>2</sub>
Metformin	Antidiabetic	657-24-9	Y	C <sub>4</sub> H <sub>11</sub> N <sub>5</sub>
Methacholine	Cholinergic	55-92-5		C <sub>8</sub> H <sub>18</sub> NO <sub>2</sub>
Methacycline	Antibiotic	914-00-1		C <sub>22</sub> H <sub>22</sub> N <sub>2</sub> O <sub>8</sub>
Methadone	Analgesic	76-99-3	Y	C <sub>21</sub> H <sub>27</sub> NO
Methadyl Acetate	Analgesic	509-74-0		C <sub>23</sub> H <sub>31</sub> NO <sub>2</sub>
Methafurylene Fumarate	Antihistaminic	531-06-6		C <sub>14</sub> H <sub>19</sub> N <sub>3</sub> O
Methallatal	Antiemetic	115-56-0		C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> S
Methalleneestril	Estrogen	517-18-0		C <sub>18</sub> H <sub>22</sub> O <sub>3</sub>
Methallibure	Pituitary	926-93-2		C <sub>7</sub> H <sub>14</sub> N <sub>4</sub> S <sub>2</sub>
Methalthiazide	Diuretic	5611-64-3		C <sub>12</sub> H <sub>16</sub> ClN <sub>3</sub> O <sub>4</sub> S <sub>3</sub>
Methamphetamine	Anorexic	537-46-2	Y	C <sub>10</sub> H <sub>15</sub> N
Methandriol	Steroid	521-10-8		C <sub>20</sub> H <sub>32</sub> O <sub>2</sub>
Methandrostenolone	Androgen	72-63-9		C <sub>20</sub> H <sub>28</sub> O <sub>2</sub>
Methaniazide	Antibacterial	13447-95-5		C <sub>7</sub> H <sub>9</sub> N <sub>3</sub> O <sub>4</sub> S
Methantheline	Antispasmodic	5818-17-7		C <sub>21</sub> H <sub>26</sub> BrNO <sub>3</sub>
Methaphenilene	Antihistaminic	493-78-7		C <sub>15</sub> H <sub>20</sub> N <sub>2</sub> S
Methapyrilene	Antihistaminic	91-80-5		C <sub>14</sub> H <sub>19</sub> N <sub>3</sub> S
Methaqualone	Sedative	72-44-6		C <sub>16</sub> H <sub>14</sub> N <sub>2</sub> O
Metharbital	Anticonvulsant	50-11-3		C <sub>9</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>
Methastyrindone	Antipsychotic	721-19-7		C <sub>13</sub> H <sub>15</sub> NO <sub>2</sub>
Methazolamide	Diuretic	554-57-4		C <sub>5</sub> H <sub>8</sub> N <sub>4</sub> O <sub>3</sub> S <sub>2</sub>
Methdilazine	Dermatologic	1982-37-2		C <sub>18</sub> H <sub>20</sub> N <sub>2</sub> S

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Methenamine	Antibacterial	100-97-0		C <sub>6</sub> H <sub>12</sub> N <sub>4</sub>
Methenolone Acetate	Steroid	434-05-9		C <sub>22</sub> H <sub>32</sub> O <sub>3</sub>
Methenolone Enanthate	Steroid	303-42-4		C <sub>27</sub> H <sub>42</sub> O <sub>3</sub>
Metheptazine	Analgesic	469-78-3		C <sub>16</sub> H <sub>23</sub> NO <sub>2</sub>
Methestrol	Estrogen	130-73-4		C <sub>20</sub> H <sub>26</sub> O <sub>2</sub>
Methetoin	Anticonvulsant	5696-06-0		C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Methicillin	Antibiotic	61-32-5		C <sub>17</sub> H <sub>20</sub> N <sub>2</sub> O <sub>6</sub> S
Methimazole	Thyroid	60-56-0	Y	C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> S
Methiodal	Anesthetic	143-47-5		CH <sub>3</sub> IO <sub>3</sub> S
Methiomeprazine	Analgesic	7009-43-0		C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> S <sub>2</sub>
Methionine	Hepatoprotectant	63-68-3		C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub> S
Methisazone	Antiviral	1910-68-5		C <sub>10</sub> H <sub>10</sub> N <sub>4</sub> OS
Methitural	Sedative	467-43-6		C <sub>12</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub> S <sub>2</sub>
Methixene	Muscle Relaxant	4969-02-2	Y	C <sub>20</sub> H <sub>23</sub> NS
Methocarbamol	Muscle Relaxant	532-03-6	Y	C <sub>11</sub> H <sub>15</sub> NO <sub>5</sub>
Methohexital	Anesthetic	151-83-7		C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>
Methopholine	Analgesic	2154-02-1		C <sub>20</sub> H <sub>24</sub> ClNO <sub>2</sub>
Methoprene	Dermatologic	40596-69-8		C <sub>19</sub> H <sub>34</sub> O <sub>3</sub>
Methoserpidine	Antihypertensive	865-04-3		C <sub>33</sub> H <sub>40</sub> N <sub>2</sub> O <sub>9</sub>
Methotrexate	Antineoplastic	59-05-2	Y	C <sub>20</sub> H <sub>22</sub> N <sub>6</sub> O <sub>5</sub>
Methotrimeprazine	Analgesic	60-99-1		C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> OS
Methoxamine	Antihypotensive	390-28-3		C <sub>11</sub> H <sub>17</sub> NO <sub>3</sub>
Methoxsalen	Dermatologic	298-81-7	Y	C <sub>12</sub> H <sub>8</sub> O <sub>4</sub>
Methoxyflurane	Anesthetic	76-38-0		C <sub>3</sub> H <sub>4</sub> Cl <sub>2</sub> F <sub>2</sub> O
2--5-Nitrofurran	Antifungal	586-84-5		C <sub>6</sub> H <sub>7</sub> NO <sub>4</sub>
Methoxyphedrine	Bronchodilator	530-54-1		C <sub>11</sub> H <sub>15</sub> NO <sub>2</sub>
Methoxyphenamine	Bronchodilator	93-30-1		C <sub>11</sub> H <sub>17</sub> NO
Methoxypromazine Maleate	Antipsychotic	61-01-8		C <sub>18</sub> H <sub>22</sub> N <sub>2</sub> OS
Methscopolamine	Antispasmodic	13265-10-6	Y	C <sub>18</sub> H <sub>24</sub> NO <sub>4</sub>
Methsuximide	Anticonvulsant	77-41-8	Y	C <sub>12</sub> H <sub>13</sub> NO <sub>2</sub>
Methylclothiazide	Diuretic	135-07-9	Y	C <sub>9</sub> H <sub>11</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>4</sub> S <sub>2</sub>
Methyl Aminolevulinate	Antineoplastic	33320-16-0		C <sub>6</sub> H <sub>11</sub> NO <sub>3</sub>
Methyl Nicotinate	Dermatologic	93-60-7		C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub>
Methyl Palmoxirate	Antidiabetic	69207-52-9		C <sub>18</sub> H <sub>34</sub> O <sub>3</sub>
Methyl Salicylate	Dermatologic	119-36-8		C <sub>8</sub> H <sub>8</sub> O <sub>3</sub>
Methylatropine Nitrate	Mydriatic	52-88-0		C <sub>18</sub> H <sub>26</sub> N <sub>2</sub> O <sub>6</sub>
Methylbenactyzium Bromide	Antidepressant	3166-62-9		C <sub>21</sub> H <sub>28</sub> BrNO <sub>3</sub>
Methylchromone	Antispasmodic	85-90-5		C <sub>10</sub> H <sub>8</sub> O <sub>2</sub>
Methyldesorphine	Analgesic	16008-36-9		C <sub>18</sub> H <sub>21</sub> NO <sub>2</sub>
Methyldihydromorphine	Analgesic	509-56-8		C <sub>18</sub> H <sub>23</sub> NO <sub>3</sub>
Methyldopa	Antihypertensive	555-30-6		C <sub>10</sub> H <sub>13</sub> NO <sub>4</sub>
Methylene Blue	Hemantic	61-73-4		C <sub>16</sub> H <sub>18</sub> ClN <sub>3</sub> S
Methylephedrine	Nootropic	552-79-4		C <sub>11</sub> H <sub>17</sub> NO
Methylergonovine	Oxytocic	113-42-8	Y	C <sub>20</sub> H <sub>25</sub> N <sub>3</sub> O <sub>2</sub>
Methylhexaneamine	Antihypotensive	105-41-9		C <sub>7</sub> H <sub>17</sub> N
Methylmethionine Sulfonium Chloride	Unclassified	1115-84-0		C <sub>6</sub> H <sub>14</sub> ClNO <sub>2</sub> S
Methylphenidate	Nootropic	113-45-1	Y	C <sub>14</sub> H <sub>19</sub> NO <sub>2</sub>
Methylprednisolone	Glucocorticoid	83-43-2	Y	C <sub>22</sub> H <sub>30</sub> O <sub>5</sub>
Methylprednisolone Aceponate	Glucocorticoid	86401-95-8		C <sub>27</sub> H <sub>36</sub> O <sub>7</sub>
Methylprednisolone Acetate	Glucocorticoid	53-36-1	Y	C <sub>24</sub> H <sub>32</sub> O <sub>6</sub>
Methylprednisolone Hemisuccinate	Glucocorticoid	2921-57-5		C <sub>26</sub> H <sub>34</sub> O <sub>8</sub>
Methylprednisolone Sodium Phosphate	Glucocorticoid	22252-38-6		C <sub>22</sub> H <sub>31</sub> O <sub>8</sub> P
Methylprednisolone Suleptanate	Antiinflammatory	121807-10-1		C <sub>33</sub> H <sub>49</sub> NO <sub>10</sub> S
Methylpromazine	Dermatologic	84-96-8		C <sub>18</sub> H <sub>22</sub> N <sub>2</sub> S
Methyltestosterone	Androgen	58-18-4	Y	C <sub>20</sub> H <sub>30</sub> O <sub>2</sub>
Methylthiouracil	Thyroid	56-04-2		C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> OS
Methynodiol Diacetate	Progestogen	23163-51-1		C <sub>25</sub> H <sub>34</sub> O <sub>4</sub>
Methypylon	Sedative	125-64-4		C <sub>10</sub> H <sub>17</sub> NO <sub>2</sub>
Methysergide	Antimigraine	361-37-5	Y	C <sub>21</sub> H <sub>27</sub> N <sub>3</sub> O <sub>2</sub>
Metiamide	Antitumor	34839-70-8		C <sub>9</sub> H <sub>16</sub> N <sub>4</sub> S <sub>2</sub>
Metiapine	Antipsychotic	5800-19-1		C <sub>19</sub> H <sub>21</sub> N <sub>3</sub> S

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Metiazinic Acid	Antiinflammatory	13993-65-2		C <sub>15</sub> H <sub>13</sub> NO <sub>2</sub> S
Metibride	Antithrombotic	77989-60-7		C <sub>18</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>2</sub> S <sub>2</sub>
Meticrane	Diuretic	1084-65-7		C <sub>10</sub> H <sub>13</sub> NO <sub>4</sub> S <sub>2</sub>
Metildigoxin	Cardiotonic	30685-43-9	Y	C <sub>42</sub> H <sub>66</sub> O <sub>14</sub>
Metindizate	Antispasmodic	15687-33-9		C <sub>25</sub> H <sub>31</sub> NO <sub>3</sub>
Metioprim	Antibacterial	68902-57-8		C <sub>14</sub> H <sub>18</sub> N <sub>4</sub> O <sub>2</sub> S
Metioxate	Antidepressant	42110-58-7		C <sub>22</sub> H <sub>27</sub> N <sub>3</sub> O <sub>4</sub> S
Metipirox	Antibacterial	29342-02-7		C <sub>7</sub> H <sub>9</sub> NO <sub>2</sub>
Metipranolol	Antihypertensive	22664-55-7		C <sub>17</sub> H <sub>27</sub> NO <sub>4</sub>
Metiprenaline	Bronchodilator	1212-03-9		C <sub>12</sub> H <sub>19</sub> NO <sub>3</sub>
Metitepine	Antipsychotic	20229-30-5		C <sub>20</sub> H <sub>24</sub> N <sub>2</sub> S <sub>2</sub>
Metizoline	Adrenergic	17692-22-7		C <sub>13</sub> H <sub>14</sub> N <sub>2</sub> S
Metkephamid Acetate	Analgesic	66960-34-7		C <sub>29</sub> H <sub>40</sub> N <sub>6</sub> O <sub>6</sub> S
Metochalcone	Choleric	18493-30-6		C <sub>18</sub> H <sub>18</sub> O <sub>4</sub>
Metoclopramide	Antiemetic	364-62-5	Y	C <sub>14</sub> H <sub>22</sub> ClN <sub>3</sub> O <sub>2</sub>
Metocurine	Muscle Relaxant	5152-30-7		C <sub>40</sub> H <sub>48</sub> N <sub>2</sub> O <sub>6</sub>
Metocurine Iodide	Muscle Relaxant	7601-55-0		C <sub>40</sub> H <sub>48</sub> I <sub>2</sub> N <sub>2</sub> O <sub>6</sub>
Metofenazate	Antipsychotic	388-51-2		C <sub>31</sub> H <sub>36</sub> ClN <sub>3</sub> O <sub>5</sub> S
Metogest	Steroid	52279-58-0		C <sub>20</sub> H <sub>30</sub> O <sub>2</sub>
Metolazone	Diuretic	17560-51-9	Y	C <sub>16</sub> H <sub>16</sub> ClN <sub>3</sub> O <sub>3</sub> S
Metomidate	Sedative	5377-20-8		C <sub>13</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Metopimazine	Antiemetic	14008-44-7		C <sub>22</sub> H <sub>27</sub> N <sub>3</sub> O <sub>3</sub> S <sub>2</sub>
Metopon	Analgesic	143-52-2		C <sub>18</sub> H <sub>21</sub> NO <sub>3</sub>
Metoprine	Antineoplastic	7761-45-7		C <sub>11</sub> H <sub>10</sub> Cl <sub>2</sub> N <sub>4</sub>
Metoprolol	Antihypertensive	51384-51-1	Y	C <sub>15</sub> H <sub>25</sub> NO <sub>3</sub>
Metoquizine	Mydriatic	7125-67-9		C <sub>22</sub> H <sub>27</sub> N <sub>5</sub> O
Metoserpate	Sedative	1178-28-5		C <sub>24</sub> H <sub>32</sub> N <sub>2</sub> O <sub>5</sub>
Metostilenol	Steroid	103980-45-6		C <sub>15</sub> H <sub>21</sub> NO <sub>3</sub>
Metoxepin	Antipsychotic	22013-23-6		C <sub>20</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>
Metrafazoline	Decongestant	38349-38-1		C <sub>17</sub> H <sub>22</sub> N <sub>2</sub>
Metralindole	Antidepressant	54188-38-4		C <sub>15</sub> H <sub>17</sub> N <sub>3</sub> O
Metrazifone	Nootropic	68289-14-5		C <sub>20</sub> H <sub>23</sub> N <sub>5</sub> O
Metrenperone	Steroid	81043-56-3		C <sub>24</sub> H <sub>26</sub> FN <sub>3</sub> O <sub>2</sub>
Metribolone	Steroid	965-93-5		C <sub>19</sub> H <sub>24</sub> O <sub>2</sub>
Metrifonate	Anthelminthic	52-68-6		C <sub>4</sub> H <sub>8</sub> Cl <sub>3</sub> O <sub>4</sub> P
Metrifudil	Antiseizure	23707-33-7		C <sub>18</sub> H <sub>21</sub> N <sub>5</sub> O <sub>4</sub>
Metronidazole	Antiprotozoal	443-48-1	Y	C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> O <sub>3</sub>
Meturedepa	Antineoplastic	661-29-6		C <sub>11</sub> H <sub>22</sub> N <sub>3</sub> O <sub>3</sub> P
Metyridine	Analgesic	14-91-0		C <sub>8</sub> H <sub>11</sub> NO
Metyrosine	Antineoplastic	672-87-7	Y	C <sub>10</sub> H <sub>13</sub> NO <sub>3</sub>
Mevastatin	Antihyperlipidemic	73573-88-3		C <sub>23</sub> H <sub>34</sub> O <sub>5</sub>
Mexafylline	Bronchodilator	80294-25-3		C <sub>14</sub> H <sub>18</sub> N <sub>4</sub> O <sub>2</sub>
Mexazolam	Anxiolytic	31868-18-5		C <sub>18</sub> H <sub>16</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Mexenone	Dermatologic	1641-17-4		C <sub>15</sub> H <sub>14</sub> O <sub>3</sub>
Mexiletine	Antiarrhythmic	31828-71-4	Y	C <sub>11</sub> H <sub>17</sub> NO
Mexiprostil	Antiulcerative	88980-20-5		C <sub>23</sub> H <sub>40</sub> O <sub>6</sub>
Mexoprofen	Analgesic	37529-08-1		C <sub>16</sub> H <sub>22</sub> O <sub>2</sub>
Mexrenoate Potassium	Antihypertensive	41020-68-2		C <sub>24</sub> H <sub>34</sub> O <sub>6</sub>
Mezacopride	Antiemetic	89613-77-4		C <sub>16</sub> H <sub>22</sub> ClN <sub>3</sub> O <sub>2</sub>
Mezepine	Analgesic	27432-00-4		C <sub>18</sub> H <sub>22</sub> N <sub>2</sub>
Mezilamine	Antidepressant	50335-55-2		C <sub>11</sub> H <sub>18</sub> ClN <sub>5</sub> S
Mezlocillin	Antibiotic	51481-65-3		C <sub>21</sub> H <sub>25</sub> N <sub>5</sub> O <sub>8</sub> S <sub>2</sub>
Mianserin	Antidepressant	24219-97-4	Y	C <sub>18</sub> H <sub>20</sub> N <sub>2</sub>
Mibefradil	Antihypertensive	116644-53-2	Y	C <sub>29</sub> H <sub>38</sub> FN <sub>3</sub> O <sub>3</sub>
Mibolerone	Androgen	3704-09-4		C <sub>20</sub> H <sub>30</sub> O <sub>2</sub>
Micinate	Vasodilator	39537-99-0		C <sub>23</sub> H <sub>27</sub> NO <sub>4</sub>
Miconazole	Antifungal	22916-47-8		C <sub>18</sub> H <sub>14</sub> Cl <sub>4</sub> N <sub>2</sub> O
Micronomicin	Antibiotic	52093-21-7		C <sub>20</sub> H <sub>41</sub> N <sub>5</sub> O <sub>7</sub>
Midafalur	Sedative	23757-42-8		C <sub>7</sub> H <sub>3</sub> F <sub>12</sub> N <sub>3</sub>
Midafotel	Analgesic	117414-74-1		C <sub>8</sub> H <sub>15</sub> N <sub>2</sub> O <sub>5</sub> P
Midaglizole	Antihypertensive	66529-17-7		C <sub>16</sub> H <sub>17</sub> N <sub>3</sub>
Midamaline	Antihypertensive	496-38-8		C <sub>18</sub> H <sub>21</sub> ClN <sub>4</sub>
Midaxifylline	Bronchodilator	151159-23-8		C <sub>16</sub> H <sub>25</sub> N <sub>5</sub> O <sub>2</sub>



Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Midazolgel	Unclassified	80614-27-3		C <sub>18</sub> H <sub>24</sub> N <sub>2</sub> O
Midazolam	Anesthetic	59467-70-8		C <sub>18</sub> H <sub>15</sub> ClFN <sub>3</sub>
Midecamycin	Antibiotic	35457-80-8		C <sub>41</sub> H <sub>67</sub> NO <sub>15</sub>
Midesteine	Antitussive	94149-41-4		C <sub>12</sub> H <sub>13</sub> NO <sub>5</sub> S <sub>3</sub>
Midodrine	Antihypertensive	42794-76-3	Y	C <sub>12</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub>
Midostaurin	Antineoplastic	120685-11-2	Y	C <sub>35</sub> H <sub>30</sub> N <sub>4</sub> O <sub>4</sub>
Mifentidine	Antihistaminic	83184-43-4		C <sub>13</sub> H <sub>16</sub> N <sub>4</sub>
Mifepristone	Abortifacient	84371-65-3		C <sub>29</sub> H <sub>35</sub> NO <sub>2</sub>
Mifobate	Antihyperlipidemic	76541-72-5		C <sub>11</sub> H <sub>17</sub> ClO <sub>7</sub> P <sub>2</sub>
Migalastat	Antihypertensive	108147-54-2	Y	C <sub>6</sub> H <sub>13</sub> NO <sub>4</sub>
Miglitol	Antidiabetic	72432-03-2	Y	C <sub>8</sub> H <sub>17</sub> NO <sub>5</sub>
Miglustat	Antihypertensive	72599-27-0	Y	C <sub>10</sub> H <sub>21</sub> NO <sub>4</sub>
Milacainide	Antiarrhythmic	141725-09-9		C <sub>19</sub> H <sub>25</sub> N <sub>3</sub> O
Milacemide	Anticonvulsant	76990-56-2		C <sub>7</sub> H <sub>16</sub> N <sub>2</sub> O
Milameline	Nootropic	139886-32-1		C <sub>8</sub> H <sub>14</sub> N <sub>2</sub> O
Milataxel	Antineoplastic	393101-41-2		C <sub>44</sub> H <sub>55</sub> NO <sub>16</sub>
Milenperone	Antipsychotic	59831-64-0		C <sub>22</sub> H <sub>23</sub> ClFN <sub>3</sub> O <sub>2</sub>
Milfasartan	Antihypertensive	148564-47-0		C <sub>30</sub> H <sub>30</sub> N <sub>6</sub> O <sub>5</sub> S
Milipertine	Antipsychotic	24360-55-2		C <sub>24</sub> H <sub>31</sub> N <sub>3</sub> O <sub>3</sub>
Milnacipran	Antidepressant	92623-85-3	Y	C <sub>15</sub> H <sub>22</sub> N <sub>2</sub> O
Miloxacin	Antibiotic	37065-29-5		C <sub>12</sub> H <sub>9</sub> NO <sub>6</sub>
Milrinone	Cardiotonic	78415-72-2		C <sub>12</sub> H <sub>9</sub> N <sub>3</sub> O
Miltefosine	Antineoplastic	58066-85-6	Y	C <sub>21</sub> H <sub>46</sub> NO <sub>4</sub> P
Milverine	Antispasmodic	75437-14-8		C <sub>20</sub> H <sub>20</sub> N <sub>2</sub>
Mimbane	Analgesic	3277-59-6		C <sub>20</sub> H <sub>26</sub> N <sub>2</sub>
Minalrestat	Antidiabetic	129688-50-2		C <sub>19</sub> H <sub>11</sub> BrF <sub>2</sub> N <sub>2</sub> O <sub>4</sub>
Minamestane	Antineoplastic	105051-87-4		C <sub>19</sub> H <sub>23</sub> NO <sub>2</sub>
Minaprine	Antidepressant	25905-77-5		C <sub>17</sub> H <sub>22</sub> N <sub>4</sub> O
Minaxolone	Anesthetic	62571-87-3		C <sub>25</sub> H <sub>43</sub> NO <sub>3</sub>
Mindodilol	Unclassified	70260-53-6		C <sub>23</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub>
Mindoperone	Antipsychotic	52157-83-2		C <sub>25</sub> H <sub>29</sub> FN <sub>2</sub> O <sub>2</sub>
Minepentate	Unclassified	13877-99-1		C <sub>18</sub> H <sub>27</sub> NO <sub>3</sub>
Minocromil	Antihistaminic	85118-44-1		C <sub>18</sub> H <sub>16</sub> N <sub>2</sub> O <sub>6</sub>
Minocycline	Antibiotic	10118-90-8	Y	C <sub>23</sub> H <sub>27</sub> N <sub>3</sub> O <sub>7</sub>
Minodronic Acid	Bone Resorption Inhibitor	180064-38-4	Y	C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O <sub>7</sub> P <sub>2</sub>
Minopafant	Antithrombotic	128420-61-1		C <sub>46</sub> H <sub>73</sub> ClN <sub>4</sub> O <sub>9</sub>
Minoxidil	Antihypertensive	38304-91-5		C <sub>9</sub> H <sub>15</sub> N <sub>5</sub> O
Mioflazine	Vasodilator	79467-23-5		C <sub>29</sub> H <sub>30</sub> Cl <sub>2</sub> F <sub>2</sub> N <sub>4</sub> O <sub>2</sub>
Mipimazole	Antibiotic	20406-60-4		C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> S
Mipitroban	Anticoagulant	136122-46-8		C <sub>19</sub> H <sub>19</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>2</sub>
Miproxifene	Antineoplastic	129612-87-9		C <sub>29</sub> H <sub>35</sub> NO <sub>2</sub>
Mirfentanil	Analgesic	117523-47-4		C <sub>22</sub> H <sub>24</sub> N <sub>4</sub> O <sub>2</sub>
Mirincamycin	Antibacterial	31101-25-4		C <sub>19</sub> H <sub>35</sub> ClN <sub>2</sub> O <sub>5</sub> S
Mirisetron Maleate	Anxiolytic	135905-89-4		C <sub>24</sub> H <sub>31</sub> N <sub>3</sub> O <sub>2</sub>
Mioprofen	Analgesic	55843-86-2		C <sub>16</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Mirosamicin	Antibacterial	3684-69-2		C <sub>37</sub> H <sub>61</sub> NO <sub>13</sub>
Mirtazapine	Antidepressant	85650-52-8	Y	C <sub>17</sub> H <sub>19</sub> N <sub>3</sub>
Misonidazole	Antiprotozoal	13551-87-6		C <sub>7</sub> H <sub>11</sub> N <sub>3</sub> O <sub>4</sub>
Misoprostol	Antilucerative	59122-46-2		C <sub>22</sub> H <sub>38</sub> O <sub>5</sub>
Mitemincal Fumarate	Gastroprokinetic	154738-42-8		C <sub>40</sub> H <sub>69</sub> NO <sub>12</sub>
Mitiglinide	Antidiabetic	145375-43-5	Y	C <sub>19</sub> H <sub>25</sub> NO <sub>3</sub>
Mitindomide	Antineoplastic	10403-51-7		C <sub>14</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub>
Mitobronitol	Antineoplastic	488-41-5		C <sub>6</sub> H <sub>12</sub> Br <sub>2</sub> O <sub>4</sub>
Mitocloimine	Antispasmodic	17692-54-5		C <sub>16</sub> H <sub>19</sub> Cl <sub>2</sub> NO
Mitoflaxone	Antineoplastic	87626-55-9		C <sub>17</sub> H <sub>12</sub> O <sub>4</sub>
Mitoguazone	Antineoplastic	459-86-9		C <sub>5</sub> H <sub>12</sub> N <sub>8</sub>
Mitolactol	Antineoplastic	10318-26-0		C <sub>6</sub> H <sub>12</sub> Br <sub>2</sub> O <sub>4</sub>
Mitomycin	Antineoplastic	50-07-7		C <sub>15</sub> H <sub>18</sub> N <sub>4</sub> O <sub>5</sub>
Mitonafide	Antineoplastic	54824-17-8		C <sub>16</sub> H <sub>15</sub> N <sub>3</sub> O <sub>4</sub>
Mitopodozide	Antineoplastic	1508-45-8		C <sub>24</sub> H <sub>30</sub> N <sub>2</sub> O <sub>8</sub>
Mitoquidone	Antineoplastic	91753-07-0		C <sub>20</sub> H <sub>13</sub> NO <sub>2</sub>
Mitotane	Antineoplastic	53-19-0	Y	C <sub>14</sub> H <sub>10</sub> Cl <sub>4</sub>
Mitotenamine	Antihypertensive	7696-00-6		C <sub>13</sub> H <sub>15</sub> Br <sub>2</sub> ClNS

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Mitoxantrone	Antineoplastic	65271-80-9		C <sub>22</sub> H <sub>28</sub> N <sub>4</sub> O <sub>6</sub>
Mitozolomide	Antineoplastic	85622-95-3		C <sub>7</sub> H <sub>7</sub> ClN <sub>6</sub> O <sub>2</sub>
Mitratapide	Antiobesity	179602-65-4		C <sub>36</sub> H <sub>41</sub> ClN <sub>8</sub> O <sub>4</sub> S
Mivazerol	Antihypotensive	125472-02-8		C <sub>11</sub> H <sub>11</sub> N <sub>3</sub> O <sub>2</sub>
Mivobulin Isethionate	Antineoplastic	122332-18-7		C <sub>17</sub> H <sub>19</sub> N <sub>5</sub> O <sub>2</sub>
Mivotilate	Hepatic Protectant	130112-42-4		C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub> S <sub>3</sub>
Mixidine	Vasodilator	27737-38-8		C <sub>15</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>
Mizolastine	Antihistaminic	108612-45-9	Y	C <sub>24</sub> H <sub>25</sub> FN <sub>6</sub> O
Mizoribine	Immunosuppressant	50924-49-7	Y	C <sub>9</sub> H <sub>13</sub> N <sub>3</sub> O <sub>6</sub>
Mobenzoxamine	Antiemetic	65329-79-5		C <sub>30</sub> H <sub>35</sub> FN <sub>2</sub> O <sub>3</sub>
Mocimycin	Antibiotic	50935-71-2		C <sub>43</sub> H <sub>60</sub> N <sub>2</sub> O <sub>12</sub>
Mociprazine	Antiemetic	56693-13-1		C <sub>22</sub> H <sub>32</sub> N <sub>2</sub> O <sub>3</sub>
Moclobemide	Antidepressant	71320-77-9	Y	C <sub>13</sub> H <sub>17</sub> ClN <sub>2</sub> O <sub>2</sub>
Moctamide	Antithrombotic	29619-86-1		C <sub>33</sub> H <sub>47</sub> NO
Modafinil	Nootropic	68693-11-8	Y	C <sub>15</sub> H <sub>15</sub> N <sub>2</sub> O <sub>2</sub> S
Modaline Sulfate	Antidepressant	2856-74-8		C <sub>10</sub> H <sub>15</sub> N <sub>3</sub>
Modecainide	Antiarrhythmic	81329-71-7		C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub>
Modipafant	Antithrombotic	122957-06-6		C <sub>34</sub> H <sub>29</sub> ClN <sub>6</sub> O <sub>3</sub>
Moexipril	Antihypertensive	103775-10-6	Y	C <sub>27</sub> H <sub>34</sub> N <sub>2</sub> O <sub>7</sub>
Moexiprilat	Antihypertensive	103775-14-0		C <sub>25</sub> H <sub>30</sub> N <sub>2</sub> O <sub>7</sub>
Mofarotene	Antineoplastic	125533-88-2		C <sub>29</sub> H <sub>39</sub> NO <sub>2</sub>
Mofebutazone	Antiinflammatory	2210-63-1		C <sub>13</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>
Mofegiline	Antiparkinsonian	119386-96-8		C <sub>11</sub> H <sub>13</sub> F <sub>2</sub> N
Mofezolac	Antiinflammatory	78967-07-4	Y	C <sub>19</sub> H <sub>17</sub> NO <sub>5</sub>
Mofloverine	Antispasmodic	54063-50-2		C <sub>16</sub> H <sub>23</sub> NO <sub>6</sub>
Mofoxime	Analgesic	29936-79-6		C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub>
Moguisteine	Antitussive	19637-67-1		C <sub>16</sub> H <sub>21</sub> NO <sub>5</sub> S
Molfarnate	Antiulcerative	83689-23-0		C <sub>31</sub> H <sub>50</sub> O <sub>2</sub>
Molinazone	Analgesic	5581-46-4		C <sub>11</sub> H <sub>12</sub> N <sub>4</sub> O <sub>2</sub>
Molindone	Antipsychotic	7416-34-4	Y	C <sub>16</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub>
Molracetam	Nootropic	94746-78-8		C <sub>18</sub> H <sub>25</sub> N <sub>3</sub> O <sub>4</sub>
Molsidomine	Antianginal	25717-80-0	Y	C <sub>9</sub> H <sub>14</sub> N <sub>4</sub> O <sub>4</sub>
Mometasone Furoate	Steroid	83919-23-7		C <sub>27</sub> H <sub>30</sub> Cl <sub>2</sub> O <sub>6</sub>
Monalazone Disodium	Antiinflammatory	106145-03-3		C <sub>7</sub> H <sub>6</sub> ClNO <sub>4</sub> S
Monatepil Maleate	Antianginal	103377-41-9		C <sub>28</sub> H <sub>30</sub> FN <sub>3</sub> OS
Monensin	Antibiotic	17090-79-8		C <sub>36</sub> H <sub>62</sub> O <sub>11</sub>
Monobenzone	Dermatologic	103-16-2		C <sub>13</sub> H <sub>12</sub> O <sub>2</sub>
Monooctanoin	Anticholelithogenic	502-54-5		C <sub>11</sub> H <sub>22</sub> O <sub>4</sub>
Monometacrine	Antidepressant	4757-49-7		C <sub>19</sub> H <sub>24</sub> N <sub>2</sub>
Monoxerutin	Capillary Protectant	23869-24-1		C <sub>29</sub> H <sub>34</sub> O <sub>17</sub>
Montelukast	Bronchodilator	158966-92-8	Y	C <sub>35</sub> H <sub>36</sub> ClNO <sub>3</sub> S
Montirelin	Thyroid	90243-66-6		C <sub>17</sub> H <sub>24</sub> N <sub>6</sub> O <sub>4</sub> S
Moperone	Antipsychotic	1050-79-9		C <sub>22</sub> H <sub>26</sub> FNO <sub>2</sub>
Mopidamol	Antineoplastic	13665-88-8		C <sub>19</sub> H <sub>31</sub> N <sub>7</sub> O <sub>4</sub>
Mopidralazine	Antihypertensive	75841-82-6		C <sub>14</sub> H <sub>19</sub> N <sub>5</sub> O
Moprolol	Antihypertensive	5741-22-0		C <sub>13</sub> H <sub>21</sub> NO <sub>3</sub>
Moquizone	Choleretic	19395-58-5		C <sub>20</sub> H <sub>21</sub> N <sub>3</sub> O <sub>3</sub>
Morantel Tartrate	Anthelminthic	20574-50-9		C <sub>12</sub> H <sub>16</sub> N <sub>2</sub> S
Morazone	Analgesic	6536-18-1		C <sub>23</sub> H <sub>27</sub> N <sub>3</sub> O <sub>2</sub>
Morclofone	Antitussive	31848-01-8		C <sub>21</sub> H <sub>24</sub> ClNO <sub>5</sub>
Morforex	Anorexic	41152-17-4		C <sub>15</sub> H <sub>24</sub> N <sub>2</sub> O
Moricizine	Antiarrhythmic	31883-05-3	Y	C <sub>22</sub> H <sub>25</sub> N <sub>3</sub> O <sub>4</sub> S
Morinamide	Antibacterial	952-54-5		C <sub>10</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub>
Morniflumate	Antiinflammatory	65847-85-0		C <sub>19</sub> H <sub>20</sub> F <sub>3</sub> N <sub>3</sub> O <sub>3</sub>
Morocromen	Antithrombotic	35843-07-3		C <sub>21</sub> H <sub>27</sub> N <sub>3</sub> O <sub>5</sub>
Moroxydine	Antiviral	3731-59-7		C <sub>6</sub> H <sub>13</sub> N <sub>5</sub> O
Morpheridine	Analgesic	469-81-8		C <sub>20</sub> H <sub>30</sub> N <sub>2</sub> O <sub>3</sub>
Morphine Glucuronide	Nootropic	20290-10-2		C <sub>23</sub> H <sub>27</sub> NO <sub>9</sub>
Morphine	Analgesic	57-27-2	Y	C <sub>17</sub> H <sub>19</sub> NO <sub>3</sub>
Morsuximide	Anticonvulsant	3780-72-1		C <sub>16</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub>
Mosapramine	Antipsychotic	89419-40-9		C <sub>28</sub> H <sub>35</sub> ClN <sub>4</sub> O
Mosapride	Gastroprokinetic	112885-41-3	Y	C <sub>21</sub> H <sub>25</sub> ClFN <sub>3</sub> O <sub>3</sub>
Motapizone	Bronchodilator	90697-57-7		C <sub>12</sub> H <sub>12</sub> N <sub>4</sub> OS

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Motexafin	Antineoplastic	189752-49-6		C <sub>48</sub> H <sub>67</sub> N <sub>5</sub> O <sub>10</sub>
Motrazepam	Anxiolytic	29442-58-8		C <sub>17</sub> H <sub>15</sub> N <sub>3</sub> O <sub>4</sub>
Motretinide	Dermatologic	56281-36-8		C <sub>23</sub> H <sub>31</sub> NO <sub>2</sub>
Moveltipril	Antihypertensive	85856-54-8		C <sub>19</sub> H <sub>30</sub> N <sub>2</sub> O <sub>5</sub> S
Moxadolen	Unclassified	75992-53-9		C <sub>11</sub> H <sub>13</sub> NO <sub>4</sub>
Moxalactam	Antibiotic	64952-97-2		C <sub>20</sub> H <sub>20</sub> N <sub>6</sub> O <sub>5</sub> S
Moxaprine	Antiarrhythmic	53076-26-9		C <sub>23</sub> H <sub>32</sub> N <sub>2</sub> O
Moxastine	Antihistaminic	3572-74-5		C <sub>18</sub> H <sub>23</sub> NO
Moxaverine	Antispasmodic	10539-19-2		C <sub>20</sub> H <sub>21</sub> NO <sub>2</sub>
Moxazocine	Analgesic	58239-89-7		C <sub>18</sub> H <sub>25</sub> NO <sub>2</sub>
Moxestrol	Estrogen	34816-55-2		C <sub>21</sub> H <sub>26</sub> O <sub>3</sub>
Moxicoumone	Unclassified	17692-56-7		C <sub>22</sub> H <sub>30</sub> N <sub>2</sub> O <sub>6</sub>
Moxidectin	Antiprotozoal	113507-06-5		C <sub>37</sub> H <sub>53</sub> NO <sub>8</sub>
Moxifloxacin	Antibiotic	151096-09-2	Y	C <sub>21</sub> H <sub>24</sub> FN <sub>3</sub> O <sub>4</sub>
Moxilubant Maleate	Antirheumatic	146978-48-5		C <sub>26</sub> H <sub>37</sub> N <sub>3</sub> O <sub>4</sub>
Moxipraquine	Antiprotozoal	23790-08-1		C <sub>24</sub> H <sub>38</sub> N <sub>4</sub> O <sub>2</sub>
Moxiraprine	Muscle Relaxant	82239-52-9		C <sub>17</sub> H <sub>22</sub> N <sub>4</sub> O <sub>2</sub>
Moxisylyte	Vasodilator	54-32-0	Y	C <sub>16</sub> H <sub>25</sub> NO <sub>3</sub>
Moxnidazole	Antiprotozoal	52279-59-1		C <sub>13</sub> H <sub>18</sub> N <sub>6</sub> O <sub>5</sub>
Moxonidine	Antihypertensive	75438-57-2		C <sub>9</sub> H <sub>12</sub> ClN <sub>5</sub> O
Mozavaptan	Plasma Volume Expander	137975-06-5	Y	C <sub>27</sub> H <sub>29</sub> N <sub>3</sub> O <sub>2</sub>
Mozenavir	Antiviral	174391-92-5		C <sub>33</sub> H <sub>36</sub> N <sub>4</sub> O <sub>3</sub>
Mubritinib	Antineoplastic	366017-09-6		C <sub>25</sub> H <sub>23</sub> F <sub>3</sub> N <sub>4</sub> O <sub>2</sub>
Mupirocin	Antibacterial	12650-69-0		C <sub>26</sub> H <sub>44</sub> O <sub>9</sub>
Murabutide	Immunomodulator	74817-61-1		C <sub>23</sub> H <sub>40</sub> N <sub>4</sub> O <sub>11</sub>
Muraglitazar	Antidiabetic	331741-94-7		C <sub>29</sub> H <sub>28</sub> N <sub>2</sub> O <sub>7</sub>
Murocainide	Antiarrhythmic	66203-94-9		C <sub>19</sub> H <sub>27</sub> N <sub>3</sub> O <sub>5</sub>
Muzolimine	Diuretic	55294-15-0		C <sub>11</sub> H <sub>11</sub> Cl <sub>2</sub> N <sub>5</sub> O
Mycophenolate Mofetil	Immunomodulator	128794-94-5	Y	C <sub>23</sub> H <sub>31</sub> NO <sub>7</sub>
Mycophenolic Acid	Immunosuppressant	24280-93-1		C <sub>17</sub> H <sub>20</sub> O <sub>6</sub>
Myfadol	Analgesic	4575-34-2		C <sub>21</sub> H <sub>25</sub> NO <sub>2</sub>
Myralact	Unclassified	25737-87-5		C <sub>16</sub> H <sub>35</sub> NO
Myrophine	Analgesic	467-18-5		C <sub>38</sub> H <sub>51</sub> NO <sub>4</sub>
Myrtecaine	Anesthetic	7712-50-7		C <sub>17</sub> H <sub>31</sub> NO
N Pyridinium Chloride	Unclassified	6272-74-8		C <sub>21</sub> H <sub>35</sub> ClN <sub>2</sub> O <sub>3</sub>
N,1-Dimethylhexylamine	Decongestant	540-43-2		C <sub>8</sub> H <sub>19</sub> N
N,N Dimethyl P Toluidine	Unclassified	99-97-8		C <sub>9</sub> H <sub>13</sub> N
Nabazenil	Anticonvulsant	58019-65-1		C <sub>35</sub> H <sub>55</sub> NO <sub>3</sub>
Nabilone	Antiemetic	51022-71-0	Y	C <sub>24</sub> H <sub>36</sub> O <sub>3</sub>
Nabitan	Analgesic	66556-74-9		C <sub>35</sub> H <sub>52</sub> N <sub>2</sub> O <sub>3</sub>
Naboctate	Antiglaucoma	74912-19-9		C <sub>33</sub> H <sub>53</sub> NO <sub>3</sub>
Nabumetone	Antiinflammatory	42924-53-8	Y	C <sub>15</sub> H <sub>16</sub> O <sub>2</sub>
Nacartocin	Oxytocic	77727-10-7		C <sub>46</sub> H <sub>71</sub> N <sub>11</sub> O <sub>11</sub> S
Nadide	Antidote	53-84-9		C <sub>21</sub> H <sub>27</sub> N <sub>7</sub> O <sub>14</sub> P <sub>2</sub>
Nadifloxacin	Antibiotic	124858-35-1		C <sub>19</sub> H <sub>21</sub> FN <sub>2</sub> O <sub>4</sub>
Nadolol	Antihypertensive	42200-33-9	Y	C <sub>17</sub> H <sub>27</sub> NO <sub>4</sub>
Nadoxolol	Antiarrhythmic	54063-51-3		C <sub>14</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>
Naepaine	Anesthetic	2188-67-2		C <sub>14</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>
Nafagrel	Antiinflammatory	97901-21-8		C <sub>15</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>
Nafamostat Mesylate	Anticoagulant	81525-10-2		C <sub>19</sub> H <sub>17</sub> N <sub>5</sub> O <sub>2</sub>
Nafazatom	Antithrombotic	59040-30-1		C <sub>16</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>
Nafcaproic Acid	Hemostatic	1085-91-2		C <sub>16</sub> H <sub>18</sub> O <sub>2</sub>
Nafcillin	Antibiotic	147-52-4		C <sub>21</sub> H <sub>22</sub> N <sub>2</sub> O <sub>5</sub> S
Nafenodone	Antidepressant	92615-20-8		C <sub>20</sub> H <sub>23</sub> NO
Nafenopin	Antihyperlipidemic	3771-19-5		C <sub>20</sub> H <sub>22</sub> O <sub>3</sub>
Nafetolol	Antihypertensive	42050-23-7		C <sub>19</sub> H <sub>29</sub> NO <sub>3</sub>
Nafimidone	Anticonvulsant	64212-22-2		C <sub>15</sub> H <sub>12</sub> N <sub>2</sub> O
Nafiverine	Antispasmodic	5061-22-3		C <sub>34</sub> H <sub>38</sub> N <sub>2</sub> O <sub>4</sub>
Naflocort	Steroid	59497-39-1		C <sub>29</sub> H <sub>33</sub> FO <sub>4</sub>
Nafomine Malate	Muscle Relaxant	46263-35-8		C <sub>12</sub> H <sub>13</sub> NO
Nafoxadol	Analgesic	84145-90-4		C <sub>15</sub> H <sub>15</sub> NO <sub>2</sub>
Nafoxidine	Steroid	1845-11-0		C <sub>29</sub> H <sub>31</sub> NO <sub>2</sub>
Nafrotyl	Vasodilator	31329-57-4	Y	C <sub>24</sub> H <sub>33</sub> NO <sub>3</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Naftalofos	Anthelminthic	1491-41-4		C <sub>16</sub> H <sub>16</sub> NO <sub>6</sub> P
Naftazone	Capillary Protectant	15687-37-3	Y	C <sub>11</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub>
Naftifine	Antifungal	65472-88-0		C <sub>21</sub> H <sub>21</sub> N
Naftopidil	Antihypertensive	57149-07-2	Y	C <sub>24</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub>
Naftoxate	Unclassified	28820-28-2		C <sub>19</sub> H <sub>14</sub> N <sub>2</sub> OS <sub>2</sub>
Naftypramide	Antiemetic	1505-95-9		C <sub>19</sub> H <sub>26</sub> N <sub>2</sub> O
Naglvian	Antidiabetic	122575-28-4		C <sub>22</sub> H <sub>46</sub> N <sub>4</sub> O <sub>3S2V</sub>
Nalbuphine	Analgesic	20594-83-6	Y	C <sub>21</sub> H <sub>27</sub> NO <sub>4</sub>
Nalfurafine	Dermatologic	152657-84-6		C <sub>28</sub> H <sub>32</sub> N <sub>2</sub> O <sub>5</sub>
Nalidixic Acid	Antibiotic	389-08-2		C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>
Nalmefene	Antidote	55096-26-9		C <sub>21</sub> H <sub>25</sub> NO <sub>3</sub>
Nalmexone	Analgesic	16676-26-9	Y	C <sub>21</sub> H <sub>25</sub> NO <sub>4</sub>
Nalorphine	Antidote	62-67-9		C <sub>19</sub> H <sub>21</sub> NO <sub>3</sub>
Naloxone	Antidote	465-65-6	Y	C <sub>19</sub> H <sub>21</sub> NO <sub>4</sub>
Naltrexone	Antidote	16590-41-3		C <sub>20</sub> H <sub>23</sub> NO <sub>4</sub>
Naminidil	Vasodilator	220641-11-2	Y	C <sub>15</sub> H <sub>19</sub> N <sub>5</sub>
Naminterol	Bronchodilator	93047-40-6		C <sub>19</sub> H <sub>26</sub> N <sub>2</sub> O <sub>3</sub>
Namirotene	Immunomodulator	101506-83-6		C <sub>17</sub> H <sub>18</sub> O <sub>2</sub> S
Nanafrocic	Antibiotic	52934-83-5		C <sub>16</sub> H <sub>14</sub> O <sub>6</sub>
Nandrolone Cyclotate	Steroid	22263-51-0		C <sub>28</sub> H <sub>38</sub> O <sub>3</sub>
Nandrolone Decanoate	Steroid	360-70-3		C <sub>28</sub> H <sub>44</sub> O <sub>3</sub>
Nandrolone Phenpropionate	Androgen	62-90-8		C <sub>27</sub> H <sub>34</sub> O <sub>3</sub>
Nanofin	Antirheumatic	504-03-0		C <sub>7</sub> H <sub>15</sub> N
Nanterinone	Vasodilator	102791-47-9		C <sub>15</sub> H <sub>15</sub> N <sub>3</sub> O
Nantradol	Analgesic	72028-54-7		C <sub>27</sub> H <sub>35</sub> NO <sub>4</sub>
Napactadine	Antidepressant	76631-45-3		C <sub>14</sub> H <sub>16</sub> N <sub>2</sub>
Napamezole	Antidepressant	91524-14-0		C <sub>14</sub> H <sub>16</sub> N <sub>2</sub>
Naphazoline	Decongestant	835-31-4		C <sub>14</sub> H <sub>14</sub> N <sub>2</sub>
Naphthalene	Anthelminthic	91-20-3		C <sub>10</sub> H <sub>8</sub>
Naphthocaine	Analgesic	5656-83-7		C <sub>17</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>
Naphthonone	Unclassified	7114-11-6		C <sub>16</sub> H <sub>16</sub> O <sub>2</sub>
Napirimus	Immunosuppressant	70696-66-1		C <sub>17</sub> H <sub>13</sub> NO <sub>3</sub>
Napitane Mesylate	Antidepressant	148152-63-0		C <sub>22</sub> H <sub>25</sub> NO <sub>2</sub>
Naproxime	Analgesic	57925-64-1		C <sub>13</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Naproxen	Antiinflammatory	22204-53-1	Y	C <sub>14</sub> H <sub>14</sub> O <sub>3</sub>
Naproxol	Antiinflammatory	26159-36-4		C <sub>14</sub> H <sub>16</sub> O <sub>2</sub>
Napsagatran	Antithrombotic	154397-77-0		C <sub>26</sub> H <sub>34</sub> N <sub>6</sub> O <sub>6</sub> S
Naranol	Antipsychotic	22292-91-7		C <sub>18</sub> H <sub>21</sub> NO <sub>2</sub>
Narasin	Antibacterial	55134-13-9		C <sub>43</sub> H <sub>72</sub> O <sub>11</sub>
Naratriptan	Antimigraine	121679-13-8	Y	C <sub>17</sub> H <sub>25</sub> N <sub>3</sub> O <sub>2</sub> S
Narceine	Analgesic	131-28-2		C <sub>23</sub> H <sub>27</sub> NO <sub>8</sub>
Nardeterol	Bronchodilator	73865-18-6		C <sub>20</sub> H <sub>24</sub> FN <sub>3</sub> O <sub>2</sub>
Naringin	Antiinflammatory	10236-47-2		C <sub>27</sub> H <sub>32</sub> O <sub>14</sub>
Naroparicil	Antithrombotic	120819-70-7		C <sub>19</sub> H <sub>17</sub> NO <sub>4</sub> S <sub>2</sub>
Natamycin	Antifungal	7681-93-8		C <sub>33</sub> H <sub>47</sub> NO <sub>13</sub>
Nateglinide	Antidiabetic	105816-04-4	Y	C <sub>19</sub> H <sub>27</sub> NO <sub>3</sub>
Naveglitazar	Antidiabetic	476436-68-7		C <sub>25</sub> H <sub>26</sub> O <sub>6</sub>
Navuridine	Antiviral	84472-85-5		C <sub>9</sub> H <sub>11</sub> N <sub>5</sub> O <sub>4</sub>
Naxagolide	Antiparkinsonian	88058-88-2		C <sub>15</sub> H <sub>21</sub> NO <sub>2</sub>
Naxaprostene	Prostaglandin	87269-59-8		C <sub>25</sub> H <sub>32</sub> O <sub>4</sub>
Naxifylline	Cardiotonic	166374-49-8		C <sub>18</sub> H <sub>24</sub> N <sub>4</sub> O <sub>3</sub>
Nealbarbital	Sedative	561-83-1		C <sub>12</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>
Nebentan	Unclassified	403604-85-3		C <sub>24</sub> H <sub>21</sub> N <sub>5</sub> O <sub>5</sub> S
Nebicapone	Antiparkinsonian	274925-86-9		C <sub>14</sub> H <sub>11</sub> NO <sub>5</sub>
Nebidrazine	Anorexic	55248-23-2		C <sub>9</sub> H <sub>8</sub> Cl <sub>2</sub> N <sub>6</sub>
Nebivolol	Antihypertensive	118457-14-0	Y	C <sub>22</sub> H <sub>25</sub> F <sub>2</sub> NO <sub>4</sub>
Neboglamine	Antifungal	163000-63-3		C <sub>13</sub> H <sub>24</sub> N <sub>2</sub> O <sub>3</sub>
Nebracetam	Nootropic	97205-34-0		C <sub>12</sub> H <sub>16</sub> N <sub>2</sub> O
Necopidem	Sedative	103844-77-5		C <sub>23</sub> H <sub>29</sub> N <sub>3</sub> O
Nedocromil	Antihistaminic	69049-73-6		C <sub>19</sub> H <sub>17</sub> NO <sub>7</sub>
Nefazodone	Antidepressant	83366-66-9		C <sub>25</sub> H <sub>32</sub> ClN <sub>5</sub> O <sub>2</sub>
Nefiracetam	Nootropic	77191-36-7		C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>
Neflumozide	Antipsychotic	86636-93-3		C <sub>22</sub> H <sub>23</sub> FN <sub>4</sub> O <sub>2</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Nefopam	Analgesic	13669-70-0		C <sub>17</sub> H <sub>19</sub> NO
Nelarabine	Antineoplastic	121032-29-9		C <sub>11</sub> H <sub>15</sub> N <sub>5</sub> O <sub>5</sub>
Neldazosin	Antihypertensive	109713-79-3		C <sub>18</sub> H <sub>25</sub> N <sub>5</sub> O <sub>4</sub>
Nelezaprine Maleate	Muscle Relaxant	69624-60-8		C <sub>18</sub> H <sub>21</sub> ClN <sub>2</sub>
Nelfinavir	Antiviral	159989-64-7	Y	C <sub>32</sub> H <sub>45</sub> N <sub>3</sub> O <sub>4</sub> S
Neltenexine	Respiratory Stimulant	99453-84-6		C <sub>18</sub> H <sub>20</sub> Br <sub>2</sub> N <sub>2</sub> O <sub>2</sub> S
Nemadectin	Antiprotozoal	102130-84-7		C <sub>36</sub> H <sub>52</sub> O <sub>8</sub>
Nemazoline	Decongestant	130759-56-7		C <sub>10</sub> H <sub>11</sub> Cl <sub>2</sub> N <sub>3</sub>
Nemifitide Ditriflutate	Antidepressant	173240-15-8		C <sub>33</sub> H <sub>43</sub> FN <sub>10</sub> O <sub>6</sub>
Nemonapride	Antiemetic	75272-39-8	Y	C <sub>21</sub> H <sub>26</sub> ClN <sub>3</sub> O <sub>2</sub>
Nemorubicin	Antineoplastic	108852-90-0		C <sub>32</sub> H <sub>37</sub> NO <sub>13</sub>
Neosarsphenamine	Antibiotic	637-30-9		C <sub>13</sub> H <sub>14</sub> As <sub>2</sub> N <sub>2</sub> O <sub>4</sub> S
Neocinchophen	Analgesic	485-34-7		C <sub>19</sub> H <sub>17</sub> NO <sub>2</sub>
Neostigmine Bromide	Cholinergic	114-80-7		C <sub>12</sub> H <sub>19</sub> BrN <sub>2</sub> O <sub>2</sub>
Nepadutant	Bronchodilator	183747-35-5	Y	C <sub>45</sub> H <sub>58</sub> N <sub>10</sub> O <sub>13</sub>
Nepafenac	Antiinflammatory	78281-72-8		C <sub>15</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Nepaprazole	Antiulcerative	156601-79-5		C <sub>18</sub> H <sub>19</sub> N <sub>3</sub> O <sub>2</sub> S
Nepicostat	Cardiotonic	173997-05-2	Y	C <sub>14</sub> H <sub>15</sub> F <sub>2</sub> N <sub>3</sub> S
Nepinalone	Hemostatic	22443-11-4	Y	C <sub>18</sub> H <sub>25</sub> NO
Nequinat	Antibacterial	13997-19-8		C <sub>22</sub> H <sub>23</sub> NO <sub>4</sub>
Neramexane Mesylate	Antidepressant	219810-59-0	Y	C <sub>11</sub> H <sub>23</sub> N
Neraminol	Antihypotensive	86140-10-5		C <sub>20</sub> H <sub>26</sub> N <sub>4</sub> O <sub>2</sub>
Nerbacadol	Unclassified	99803-72-2		C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Neridronic Acid	Bone Resorption Inhibitor	79778-41-9		C <sub>6</sub> H <sub>17</sub> NO <sub>7</sub> P <sub>2</sub>
Nerisopam	Anxiolytic	102771-12-0		C <sub>18</sub> H <sub>19</sub> N <sub>3</sub> O <sub>2</sub>
Nerispiridine	Analgesic	119229-65-1		C <sub>17</sub> H <sub>18</sub> FN <sub>3</sub>
Nesapidil	Vasodilator	118778-75-9		C <sub>23</sub> H <sub>28</sub> N <sub>4</sub> O <sub>4</sub>
Nesosteine	Mucolytic	84233-61-4		C <sub>11</sub> H <sub>11</sub> NO <sub>3</sub> S
Nestifylline	Bronchodilator	116763-36-1		C <sub>11</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub> S <sub>2</sub>
Neticonazole	Antifungal	130726-68-0		C <sub>17</sub> H <sub>22</sub> N <sub>2</sub> OS
Netilmicin	Antibiotic	56391-56-1		C <sub>21</sub> H <sub>41</sub> N <sub>5</sub> O <sub>7</sub>
Netivudine	Antiviral	84558-93-0		C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> O <sub>6</sub>
Netobimin	Anthelminthic	88255-01-0		C <sub>14</sub> H <sub>20</sub> N <sub>4</sub> O <sub>7</sub> S <sub>2</sub>
Netoglitazone	Antidiabetic	161600-01-7		C <sub>21</sub> H <sub>16</sub> FNO <sub>3</sub> S
Netupitant	Antiemetic	290297-26-6		C <sub>30</sub> H <sub>32</sub> F <sub>6</sub> N <sub>4</sub> O
Neutramycin	Antibacterial	1404-08-6		C <sub>34</sub> H <sub>54</sub> O <sub>14</sub>
Nevirapine	Antiviral	129618-40-2	Y	C <sub>15</sub> H <sub>14</sub> N <sub>4</sub> O
Nexeridine	Analgesic	53716-48-6		C <sub>19</sub> H <sub>29</sub> NO <sub>2</sub>
Nexopamil	Antiarrhythmic	136033-49-3		C <sub>24</sub> H <sub>40</sub> N <sub>2</sub> O <sub>3</sub>
Niacin	Dermatologic	59-67-6	Y	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>
Niacinamide	Dermatologic	98-92-0		C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O
Nialamide	Antidepressant	51-12-7		C <sub>16</sub> H <sub>18</sub> N <sub>4</sub> O <sub>2</sub>
Niaprazine	Sedative	27367-90-4		C <sub>20</sub> H <sub>25</sub> FN <sub>4</sub> O
Nibroxane	Antibacterial	53983-00-9		C <sub>5</sub> H <sub>8</sub> BrNO <sub>4</sub>
Nicafenine	Analgesic	64039-88-9		C <sub>24</sub> H <sub>19</sub> ClN <sub>4</sub> O <sub>3</sub>
Nicainoprol	Antihypertensive	76252-06-7		C <sub>21</sub> H <sub>27</sub> N <sub>3</sub> O <sub>3</sub>
Nicametate	Vasodilator	3099-52-3		C <sub>12</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>
Nicanartine	Antihyperlipidemic	150443-71-3		C <sub>23</sub> H <sub>33</sub> NO <sub>2</sub>
Nicaraven	Cardiotonic	79455-30-4		C <sub>15</sub> H <sub>16</sub> N <sub>4</sub> O <sub>2</sub>
Nicarbazine	Antibacterial	587-90-6		C <sub>13</sub> H <sub>10</sub> N <sub>4</sub> O <sub>5</sub>
Nicarbazine	Antibacterial	108-79-2		C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O
Nicardipine	Antianginal	55985-32-5	Y	C <sub>26</sub> H <sub>29</sub> N <sub>3</sub> O <sub>6</sub>
Nicergoline	Vasodilator	27848-84-6	Y	C <sub>24</sub> H <sub>26</sub> BrN <sub>3</sub> O <sub>3</sub>
Niceritrol	Antihyperlipidemic	5868-05-3		C <sub>29</sub> H <sub>24</sub> N <sub>4</sub> O <sub>8</sub>
Niceverine	Antispasmodic	2545-24-6		C <sub>30</sub> H <sub>23</sub> N <sub>3</sub> O <sub>6</sub>
Niclofolan	Anthelminthic	10331-57-4		C <sub>12</sub> H <sub>6</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>6</sub>
Niclosamide	Anthelminthic	50-65-7		C <sub>13</sub> H <sub>8</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>4</sub>
Nicoboxil	Analgesic	13912-80-6		C <sub>12</sub> H <sub>17</sub> NO <sub>3</sub>
Nicoconlate	Nootropic	10571-59-2		C <sub>16</sub> H <sub>16</sub> ClNO <sub>2</sub>
Nicodine	Antitussive	3688-66-2		C <sub>24</sub> H <sub>24</sub> N <sub>2</sub> O <sub>4</sub>
Nicocortonide	Glucocorticoid	65415-41-0		C <sub>31</sub> H <sub>37</sub> NO <sub>7</sub>
Nicodicodine	Antitussive	808-24-2		C <sub>24</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub>
Nicofibrate	Antihyperlipidemic	31980-29-7		C <sub>16</sub> H <sub>16</sub> ClNO <sub>3</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Nicofuranose	Vasodilator	15351-13-0		C <sub>30</sub> H <sub>24</sub> N <sub>4</sub> O <sub>10</sub>
Nicofurate	Unclassified	4397-91-5		C <sub>35</sub> H <sub>28</sub> N <sub>4</sub> O <sub>11</sub>
Nicogrelate	Antithrombotic	80614-21-7		C <sub>17</sub> H <sub>21</sub> N <sub>3</sub> O <sub>2</sub>
Nicomol	Capillary Protectant	27959-26-8		C <sub>34</sub> H <sub>32</sub> N <sub>4</sub> O <sub>9</sub>
Nicomorphine	Analgesic	639-48-5		C <sub>29</sub> H <sub>25</sub> N <sub>3</sub> O <sub>5</sub>
Nicopholine	Analgesic	492-85-3		C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>
Nicoracetam	Nootropic	128326-80-7		C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>
Nicorandil	Vasodilator	65141-46-0	Y	C <sub>8</sub> H <sub>9</sub> N <sub>3</sub> O <sub>4</sub>
Nicothiazone	Unclassified	555-90-8		C <sub>7</sub> H <sub>8</sub> N <sub>4</sub> S
Nicotine	Nootropic	54-11-5	Y	C <sub>10</sub> H <sub>14</sub> N <sub>2</sub>
Nicotinyl Alcohol	Vasodilator	100-55-0		C <sub>6</sub> H <sub>7</sub> NO
Nicotredole	Unclassified	29876-14-0		C <sub>16</sub> H <sub>15</sub> N <sub>3</sub> O
Nicoxamat	Unclassified	5657-61-4		C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>
Nictiazem	Antihypertensive	95058-70-1		C <sub>26</sub> H <sub>27</sub> N <sub>3</sub> O <sub>4</sub> S
Nictindole	Antithrombotic	36504-64-0		C <sub>17</sub> H <sub>16</sub> N <sub>2</sub> O
Nifedipine	Antianginal	21829-25-4	Y	C <sub>17</sub> H <sub>18</sub> N <sub>2</sub> O <sub>6</sub>
Nifekalant	Cardiotonic	130636-43-0		C <sub>19</sub> H <sub>27</sub> N <sub>5</sub> O <sub>5</sub>
Nifenalol	Antiarrhythmic	7413-36-7		C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>
Nifenazone	Antiinflammatory	2139-47-1		C <sub>17</sub> H <sub>16</sub> N <sub>4</sub> O <sub>2</sub>
Niflumic Acid	Antiinflammatory	4394-00-7		C <sub>13</sub> H <sub>9</sub> F <sub>3</sub> N <sub>2</sub> O <sub>2</sub>
Nifluridide	Ectoparasiticide	61444-62-0		C <sub>10</sub> H <sub>6</sub> F <sub>7</sub> N <sub>3</sub> O <sub>3</sub>
Nifuradene	Antibiotic	555-84-0		C <sub>8</sub> H <sub>8</sub> N <sub>4</sub> O <sub>4</sub>
Nifuraldezone	Antibiotic	3270-71-1		C <sub>7</sub> H <sub>6</sub> N <sub>4</sub> O <sub>5</sub>
Nifuralide	Antibiotic	54657-96-4		C <sub>14</sub> H <sub>13</sub> N <sub>5</sub> O <sub>4</sub> S
Nifuratel	Antibiotic	4936-47-4		C <sub>10</sub> H <sub>11</sub> N <sub>3</sub> O <sub>5</sub> S
Nifuratrone	Antibiotic	19561-70-7		C <sub>7</sub> H <sub>8</sub> N <sub>2</sub> O <sub>5</sub>
Nifurdazil	Antibiotic	5036-03-3		C <sub>10</sub> H <sub>12</sub> N <sub>4</sub> O <sub>5</sub>
Nifurethazone	Antibiotic	5580-25-6		C <sub>10</sub> H <sub>15</sub> N <sub>5</sub> O <sub>4</sub>
Nifurfoline	Antibiotic	3363-58-4		C <sub>13</sub> H <sub>15</sub> N <sub>5</sub> O <sub>6</sub>
Nifurimide	Antibiotic	21638-36-8		C <sub>9</sub> H <sub>10</sub> N <sub>4</sub> O <sub>4</sub>
Nifurizone	Antibiotic	26350-39-0		C <sub>12</sub> H <sub>13</sub> N <sub>5</sub> O <sub>5</sub>
Nifurmazole	Antibiotic	18857-59-5		C <sub>11</sub> H <sub>10</sub> N <sub>4</sub> O <sub>6</sub>
Nifurmerone	Antibiotic	5579-95-3		C <sub>6</sub> H <sub>4</sub> CINO <sub>4</sub>
Nifuroquine	Antibiotic	57474-29-0		C <sub>14</sub> H <sub>8</sub> N <sub>2</sub> O <sub>6</sub>
Nifuroxazide	Antibiotic	965-52-6		C <sub>12</sub> H <sub>9</sub> N <sub>3</sub> O <sub>5</sub>
Nifuroxime	Antibacterial	6236-05-1		C <sub>5</sub> H <sub>4</sub> N <sub>2</sub> O <sub>4</sub>
Nifurpipone	Antibiotic	24632-47-1		C <sub>12</sub> H <sub>17</sub> N <sub>5</sub> O <sub>4</sub>
Nifurpirinol	Antibiotic	13411-16-0		C <sub>12</sub> H <sub>10</sub> N <sub>2</sub> O <sub>4</sub>
Nifurprazine	Antibiotic	1614-20-6		C <sub>10</sub> H <sub>8</sub> N <sub>4</sub> O <sub>3</sub>
Nifurquinazol	Antibiotic	5055-20-9		C <sub>16</sub> H <sub>16</sub> N <sub>4</sub> O <sub>5</sub>
Nifursemizone	Antiprotozoal	5579-89-5		C <sub>8</sub> H <sub>10</sub> N <sub>4</sub> O <sub>4</sub>
Nifursol	Antiprotozoal	16915-70-1		C <sub>12</sub> H <sub>7</sub> N <sub>5</sub> O <sub>9</sub>
Nifurthiazole	Antibiotic	3570-75-0		C <sub>8</sub> H <sub>6</sub> N <sub>4</sub> O <sub>4</sub> S
Nifurtimox	Antibiotic	23256-30-6	Y	C <sub>10</sub> H <sub>13</sub> N <sub>3</sub> O <sub>5</sub> S
Nifurtoinol	Antibiotic	1088-92-2		C <sub>9</sub> H <sub>8</sub> N <sub>4</sub> O <sub>6</sub>
Nifurvidine	Antibiotic	1900-13-6		C <sub>11</sub> H <sub>9</sub> N <sub>3</sub> O <sub>4</sub>
Nifurzide	Antibiotic	39978-42-2	Y	C <sub>12</sub> H <sub>8</sub> N <sub>4</sub> O <sub>6</sub> S
Niguldipine	Antihypertensive	113165-32-5		C <sub>36</sub> H <sub>39</sub> N <sub>3</sub> O <sub>6</sub>
Nihydrazone	Antibacterial	67-28-7		C <sub>7</sub> H <sub>7</sub> N <sub>3</sub> O <sub>4</sub>
Nikethamide	Nootropic	59-26-7		C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O
Nileprost	Prostaglandin	71097-83-1		C <sub>22</sub> H <sub>33</sub> NO <sub>5</sub>
Nilprazole	Antitumor	60662-19-3		C <sub>26</sub> H <sub>33</sub> N <sub>5</sub> O <sub>2</sub>
Niludipine	Antianginal	22609-73-0		C <sub>25</sub> H <sub>34</sub> N <sub>2</sub> O <sub>8</sub>
Nilutamide	Antineoplastic	63612-50-0	Y	C <sub>12</sub> H <sub>10</sub> F <sub>3</sub> N <sub>3</sub> O <sub>4</sub>
Nilvadipine	Antianginal	75530-68-6	Y	C <sub>19</sub> H <sub>19</sub> N <sub>3</sub> O <sub>6</sub>
Nimazone	Antiinflammatory	17230-89-6		C <sub>11</sub> H <sub>9</sub> CIN <sub>4</sub> O
Nimesulide	Antiinflammatory	51803-78-2	Y	C <sub>13</sub> H <sub>12</sub> N <sub>2</sub> O <sub>5</sub> S
Nimetazepam	Muscle Relaxant	2011-67-8		C <sub>16</sub> H <sub>13</sub> N <sub>3</sub> O <sub>3</sub>
Nimidane	Antiprotozoal	50435-25-1		C <sub>9</sub> H <sub>8</sub> CINS <sub>2</sub>
Nimodipine	Vasodilator	66085-59-4	Y	C <sub>21</sub> H <sub>26</sub> N <sub>2</sub> O <sub>7</sub>
Nimorazole	Antiprotozoal	6506-37-2		C <sub>9</sub> H <sub>14</sub> N <sub>4</sub> O <sub>3</sub>
Nimustine	Antineoplastic	42471-28-3		C <sub>9</sub> H <sub>13</sub> CIN <sub>6</sub> O <sub>2</sub>
Niometacin	Antiinflammatory	16426-83-8		C <sub>18</sub> H <sub>16</sub> N <sub>2</sub> O <sub>4</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Niperotidine	Antiulcerative	84845-75-0		C <sub>20</sub> H <sub>26</sub> N <sub>4</sub> O <sub>5</sub> S
Nipradilol	Antianginal	81486-22-8	Y	C <sub>15</sub> H <sub>22</sub> N <sub>2</sub> O <sub>6</sub>
Niprofazon	Antiinflammatory	15387-10-7		C <sub>21</sub> H <sub>25</sub> N <sub>5</sub> O <sub>2</sub>
Niravoline	Diuretic	130610-93-4		C <sub>22</sub> H <sub>25</sub> N <sub>3</sub> O <sub>3</sub>
Niridazole	Anthelminthic	61-57-4		C <sub>6</sub> H <sub>6</sub> N <sub>4</sub> O <sub>3</sub> S
Nisbuterol Mesylate	Bronchodilator	57540-78-0		C <sub>22</sub> H <sub>27</sub> NO <sub>6</sub>
Nisobamate	Sedative	25269-04-9		C <sub>13</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub>
Nisoldipine	Antihypertensive	63675-72-9	Y	C <sub>20</sub> H <sub>24</sub> N <sub>2</sub> O <sub>6</sub>
Nisoxetine	Antidepressant	53179-07-0		C <sub>17</sub> H <sub>21</sub> NO <sub>2</sub>
Nisterime Acetate	Androgen	51354-31-5		C <sub>27</sub> H <sub>35</sub> N <sub>2</sub> O <sub>5</sub>
Nitarson	Antiprotozoal	98-72-6		C <sub>6</sub> H <sub>6</sub> AsNO <sub>5</sub>
Nitazoxanide	Anthelminthic	55981-09-4	Y	C <sub>12</sub> H <sub>9</sub> N <sub>3</sub> O <sub>5</sub> S
Nitecapone	Capillary Protectant	116313-94-1		C <sub>12</sub> H <sub>11</sub> NO <sub>6</sub>
Nithiamide	Antiprotozoal	140-40-9		C <sub>5</sub> H <sub>5</sub> N <sub>3</sub> O <sub>3</sub> S
Nitisinone	Dermatologic	104206-65-7	Y	C <sub>14</sub> H <sub>10</sub> F <sub>3</sub> NO <sub>5</sub>
Nitracrine	Antidepressant	4533-39-5		C <sub>18</sub> H <sub>20</sub> N <sub>4</sub> O <sub>2</sub>
Nitrafudam	Antidepressant	64743-09-5		C <sub>11</sub> H <sub>9</sub> N <sub>3</sub> O <sub>3</sub>
Nitralamine	Antifungal	71872-90-7		C <sub>10</sub> H <sub>13</sub> ClN <sub>2</sub> O <sub>2</sub> S
Nitramisole	Anthelminthic	6646-49-7		C <sub>11</sub> H <sub>11</sub> N <sub>3</sub> O <sub>2</sub> S
Nitraquazone	Antiinflammatory	56739-21-0		C <sub>16</sub> H <sub>13</sub> N <sub>3</sub> O <sub>4</sub>
Nitrazepam	Anticonvulsant	146-22-5	Y	C <sub>15</sub> H <sub>11</sub> N <sub>3</sub> O <sub>3</sub>
Nitrefazole	Alcohol Deterrant	21721-92-6		C <sub>10</sub> H <sub>8</sub> N <sub>4</sub> O <sub>4</sub>
Nitrendipine	Antihypertensive	39562-70-4	Y	C <sub>18</sub> H <sub>20</sub> N <sub>2</sub> O <sub>6</sub>
Nitricholine Perchlorate	Cholinergic	7009-91-8		C <sub>5</sub> H <sub>13</sub> ClN <sub>2</sub> O <sub>7</sub>
Nitrocefin	Antibiotic	41906-86-9		C <sub>21</sub> H <sub>16</sub> N <sub>4</sub> O <sub>8</sub> S <sub>2</sub>
Nitroclofene	Anthelminthic	39224-48-1		C <sub>13</sub> H <sub>8</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>6</sub>
Nitrocycline	Antibacterial	5585-59-1		C <sub>21</sub> H <sub>21</sub> N <sub>3</sub> O <sub>9</sub>
Nitrodan	Anthelminthic	962-02-7		C <sub>10</sub> H <sub>8</sub> N <sub>4</sub> O <sub>5</sub> S <sub>2</sub>
Nitrofurantoin	Antibiotic	67-20-9	Y	C <sub>8</sub> H <sub>6</sub> N <sub>4</sub> O <sub>5</sub>
Nitroglycerin	Antianginal	55-63-0		C <sub>3</sub> H <sub>5</sub> N <sub>3</sub> O <sub>9</sub>
Nitromide	Antibacterial	121-81-3		C <sub>7</sub> H <sub>5</sub> N <sub>3</sub> O <sub>5</sub>
Nitromifene	Steroid	10448-84-7		C <sub>27</sub> H <sub>28</sub> N <sub>2</sub> O <sub>4</sub>
Nitroscanate	Anthelminthic	19881-18-6		C <sub>13</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub> S
Nitrovin	Antibacterial	804-36-4		C <sub>14</sub> H <sub>12</sub> N <sub>6</sub> O <sub>6</sub>
Nitroxinil	Anthelminthic	1689-89-0		C <sub>7</sub> H <sub>3</sub> IN <sub>2</sub> O <sub>3</sub>
Nitroxoline	Antibiotic	4008-48-4		C <sub>9</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub>
Nivazol	Glucocorticoid	24358-76-7		C <sub>28</sub> H <sub>31</sub> FN <sub>2</sub> O
Nixylic Acid	Unclassified	4394-05-2		C <sub>14</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Nizatidine	Antiulcerative	76963-41-2	Y	C <sub>12</sub> H <sub>21</sub> N <sub>5</sub> O <sub>2</sub> S <sub>2</sub>
Nizofenone	Nootropic	54533-85-6		C <sub>21</sub> H <sub>21</sub> ClN <sub>4</sub> O <sub>3</sub>
N Methylepinephrine	Antihypotensive	554-99-4		C <sub>10</sub> H <sub>15</sub> NO <sub>3</sub>
N Myristyl 3 Hydroxybutylamine	Unclassified	143-26-0		C <sub>18</sub> H <sub>39</sub> NO
Noberastine	Antihistaminic	110588-56-2		C <sub>17</sub> H <sub>21</sub> N <sub>5</sub> O
Nocloprost	Prostaglandin	79360-43-3		C <sub>22</sub> H <sub>37</sub> ClO <sub>4</sub>
Nocodazole	Antineoplastic	31430-18-9		C <sub>14</sub> H <sub>11</sub> N <sub>3</sub> O <sub>3</sub> S
Nofecainide	Antiarrhythmic	50516-43-3		C <sub>20</sub> H <sub>24</sub> N <sub>2</sub> O <sub>3</sub>
Nogalamycin	Antineoplastic	1404-15-5		C <sub>39</sub> H <sub>49</sub> NO <sub>16</sub>
Nolatrexed	Antineoplastic	147149-76-6		C <sub>14</sub> H <sub>12</sub> N <sub>4</sub> OS
Nolinium Bromide	Antiulcerative	40759-33-9		C <sub>15</sub> H <sub>11</sub> BrCl <sub>2</sub> N <sub>2</sub>
Nolomirole	Cardiotonic	90060-42-7		C <sub>19</sub> H <sub>27</sub> NO <sub>4</sub>
Nolpitantium Besilate	Bronchodilator	155418-06-7		C <sub>43</sub> H <sub>50</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>5</sub> S
Nomegestrol Acetate	Progestogen	58652-20-3		C <sub>23</sub> H <sub>30</sub> O <sub>4</sub>
Nomelidine	Anesthetic	60324-59-6		C <sub>15</sub> H <sub>15</sub> BrN <sub>2</sub>
Nomifensine	Antidepressant	24526-64-5		C <sub>16</sub> H <sub>18</sub> N <sub>2</sub>
Nonabine	Antiemetic	16985-03-8		C <sub>25</sub> H <sub>33</sub> NO <sub>2</sub>
Nonaperone	Antipsychotic	15997-76-9		C <sub>18</sub> H <sub>24</sub> FNO
Nonapyrimine	Unclassified	5626-36-8		C <sub>15</sub> H <sub>24</sub> N <sub>4</sub>
Nonathymulin	Thyroid	63958-90-7		C <sub>33</sub> H <sub>54</sub> N <sub>12</sub> O <sub>15</sub>
Nonivamide	Nootropic	2444-46-4		C <sub>17</sub> H <sub>27</sub> NO <sub>3</sub>
Noracymethadol	Analgesic	1477-39-0		C <sub>22</sub> H <sub>29</sub> NO <sub>2</sub>
Norbolethone	Steroid	1235-15-0		C <sub>21</sub> H <sub>32</sub> O <sub>2</sub>
Norbudrine	Antihypotensive	127560-12-7		C <sub>12</sub> H <sub>17</sub> NO <sub>3</sub>
Norclostebol	Steroid	13583-21-6		C <sub>18</sub> H <sub>25</sub> ClO <sub>2</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Norcodeine	Analgesic	467-15-2		C <sub>17</sub> H <sub>19</sub> NO <sub>3</sub>
Nordazepam	Anxiolytic	1088-11-5	Y	C <sub>15</sub> H <sub>11</sub> ClN <sub>2</sub> O
Nordefrin	Antihypotensive	74812-63-8		C <sub>9</sub> H <sub>13</sub> NO <sub>3</sub>
Nordihydroguaiaretic Acid	Antiinflammatory	500-38-9		C <sub>18</sub> H <sub>22</sub> O <sub>4</sub>
Norelgestromin	Contraceptive	53016-31-2		C <sub>21</sub> H <sub>29</sub> NO <sub>2</sub>
Norepinephrine	Antihypotensive	51-41-2		C <sub>8</sub> H <sub>11</sub> NO <sub>3</sub>
Norethandrolone	Androgen	52-78-8		C <sub>20</sub> H <sub>30</sub> O <sub>2</sub>
Norethindrone	Progestogen	68-22-4	Y	C <sub>20</sub> H <sub>26</sub> O <sub>2</sub>
Norethindrone Acetate	Progestogen	51-98-9		C <sub>22</sub> H <sub>28</sub> O <sub>3</sub>
Norethynodrel	Progestogen	68-23-5		C <sub>20</sub> H <sub>26</sub> O <sub>2</sub>
Noreximide	Sedative	6319-06-8		C <sub>9</sub> H <sub>9</sub> NO <sub>2</sub>
Norfefrine	Antihypotensive	536-21-0		C <sub>8</sub> H <sub>11</sub> NO <sub>2</sub>
Norfloxacin	Antibiotic	70458-96-7	Y	C <sub>16</sub> H <sub>18</sub> FN <sub>3</sub> O <sub>3</sub>
Norfloxacin Succinil	Antibiotic	100587-52-8		C <sub>20</sub> H <sub>22</sub> FN <sub>3</sub> O <sub>6</sub>
Norflurane	Anesthetic	811-97-2		C <sub>2</sub> H <sub>2</sub> F <sub>4</sub>
Norgesterone	Progestogen	13563-60-5		C <sub>20</sub> H <sub>28</sub> O <sub>2</sub>
Norgestimate	Progestogen	35189-28-7		C <sub>23</sub> H <sub>31</sub> NO <sub>3</sub>
Norgestomet	Progestogen	25092-41-5		C <sub>23</sub> H <sub>32</sub> O <sub>4</sub>
Norgestrel	Progestogen	6533-00-2		C <sub>21</sub> H <sub>28</sub> O <sub>2</sub>
Norgestrienone	Progestogen	848-21-5		C <sub>20</sub> H <sub>28</sub> O <sub>2</sub>
Norletimol	Unclassified	886-08-8		C <sub>14</sub> H <sub>13</sub> NO
Norlevorphanol	Analgesic	1531-12-0		C <sub>16</sub> H <sub>21</sub> NO
Normethadone	Antitussive	467-85-6		C <sub>20</sub> H <sub>25</sub> NO
Normethandrone	Androgen	514-61-4		C <sub>19</sub> H <sub>28</sub> O <sub>2</sub>
Normorphine	Analgesic	466-97-7		C <sub>16</sub> H <sub>17</sub> NO <sub>3</sub>
Norpiprane	Analgesic	561-48-8		C <sub>23</sub> H <sub>29</sub> NO
Nortetrazepam	Anxiolytic	10379-11-0		C <sub>15</sub> H <sub>15</sub> ClN <sub>2</sub> O
Nortopixantrone	Antineoplastic	156090-17-4		C <sub>20</sub> H <sub>24</sub> N <sub>6</sub> O <sub>2</sub>
Nortriptyline	Antidepressant	72-69-5	Y	C <sub>19</sub> H <sub>21</sub> N
Norvinisterone	Progestogen	6795-60-4		C <sub>20</sub> H <sub>28</sub> O <sub>2</sub>
Nosantine	Antineoplastic	76600-30-1		C <sub>14</sub> H <sub>22</sub> N <sub>4</sub> O <sub>2</sub>
Noscapine	Antitussive	128-62-1	Y	C <sub>22</sub> H <sub>23</sub> NO <sub>7</sub>
Novobiocin	Antibacterial	303-81-1		C <sub>31</sub> H <sub>36</sub> N <sub>2</sub> O <sub>11</sub>
Noxiptiline	Antidepressant	3362-45-6		C <sub>19</sub> H <sub>22</sub> N <sub>2</sub> O
Nuclomedone	Antihistamine	75963-52-9		C <sub>13</sub> H <sub>11</sub> ClN <sub>2</sub> O <sub>2</sub> S
Nuclotixene	Antidepressant	36471-39-3		C <sub>21</sub> H <sub>20</sub> ClNS
Nufenoxole	Gastroprokinetic	57726-65-5		C <sub>25</sub> H <sub>29</sub> N <sub>3</sub> O
Nupafant	Antithrombotic	139133-27-0		C <sub>23</sub> H <sub>32</sub> N <sub>4</sub> O <sub>3</sub> S
Nuvenzepine	Gastroprokinetic	96487-37-5		C <sub>19</sub> H <sub>20</sub> N <sub>4</sub> O <sub>2</sub>
Nylestriol	Estrogen	39791-20-3		C <sub>25</sub> H <sub>32</sub> O <sub>3</sub>
Nylidrin	Vasodilator	447-41-6		C <sub>19</sub> H <sub>25</sub> NO <sub>2</sub>
Oberadilol	Antianginal	114856-44-9	Y	C <sub>25</sub> H <sub>30</sub> ClN <sub>5</sub> O <sub>3</sub>
Obidoxime Chloride	Antidote	114-90-9		C <sub>14</sub> H <sub>16</sub> Cl <sub>2</sub> N <sub>4</sub> O <sub>3</sub>
Ocaperidone	Antipsychotic	129029-23-8		C <sub>24</sub> H <sub>25</sub> FN <sub>4</sub> O <sub>2</sub>
Ocfentanil	Analgesic	101343-69-5		C <sub>22</sub> H <sub>27</sub> FN <sub>2</sub> O <sub>2</sub>
Ociltide	Antidiabetic	78410-57-8		C <sub>31</sub> H <sub>40</sub> N <sub>6</sub> O <sub>7</sub> S
Ocinaplon	Anxiolytic	96604-21-6		C <sub>17</sub> H <sub>11</sub> N <sub>5</sub> O
Ocrylate	Dermatologic	6701-17-3		C <sub>12</sub> H <sub>19</sub> NO <sub>2</sub>
Octabenzone	Dermatologic	1843-05-6		C <sub>21</sub> H <sub>26</sub> O <sub>3</sub>
Octacaine	Anesthetic	13912-77-1		C <sub>14</sub> H <sub>22</sub> N <sub>2</sub> O
Octadecyltrimethylammonium	Unclassified	488-40-4		C <sub>27</sub> H <sub>46</sub> Cl <sub>5</sub> NO
Pentachlorophenate	Unclassified			
Octamoxin	Antidepressant	4684-87-1		C <sub>8</sub> H <sub>20</sub> N <sub>2</sub>
Octamylamine	Antispasmodic	502-59-0		C <sub>13</sub> H <sub>29</sub> N
Octanoic Acid	Antifungal	124-07-2		C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>
Octapinol	Antibacterial	71138-71-1		C <sub>15</sub> H <sub>31</sub> NO
Octastine	Antihistaminic	59767-12-3		C <sub>23</sub> H <sub>30</sub> ClNO
Octaverine	Antispasmodic	549-68-8		C <sub>23</sub> H <sub>27</sub> NO <sub>5</sub>
Octazamide	Analgesic	56391-55-0		C <sub>13</sub> H <sub>15</sub> NO <sub>2</sub>
Octimibate	Anticoagulant	89838-96-0		C <sub>29</sub> H <sub>30</sub> N <sub>2</sub> O <sub>3</sub>
Octinoxate	Dermatologic	5466-77-3		C <sub>18</sub> H <sub>26</sub> O <sub>3</sub>
Octisalate	Dermatologic	118-60-5		C <sub>15</sub> H <sub>22</sub> O <sub>3</sub>
Octocrylene	Dermatologic	6197-30-4		C <sub>24</sub> H <sub>27</sub> NO <sub>2</sub>



Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Octodrine	Decongestant	543-82-8		C <sub>8</sub> H <sub>19</sub> N
Octopamine	Antihypotensive	104-14-3		C <sub>8</sub> H <sub>11</sub> NO <sub>2</sub>
Octriptyline Phosphate	Antidepressant	47166-67-6		C <sub>20</sub> H <sub>21</sub> N
Octrizole	Dermatologic	3147-75-9		C <sub>20</sub> H <sub>25</sub> N <sub>3</sub> O
Odalprofen	Analgesic	137460-88-9		C <sub>20</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>
Odapipam	Sedative	131796-63-9		C <sub>19</sub> H <sub>20</sub> CINO <sub>2</sub>
Odiparil	Antithrombotic	137215-12-4		C <sub>15</sub> H <sub>16</sub> O <sub>6</sub> S
Ofloxacin	Antibiotic	82419-36-1	Y	C <sub>18</sub> H <sub>20</sub> FN <sub>3</sub> O <sub>4</sub>
Oformine	Antihypertensive	87784-12-1		C <sub>17</sub> H <sub>19</sub> N <sub>3</sub> O
Oftasceine	Antineoplastic	1461-15-0		C <sub>30</sub> H <sub>26</sub> N <sub>2</sub> O <sub>13</sub>
Oglufanide Disodium	Immunomodulator	38101-59-6		C <sub>16</sub> H <sub>19</sub> N <sub>3</sub> O <sub>5</sub>
Olafur	Antibacterial	17671-49-7		C <sub>27</sub> H <sub>58</sub> N <sub>2</sub> O <sub>3</sub>
Olamufloxacin	Antibiotic	167887-97-0		C <sub>20</sub> H <sub>23</sub> FN <sub>4</sub> O <sub>3</sub>
Olanexidine	Antibacterial	146510-36-3		C <sub>17</sub> H <sub>27</sub> Cl <sub>2</sub> N <sub>5</sub>
Olanzapine	Antipsychotic	132539-06-1	Y	C <sub>17</sub> H <sub>20</sub> N <sub>4</sub> S
Olaquinox	Antibacterial	23696-28-8		C <sub>12</sub> H <sub>13</sub> N <sub>3</sub> O <sub>4</sub>
Olcegepant	Antimigraine	204697-65-4		C <sub>38</sub> H <sub>47</sub> Br <sub>2</sub> N <sub>9</sub> O <sub>5</sub>
Oleandomycin Phosphate	Antibiotic	3922-90-5		C <sub>35</sub> H <sub>61</sub> NO <sub>12</sub>
Oletimol	Unclassified	5879-67-4		C <sub>15</sub> H <sub>15</sub> NO
Olmesartan	Antihypertensive	144689-24-7	Y	C <sub>24</sub> H <sub>26</sub> N <sub>6</sub> O <sub>3</sub>
Olmesartan Medoxomil	Antihypertensive	144689-63-4	Y	C <sub>29</sub> H <sub>30</sub> N <sub>6</sub> O <sub>6</sub>
Olmidine	Antihypertensive	31105-14-3		C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub>
Olopatadine	Antihistaminic	113806-05-6	Y	C <sub>21</sub> H <sub>23</sub> NO <sub>3</sub>
Olpadronic Acid	Bone Resorption Inhibitor	63132-39-8		C <sub>5</sub> H <sub>15</sub> NO <sub>7</sub> P <sub>2</sub>
Olpimedone	Antihistaminic	39567-20-9		C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> OS
Olprinone	Cardiotonic	106730-54-5		C <sub>14</sub> H <sub>10</sub> N <sub>4</sub> O
Olradipine	Antiparkinsonian	115972-78-6		C <sub>22</sub> H <sub>28</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>6</sub>
Olsalazine	Antiinflammatory	15722-48-2		C <sub>14</sub> H <sub>10</sub> N <sub>2</sub> O <sub>6</sub>
Oltipraz	Antiviral	64224-21-1		C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> S <sub>3</sub>
Olvanil	Analgesic	58493-49-5		C <sub>26</sub> H <sub>43</sub> NO <sub>3</sub>
Omaciclovir	Antiviral	124265-89-0		C <sub>10</sub> H <sub>15</sub> N <sub>5</sub> O <sub>3</sub>
Omapatrilat	Antihypertensive	167305-00-2		C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> O <sub>4</sub> S <sub>2</sub>
Omeprazole	Antilulcerative	73590-58-6	Y	C <sub>17</sub> H <sub>19</sub> N <sub>3</sub> O <sub>3</sub> S
Omidoline	Analgesic	21590-91-0		C <sub>22</sub> H <sub>27</sub> N <sub>3</sub> O <sub>2</sub>
Omigapil	Nootropic	181296-84-4		C <sub>19</sub> H <sub>17</sub> NO
Omiloxetine	Antidepressant	176894-09-0		C <sub>27</sub> H <sub>25</sub> F <sub>2</sub> NO <sub>4</sub>
Omoconazole Nitrate	Antifungal	74512-12-2		C <sub>20</sub> H <sub>17</sub> Cl <sub>3</sub> N <sub>2</sub> O <sub>2</sub>
Omonasteine	Mucolytic	60175-95-3		C <sub>5</sub> H <sub>9</sub> NO <sub>2</sub> S
Onapristone	Progestogen	96346-61-1		C <sub>29</sub> H <sub>39</sub> NO <sub>3</sub>
Ondansetron	Antiemetic	99614-02-5	Y	C <sub>18</sub> H <sub>19</sub> N <sub>3</sub> O
Ontazolast	Bronchodilator	147432-77-7		C <sub>21</sub> H <sub>25</sub> N <sub>3</sub> O
Ontianil	Unclassified	35727-72-1		C <sub>13</sub> H <sub>12</sub> CINO <sub>2</sub> S
Opanixil	Antihypertensive	152939-42-9		C <sub>19</sub> H <sub>21</sub> F <sub>3</sub> N <sub>6</sub> O <sub>2</sub>
Opaviraline	Antiviral	178040-94-3		C <sub>14</sub> H <sub>17</sub> FN <sub>2</sub> O <sub>3</sub>
Opiniazide	Antibacterial	2779-55-7		C <sub>16</sub> H <sub>15</sub> N <sub>3</sub> O <sub>5</sub>
Opipramol	Antidepressant	315-72-0	Y	C <sub>23</sub> H <sub>29</sub> N <sub>3</sub> O
Opratonium Iodide	Cholinergic	146919-78-0		C <sub>17</sub> H <sub>35</sub> N <sub>2</sub> O.I
Orazamide	Hepatic Protectant	360-97-4		C <sub>4</sub> H <sub>6</sub> N <sub>4</sub> O
Orazipone	Antiinflammatory	137109-78-5		C <sub>13</sub> H <sub>14</sub> O <sub>4</sub> S
Orbifloxacin	Antibiotic	113617-63-3		C <sub>19</sub> H <sub>20</sub> F <sub>3</sub> N <sub>3</sub> O <sub>3</sub>
Orbofiban Acetate	Antithrombotic	163250-90-6		C <sub>17</sub> H <sub>23</sub> N <sub>5</sub> O <sub>4</sub>
Orbutopril	Antihypertensive	108391-88-4		C <sub>20</sub> H <sub>34</sub> N <sub>2</sub> O <sub>5</sub>
Orconazole Nitrate	Antifungal	22833-02-9		C <sub>18</sub> H <sub>15</sub> Cl <sub>3</sub> N <sub>2</sub> O
Orestrate	Unclassified	13885-31-9		C <sub>27</sub> H <sub>36</sub> O <sub>3</sub>
Orlistat	Antiobesity	96829-58-2	Y	C <sub>29</sub> H <sub>53</sub> NO <sub>5</sub>
Ormeloxifene	Bone Resorption Inhibitor	31477-60-8		C <sub>30</sub> H <sub>35</sub> NO <sub>3</sub>
Ormetoprim	Antibacterial	6981-18-6		C <sub>14</sub> H <sub>18</sub> N <sub>4</sub> O <sub>2</sub>
Ornidazole	Antibacterial	16773-42-5		C <sub>7</sub> H <sub>10</sub> CIN <sub>3</sub> O <sub>3</sub>
Ornoprostil	Prostaglandin	70667-26-4		C <sub>23</sub> H <sub>38</sub> O <sub>6</sub>
Orotic Acid	Uricosuric	65-86-1		C <sub>5</sub> H <sub>4</sub> N <sub>2</sub> O <sub>4</sub>
Orotirelin	Thyroid	62305-86-6		C <sub>16</sub> H <sub>19</sub> N <sub>7</sub> O <sub>5</sub>
Orpanoxin	Antiinflammatory	60653-25-0		C <sub>13</sub> H <sub>11</sub> ClO <sub>4</sub>
Orphenadrine Citrate	Muscle Relaxant	83-98-7		C <sub>18</sub> H <sub>23</sub> NO

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Ortataxel	Antineoplastic	186348-23-2		C <sub>44</sub> H <sub>57</sub> NO <sub>17</sub>
Ortetamine	Antineoplastic	5580-32-5		C <sub>10</sub> H <sub>15</sub> N
Osalmid	Choleretic	526-18-1		C <sub>13</sub> H <sub>11</sub> NO <sub>3</sub>
Osanetant	Antihistaminic	160492-56-8		C <sub>35</sub> H <sub>41</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>2</sub>
Osaterone	Steroid	105149-04-0		C <sub>20</sub> H <sub>25</sub> ClO <sub>4</sub>
Osetamivir	Antiviral	196618-13-0	Y	C <sub>16</sub> H <sub>28</sub> N <sub>2</sub> O <sub>4</sub>
Osemozotan	Anxiolytic	137275-81-1		C <sub>19</sub> H <sub>21</sub> NO <sub>5</sub>
Osmadizone	Analgesic	27450-21-1		C <sub>23</sub> H <sub>22</sub> N <sub>2</sub> O <sub>4</sub> S
Ospemifene	Antineoplastic	128607-22-7	Y	C <sub>24</sub> H <sub>23</sub> ClO <sub>2</sub>
Ostreogrycin	Antibiotic	21411-53-0		C <sub>28</sub> H <sub>35</sub> N <sub>3</sub> O <sub>7</sub>
Osutidine	Antilucerative	140695-21-2		C <sub>19</sub> H <sub>28</sub> N <sub>4</sub> O <sub>5</sub> S <sub>2</sub>
Otamixaban	Anticoagulant	193153-04-7		C <sub>25</sub> H <sub>26</sub> N <sub>4</sub> O <sub>4</sub>
Otenzepad	Mydriatic	102394-31-0		C <sub>24</sub> H <sub>31</sub> N <sub>5</sub> O <sub>2</sub>
Oteracil	Antineoplastic	937-13-3		C <sub>4</sub> H <sub>3</sub> N <sub>3</sub> O <sub>4</sub>
Otilonium Bromide	Antispasmodic	26095-59-0	Y	C <sub>29</sub> H <sub>43</sub> BrN <sub>2</sub> O <sub>4</sub>
Ouabain	Cardiotonic	630-60-4		C <sub>29</sub> H <sub>44</sub> O <sub>12</sub>
Oxabolone Cipionate	Steroid	1254-35-9		C <sub>26</sub> H <sub>38</sub> O <sub>4</sub>
Oxabrexine	Antidepressant	65415-42-1		C <sub>18</sub> H <sub>25</sub> Br <sub>2</sub> NO <sub>3</sub>
Oxaceprol	Antiinflammatory	33996-33-7		C <sub>7</sub> H <sub>11</sub> NO <sub>4</sub>
Oxacillin	Antibiotic	66-79-5		C <sub>19</sub> H <sub>19</sub> N <sub>3</sub> O <sub>5</sub> S
Oxadimidine	Antineoplastic	16485-05-5		C <sub>18</sub> H <sub>21</sub> N <sub>3</sub> O
Oxaflozane	Antidepressant	26629-87-8		C <sub>14</sub> H <sub>18</sub> F <sub>3</sub> NO
Oxaflumazine	Antipsychotic	16498-21-8		C <sub>26</sub> H <sub>32</sub> F <sub>3</sub> N <sub>3</sub> O <sub>2</sub> S
Oxagrelate	Antithrombotic	56611-65-5		C <sub>14</sub> H <sub>16</sub> N <sub>2</sub> O <sub>4</sub>
Oxalic Acid	Hemostatic	144-62-7		C <sub>2</sub> H <sub>2</sub> O <sub>4</sub>
Oxalinast	Bronchodilator	70009-66-4		C <sub>14</sub> H <sub>13</sub> NO <sub>4</sub>
Oxamarin	Hemostatic	15301-80-1		C <sub>22</sub> H <sub>34</sub> N <sub>2</sub> O <sub>4</sub>
Oxametacin	Antiinflammatory	27035-30-9		C <sub>19</sub> H <sub>17</sub> ClN <sub>2</sub> O <sub>4</sub>
Oxamisole	Immunomodulator	99258-56-7		C <sub>15</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>
Oxamniquine	Anthelminthic	21738-42-1	Y	C <sub>14</sub> H <sub>21</sub> N <sub>3</sub> O <sub>3</sub>
Oxanamide	Anxiolytic	126-93-2		C <sub>8</sub> H <sub>15</sub> NO <sub>2</sub>
Oxandrolone	Androgen	53-39-4	Y	C <sub>19</sub> H <sub>30</sub> O <sub>3</sub>
Oxantel	Anthelminthic	36531-26-7	Y	C <sub>13</sub> H <sub>16</sub> N <sub>2</sub> O
Oxapadol	Analgesic	56969-22-3		C <sub>18</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>
Oxapium Iodide	Antispasmodic	6577-41-9		C <sub>22</sub> H <sub>34</sub> INO <sub>2</sub>
Oxapropanium Iodide	Cholinergic	541-66-2		C <sub>7</sub> H <sub>16</sub> INO <sub>2</sub>
Oxaprotiline	Antidepressant	56433-44-4		C <sub>20</sub> H <sub>23</sub> NO
Oxaprozin	Antiinflammatory	21256-18-8		C <sub>18</sub> H <sub>15</sub> NO <sub>3</sub>
Oxarbazole	Bronchodilator	35578-20-2		C <sub>21</sub> H <sub>19</sub> NO <sub>4</sub>
Oxatomide	Antihistaminic	60607-34-3	Y	C <sub>27</sub> H <sub>30</sub> N <sub>4</sub> O
Oxazafone	Sedative	70541-17-2		C <sub>19</sub> H <sub>21</sub> ClN <sub>2</sub> O <sub>3</sub>
Oxazepam	Anxiolytic	604-75-1	Y	C <sub>15</sub> H <sub>11</sub> ClN <sub>2</sub> O <sub>2</sub>
Oxazidione	Analgesic	27591-42-0		C <sub>20</sub> H <sub>19</sub> NO <sub>3</sub>
Oxazolam	Anxiolytic	24143-17-7		C <sub>18</sub> H <sub>17</sub> ClN <sub>2</sub> O <sub>2</sub>
Oxazorone	Unclassified	25392-50-1		C <sub>14</sub> H <sub>15</sub> NO <sub>4</sub>
Oxcarbazepine	Anticonvulsant	28721-07-5	Y	C <sub>15</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>
Oxdralazine	Diuretic	17259-75-5		C <sub>8</sub> H <sub>15</sub> N <sub>5</sub> O <sub>2</sub>
Oxedrine	Antihypotensive	94-07-5		C <sub>9</sub> H <sub>13</sub> NO <sub>2</sub>
Oxeglitazar	Antidiabetic	280585-34-4		C <sub>19</sub> H <sub>22</sub> O <sub>4</sub>
Oxeladin	Antitussive	468-61-1		C <sub>20</sub> H <sub>33</sub> NO <sub>3</sub>
Oxendolone	Steroid	33765-68-3		C <sub>20</sub> H <sub>30</sub> O <sub>2</sub>
Oxepinac	Antiinflammatory	55689-65-1		C <sub>16</sub> H <sub>12</sub> O <sub>4</sub>
Oxetacillin	Antibiotic	53861-02-2		C <sub>19</sub> H <sub>23</sub> N <sub>3</sub> O <sub>5</sub> S
Oxethazaine	Anesthetic	126-27-2		C <sub>28</sub> H <sub>41</sub> N <sub>3</sub> O <sub>3</sub>
Oxetorone	Analgesic	26020-55-3		C <sub>21</sub> H <sub>21</sub> NO <sub>2</sub>
Oxfendazole	Anthelminthic	53716-50-0		C <sub>15</sub> H <sub>13</sub> N <sub>3</sub> O <sub>3</sub> S
Oxfenicine	Vasodilator	32462-30-9		C <sub>8</sub> H <sub>9</sub> NO <sub>3</sub>
Oxibendazole	Anthelminthic	20559-55-1		C <sub>12</sub> H <sub>15</sub> N <sub>3</sub> O <sub>3</sub>
Oxibetaine	Antibacterial	7002-65-5		C <sub>6</sub> H <sub>13</sub> NO <sub>3</sub>
Oxiconazole	Antifungal	64211-45-6		C <sub>18</sub> H <sub>13</sub> Cl <sub>4</sub> N <sub>3</sub> O
Oxidopamine	Ophthalmic	1199-18-4		C <sub>8</sub> H <sub>11</sub> NO <sub>3</sub>
Oxidronic Acid	Bone Resorption Inhibitor	15468-10-7		CH <sub>6</sub> O <sub>7</sub> P <sub>2</sub>
Oxifentorex	Anorexic	4075-88-1		C <sub>17</sub> H <sub>21</sub> NO

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Oxifungin	Antifungal	64057-48-3		C <sub>13</sub> H <sub>12</sub> N <sub>4</sub> O
Oxiglutatione	Unclassified	27025-41-8		C <sub>20</sub> H <sub>32</sub> N <sub>6</sub> O <sub>12</sub> S <sub>2</sub>
Oxilofrine	Mydriatic	365-26-4		C <sub>10</sub> H <sub>15</sub> NO <sub>2</sub>
Oxilorphan	Antidote	42281-59-4		C <sub>20</sub> H <sub>27</sub> NO <sub>2</sub>
Oximonam	Antibacterial	90898-90-1		C <sub>12</sub> H <sub>15</sub> N <sub>5</sub> O <sub>6</sub> S
Oxindanac	Antiinflammatory	68548-99-2		C <sub>17</sub> H <sub>14</sub> O <sub>4</sub>
Oxiniac Acid	Antihyperlipidemic	2398-81-4		C <sub>6</sub> H <sub>5</sub> NO <sub>3</sub>
Oxiperomide	Antipsychotic	5322-53-2		C <sub>20</sub> H <sub>23</sub> N <sub>3</sub> O <sub>2</sub>
Oxiracetam	Nootropic	62613-82-5	Y	C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub>
Oxiramide	Antiarrhythmic	13958-40-2		C <sub>25</sub> H <sub>34</sub> N <sub>2</sub> O <sub>2</sub>
Oxisopred	Unclassified	18118-80-4		C <sub>21</sub> H <sub>28</sub> O <sub>6</sub>
Oxisuran	Antineoplastic	27302-90-5		C <sub>8</sub> H <sub>9</sub> NO <sub>2</sub> S
Oxitefonium Bromide	Antispasmodic	17692-63-6		C <sub>19</sub> H <sub>26</sub> BrNO <sub>3</sub> S
Oxitriptan	Anticonvulsant	4350-09-8		C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>
Oxitriptyline	Antidepressant	29541-85-3		C <sub>19</sub> H <sub>21</sub> NO <sub>2</sub>
Oxitropium Bromide	Bronchodilator	30286-75-0		C <sub>19</sub> H <sub>26</sub> BrNO <sub>4</sub>
Oxmetidine	Antiulcerative	72830-39-8		C <sub>19</sub> H <sub>21</sub> N <sub>5</sub> O <sub>3</sub> S
Oxodipine	Antianginal	90729-41-2		C <sub>19</sub> H <sub>21</sub> NO <sub>6</sub>
Oxogestone Phenpropionate	Progestogen	16915-80-3		C <sub>29</sub> H <sub>38</sub> O <sub>3</sub>
Oxolamine	Antiinflammatory	959-14-8		C <sub>14</sub> H <sub>19</sub> N <sub>3</sub> O
Oxolinic Acid	Antibiotic	14698-29-4		C <sub>13</sub> H <sub>11</sub> NO <sub>5</sub>
Oxomemazine	Antihistaminic	3689-50-7		C <sub>18</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub> S
Oxonazine	Antimigraine	5580-22-3		C <sub>9</sub> H <sub>14</sub> N <sub>6</sub> O
Oxophenarsine	Antiprotozoal	306-12-7		C <sub>6</sub> H <sub>6</sub> AsNO <sub>2</sub>
Oxoprostol	Antiulcerative	69648-40-4		C <sub>22</sub> H <sub>32</sub> O <sub>4</sub>
Oxpheneridine	Analgesic	546-32-7		C <sub>22</sub> H <sub>27</sub> NO <sub>3</sub>
Oxprenoate Potassium	Antihypertensive	786592-95-8		C <sub>25</sub> H <sub>38</sub> O <sub>4</sub>
Oxprenolol	Antihypertensive	6452-71-7	Y	C <sub>15</sub> H <sub>23</sub> NO <sub>3</sub>
Oxtriphylline	Bronchodilator	4499-40-5		C <sub>12</sub> H <sub>21</sub> N <sub>5</sub> O <sub>3</sub>
Oxybenzone	Dermatologic	131-57-7		C <sub>14</sub> H <sub>12</sub> O <sub>3</sub>
Oxybutynin	Urologic	5633-20-5	Y	C <sub>22</sub> H <sub>31</sub> NO <sub>3</sub>
Oxycinchophen	Uricosuric	485-89-2		C <sub>16</sub> H <sub>11</sub> NO <sub>3</sub>
Oxyclozanide	Anthelmintic	2277-92-1		C <sub>13</sub> H <sub>6</sub> Cl <sub>5</sub> NO <sub>3</sub>
Oxycodone	Analgesic	76-42-6	Y	C <sub>18</sub> H <sub>21</sub> NO <sub>4</sub>
Oxydipentonium Chloride	Muscle Relaxant	7174-23-4		C <sub>16</sub> H <sub>38</sub> N <sub>2</sub> OCl <sub>2</sub>
Oxyfedrine	Cardiotonic	15687-41-9		C <sub>19</sub> H <sub>23</sub> NO <sub>3</sub>
Oxymesterone	Steroid	145-12-0		C <sub>20</sub> H <sub>30</sub> O <sub>3</sub>
Oxymetazoline	Decongestant	1491-59-4		C <sub>16</sub> H <sub>24</sub> N <sub>2</sub> O
Oxymetholone	Androgen	434-07-1	Y	C <sub>21</sub> H <sub>32</sub> O <sub>3</sub>
Oxymorphone	Analgesic	76-41-5		C <sub>17</sub> H <sub>19</sub> NO <sub>4</sub>
Oxypendyl	Antiemetic	5585-93-3		C <sub>20</sub> H <sub>26</sub> N <sub>4</sub> OS
Oxypertine	Antidepressant	153-87-7		C <sub>23</sub> H <sub>29</sub> N <sub>3</sub> O <sub>2</sub>
Oxyphenbutazone	Antiinflammatory	129-20-4		C <sub>19</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub>
Oxyphenyclimine	Antispasmodic	125-53-1		C <sub>20</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub>
Oxyphenisatin	Laxative	125-13-3		C <sub>20</sub> H <sub>15</sub> NO <sub>3</sub>
Oxyphenonium	Antispasmodic	14214-84-7		C <sub>21</sub> H <sub>34</sub> NO <sub>3</sub>
Oxypurinol	Antiurolithic	2465-59-0		C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O <sub>2</sub>
Oxyridazine	Antipsychotic	14759-04-7		C <sub>21</sub> H <sub>26</sub> N <sub>2</sub> OS
Oxysonium Iodide	Antibacterial	3569-58-2		C <sub>18</sub> H <sub>27</sub> O <sub>3</sub> S.I
Oxytetracycline	Antibiotic	79-57-2	Y	C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>9</sub>
Ozagrel	Antianginal	82571-53-7	Y	C <sub>13</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>
Ozolinone	Diuretic	56784-39-5		C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub> S
Paclitaxel	Antineoplastic	33069-62-4	Y	C <sub>47</sub> H <sub>51</sub> NO <sub>14</sub>
Paclitaxel Ceribate	Antineoplastic	186040-50-6		C <sub>51</sub> H <sub>57</sub> NO <sub>18</sub>
Pacrinolol	Antihypertensive	65655-59-6		C <sub>23</sub> H <sub>28</sub> N <sub>2</sub> O <sub>4</sub>
Pactimibe	Antihyperlipidemic	189198-30-9		C <sub>25</sub> H <sub>40</sub> N <sub>2</sub> O <sub>3</sub>
Padimate A	Dermatologic	21245-01-2		C <sub>14</sub> H <sub>21</sub> NO <sub>2</sub>
Padimate O	Dermatologic	21245-02-3		C <sub>17</sub> H <sub>27</sub> NO <sub>2</sub>
Pafenolol	Antihypertensive	75949-61-0		C <sub>18</sub> H <sub>31</sub> N <sub>3</sub> O <sub>3</sub>
Pagoclone	Anxiolytic	133737-32-3	Y	C <sub>23</sub> H <sub>22</sub> ClN <sub>3</sub> O <sub>2</sub>
Palatrigine	Anticonvulsant	98410-36-7		C <sub>12</sub> H <sub>13</sub> Cl <sub>2</sub> N <sub>5</sub>
Palinavir	Antiviral	154612-39-2		C <sub>41</sub> H <sub>52</sub> N <sub>6</sub> O <sub>5</sub>
Paliperidone	Antipsychotic	144598-75-4	Y	C <sub>23</sub> H <sub>27</sub> FN <sub>4</sub> O <sub>3</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Paliperidone Palmitate	Antipsychotic	199739-10-1	Y	C <sub>39</sub> H <sub>57</sub> FN <sub>4</sub> O <sub>4</sub>
Palipiroden	Nootropic	188396-77-2		C <sub>26</sub> H <sub>24</sub> F <sub>3</sub> N
Palmidrol	Oxytocic	544-31-0		C <sub>18</sub> H <sub>37</sub> NO <sub>2</sub>
Palonidipine	Antianginal	96515-73-0		C <sub>29</sub> H <sub>34</sub> FN <sub>3</sub> O <sub>6</sub>
Palonosetron	Antiemetic	135729-61-2		C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> O
Palosuran	Antineoplastic	540769-28-6		C <sub>25</sub> H <sub>30</sub> N <sub>4</sub> O <sub>2</sub>
Pamabrom	Diuretic	10381-75-6		C <sub>7</sub> H <sub>7</sub> BrN <sub>4</sub> O <sub>2</sub>
Pamaqueside	Antihyperlipidemic	150332-35-7		C <sub>39</sub> H <sub>62</sub> O <sub>14</sub>
Pamaquine	Antimalarial	491-92-9		C <sub>19</sub> H <sub>29</sub> N <sub>3</sub> O
Pamatolol Sulfate	Antihypertensive	59110-35-9		C <sub>16</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub>
Pamicogrel	Antiinflammatory	101001-34-7		C <sub>25</sub> H <sub>24</sub> N <sub>2</sub> O <sub>4</sub> S
Pamidronic Acid	Bone Resorption Inhibitor	40391-99-9		C <sub>3</sub> H <sub>11</sub> NO <sub>7</sub> P <sub>2</sub>
Panadiplon	Anxiolytic	124423-84-3		C <sub>18</sub> H <sub>17</sub> N <sub>5</sub> O <sub>2</sub>
Panamesine	Antipsychotic	139225-22-2		C <sub>23</sub> H <sub>26</sub> N <sub>2</sub> O <sub>6</sub>
Pancopride	Antiemetic	121650-80-4		C <sub>18</sub> H <sub>24</sub> ClN <sub>3</sub> O <sub>2</sub>
Pancuronium	Neuromuscular Blocking Agent	15500-66-0		C <sub>35</sub> H <sub>60</sub> Br <sub>2</sub> N <sub>2</sub> O <sub>4</sub>
Panidazole	Antiprotozoal	13752-33-5		C <sub>11</sub> H <sub>12</sub> N <sub>4</sub> O <sub>2</sub>
Panipenem	Antibiotic	87726-17-8		C <sub>15</sub> H <sub>21</sub> N <sub>3</sub> O <sub>4</sub> S
Panomifene	Steroid	77599-17-8		C <sub>25</sub> H <sub>24</sub> F <sub>3</sub> NO <sub>2</sub>
Pantethine	Antihyperlipidemic	16816-67-4		C <sub>22</sub> H <sub>42</sub> N <sub>4</sub> O <sub>8</sub> S <sub>2</sub>
Pantoprazole	Ant ulcerative	102625-70-7	Y	C <sub>16</sub> H <sub>15</sub> F <sub>2</sub> N <sub>3</sub> O <sub>4</sub> S
Panuramine	Antidepressant	80349-58-2		C <sub>24</sub> H <sub>25</sub> N <sub>3</sub> O <sub>2</sub>
Papaverine	Vasodilator	58-74-2	Y	C <sub>20</sub> H <sub>21</sub> NO <sub>4</sub>
Papaveroline	Muscle Relaxant	574-77-6		C <sub>16</sub> H <sub>13</sub> NO <sub>4</sub>
Paraflutizide	Diuretic	1580-83-2		C <sub>14</sub> H <sub>13</sub> ClFN <sub>3</sub> O <sub>4</sub> S <sub>2</sub>
Paraldehyde	Sedative	123-63-7		C <sub>6</sub> H <sub>12</sub> O <sub>3</sub>
Paramethadione	Anticonvulsant	115-67-3		C <sub>7</sub> H <sub>11</sub> NO <sub>3</sub>
Paramethasone Acetate	Glucocorticoid	1597-82-6		C <sub>24</sub> H <sub>31</sub> FO <sub>6</sub>
Paranyline	Antiinflammatory	1729-61-9		C <sub>21</sub> H <sub>16</sub> N <sub>2</sub>
Parapenzolate Bromide	Mydriatic	5634-41-3		C <sub>21</sub> H <sub>26</sub> NO <sub>3</sub> Br
Parapropamol	Unclassified	1693-37-4		C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>
Pararosaniline Pamoate	Anthelminthic	479-73-2		C <sub>19</sub> H <sub>17</sub> N <sub>3</sub>
Paraxazone	Antidepressant	26513-79-1		C <sub>10</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub>
Parbendazole	Anthelminthic	14255-87-9		C <sub>13</sub> H <sub>17</sub> N <sub>3</sub> O <sub>2</sub>
Parcetasal	Unclassified	87549-36-8		C <sub>17</sub> H <sub>15</sub> NO <sub>5</sub>
Parconazole	Antifungal	68685-54-1		C <sub>17</sub> H <sub>16</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>3</sub>
Parecoxib	Antiinflammatory	198470-84-7		C <sub>19</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub> S
Pareptide Sulfate	Antiparkinsonian	61484-38-6		C <sub>14</sub> H <sub>26</sub> N <sub>4</sub> O <sub>3</sub>
Parethoxycaine	Analgesic	94-23-5		C <sub>15</sub> H <sub>23</sub> NO <sub>3</sub>
Pargeverine	Antispasmodic	13479-13-5		C <sub>21</sub> H <sub>23</sub> NO <sub>3</sub>
Pargolol	Antianginal	47082-97-3		C <sub>16</sub> H <sub>23</sub> NO <sub>3</sub>
Pargyline	Antihypertensive	555-57-7		C <sub>11</sub> H <sub>13</sub> N
Paricalcitol	Pituitary	131918-61-1		C <sub>27</sub> H <sub>44</sub> O <sub>3</sub>
Paridocaine	Analgesic	7162-37-0		C <sub>17</sub> H <sub>26</sub> N <sub>2</sub> O <sub>2</sub>
Parodilol	Antihypertensive	113854-64-1		C <sub>23</sub> H <sub>27</sub> N <sub>3</sub> O <sub>2</sub>
Paromomycin	Antibiotic	7542-37-2		C <sub>23</sub> H <sub>45</sub> N <sub>5</sub> O <sub>14</sub>
Paroxetine	Antidepressant	61869-08-7	Y	C <sub>19</sub> H <sub>20</sub> FNO <sub>3</sub>
Paroxypropione	Antispasmodic	70-70-2		C <sub>9</sub> H <sub>10</sub> O <sub>2</sub>
Parsalmide	Antifungal	30653-83-9		C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>
Parvaquone	Antiamoebic	4042-30-2		C <sub>16</sub> H <sub>16</sub> O <sub>3</sub>
Pasiniazid	Antibacterial	65-49-6		C <sub>7</sub> H <sub>7</sub> NO <sub>3</sub>
Patamostat	Antiviral	114568-26-2		C <sub>20</sub> H <sub>20</sub> N <sub>4</sub> O <sub>4</sub> S
Patupilone	Antineoplastic	152044-54-7		C <sub>27</sub> H <sub>41</sub> NO <sub>6</sub> S
Pavatrin	Muscle Relaxant	4425-78-9		C <sub>20</sub> H <sub>23</sub> NO <sub>2</sub>
Pavatrine	Muscle Relaxant	4425-78-9		C <sub>20</sub> H <sub>23</sub> NO <sub>2</sub>
Paxamate	Antihistaminic	5579-05-5		C <sub>14</sub> H <sub>13</sub> NO <sub>2</sub>
Pazelliptine	Antineoplastic	65222-35-7		C <sub>22</sub> H <sub>27</sub> N <sub>5</sub>
Pazinaclone	Anxiolytic	103255-66-9		C <sub>25</sub> H <sub>23</sub> ClN <sub>4</sub> O <sub>4</sub>
Pazopanib	Antineoplastic	444731-52-6	Y	C <sub>21</sub> H <sub>23</sub> N <sub>7</sub> O <sub>2</sub> S
Pazoxide	Antihypertensive	21132-59-2		C <sub>12</sub> H <sub>10</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub> S
Pazufloxacin	Antibiotic	127045-41-4		C <sub>16</sub> H <sub>15</sub> FN <sub>2</sub> O <sub>4</sub>
Pecilocin	Antibiotic	19504-77-9		C <sub>17</sub> H <sub>25</sub> NO <sub>3</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Pecocycline	Antibiotic	15301-82-3		C <sub>29</sub> H <sub>35</sub> N <sub>3</sub> O <sub>10</sub>
Pefloxacin	Antibacterial	70458-92-3	Y	C <sub>17</sub> H <sub>20</sub> FN <sub>3</sub> O <sub>3</sub>
Pegamotecan	Antineoplastic	203066-49-3		C <sub>52</sub> H <sub>48</sub> N <sub>6</sub> O <sub>14</sub>
Pelanserlin	Antihypertensive	2208-51-7		C <sub>21</sub> H <sub>24</sub> N <sub>4</sub> O <sub>2</sub>
Pelargonic Acid	Unclassified	112-05-0		C <sub>9</sub> H <sub>18</sub> O <sub>2</sub>
Peldesine	Antineoplastic	133432-71-0		C <sub>12</sub> H <sub>11</sub> N <sub>5</sub> O
Peliglitazar	Antidiabetic	331744-64-0		C <sub>30</sub> H <sub>30</sub> N <sub>2</sub> O <sub>7</sub>
Pelitinib	Antineoplastic	257933-82-7		C <sub>24</sub> H <sub>23</sub> ClFN <sub>5</sub> O <sub>2</sub>
Pelitrexol	Antineoplastic	446022-33-9		C <sub>20</sub> H <sub>25</sub> N <sub>5</sub> O <sub>6</sub> S
Pelretin	Dermatologic	91587-01-8		C <sub>23</sub> H <sub>28</sub> O <sub>2</sub>
Pelrinone	Cardiotonic	94386-65-9		C <sub>12</sub> H <sub>11</sub> N <sub>5</sub> O
Pelubiprofen	Analgesic	69956-77-0	Y	C <sub>16</sub> H <sub>18</sub> O <sub>3</sub>
Pemaglitazar	Antidiabetic	496050-39-6		C <sub>18</sub> H <sub>17</sub> F <sub>3</sub> O <sub>3</sub> S
Pemedolac	Analgesic	114716-16-4		C <sub>22</sub> H <sub>23</sub> NO <sub>3</sub>
Pemerid Nitrate	Antitussive	50432-78-5		C <sub>15</sub> H <sub>32</sub> N <sub>2</sub> O
Pemetrexed	Antineoplastic	137281-23-3		C <sub>20</sub> H <sub>21</sub> N <sub>5</sub> O <sub>6</sub>
Pemirolast	Antihistaminic	69372-19-6	Y	C <sub>10</sub> H <sub>8</sub> N <sub>6</sub> O
Pemoline	Nootropic	2152-34-3	Y	C <sub>9</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>
Pempidine	Antihypertensive	79-55-0		C <sub>10</sub> H <sub>21</sub> N
Penamocillin	Antibacterial	983-85-7		C <sub>19</sub> H <sub>22</sub> N <sub>2</sub> O <sub>6</sub> S
Penbutolol Sulfate	Antianginal	38363-40-5		C <sub>18</sub> H <sub>29</sub> NO <sub>2</sub>
Penciclovir	Antiviral	39809-25-1		C <sub>10</sub> H <sub>15</sub> N <sub>5</sub> O <sub>3</sub>
Penethamate Hydriodide	Mydriatic	3689-73-4		C <sub>22</sub> H <sub>31</sub> N <sub>3</sub> O <sub>4</sub> S
Penfluridol	Antipsychotic	26864-56-2		C <sub>28</sub> H <sub>27</sub> ClF <sub>5</sub> NO
Penflutizide	Diuretic	1766-91-2		C <sub>13</sub> H <sub>18</sub> F <sub>3</sub> N <sub>3</sub> O <sub>4</sub> S <sub>2</sub>
Pengitoxin	Cardiotonic	242-04-8		C <sub>51</sub> H <sub>74</sub> O <sub>19</sub>
Penicillamine	Antirheumatic	52-67-5	Y	C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub> S
Penicillin V	Antibiotic	87-08-1		C <sub>16</sub> H <sub>18</sub> N <sub>2</sub> O <sub>5</sub> S
Penicillin X	Antibiotic	525-91-7		C <sub>16</sub> H <sub>18</sub> N <sub>2</sub> O <sub>5</sub> S
Penimocycline	Antibiotic	16259-34-0		C <sub>39</sub> H <sub>43</sub> N <sub>5</sub> O <sub>12</sub> S
Penirolol	Antianginal	58503-83-6		C <sub>15</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>
Penoctonium Bromide	Antibacterial	17088-72-1		C <sub>26</sub> H <sub>50</sub> BrNO <sub>2</sub>
Penprostene	Prostaglandin	61557-12-8		C <sub>21</sub> H <sub>32</sub> O <sub>5</sub>
Pentabamate	Anxiolytic	5667-70-9		C <sub>8</sub> H <sub>16</sub> N <sub>2</sub> O <sub>4</sub>
Pentacynium Chloride	Unclassified	77-12-3		C <sub>27</sub> H <sub>39</sub> N <sub>3</sub> O <sub>2</sub> Cl
Pentaerythritol	Sedative	115-77-5		C <sub>5</sub> H <sub>12</sub> O <sub>4</sub>
Pentaerythritol Tetranitrate	Vasodilator	78-11-5		C <sub>5</sub> H <sub>8</sub> N <sub>4</sub> O <sub>12</sub>
Pentafluranol	Steroid	65634-39-1		C <sub>17</sub> H <sub>15</sub> F <sub>5</sub> O <sub>2</sub>
Pentagestrone	Progestogen	7001-56-1		C <sub>26</sub> H <sub>38</sub> O <sub>3</sub>
Pentalamide	Antifungal	5579-06-6		C <sub>12</sub> H <sub>17</sub> NO <sub>2</sub>
Pentamethonium Bromide	Antihypertensive	541-20-8		C <sub>11</sub> H <sub>28</sub> Br <sub>2</sub> N <sub>2</sub>
Pentamidine	Antiprotozoal	100-33-4		C <sub>19</sub> H <sub>24</sub> N <sub>4</sub> O <sub>2</sub>
Pentamorphone	Analgesic	68616-83-1		C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub>
Pentamoxane	Sedative	4730-07-8		C <sub>14</sub> H <sub>21</sub> NO <sub>2</sub>
Pentamustine	Antineoplastic	73105-03-0		C <sub>8</sub> H <sub>16</sub> ClN <sub>3</sub> O <sub>2</sub>
1-Pentanol	Dermatologic	71-41-0		C <sub>5</sub> H <sub>12</sub> O
Pentaphonate	Analgesic	24360-58-5		C <sub>36</sub> H <sub>40</sub> Cl <sub>5</sub> OP
Pentapiperide	Antispasmodic	7009-54-3		C <sub>18</sub> H <sub>27</sub> NO <sub>2</sub>
Pentapiperium Methylsulfate	Antispasmodic	7681-80-3		C <sub>20</sub> H <sub>33</sub> NO <sub>6</sub> S
Pentaquine Phosphate	Antimalarial	86-78-2		C <sub>18</sub> H <sub>27</sub> N <sub>3</sub> O
Pentazocine	Analgesic	359-83-1		C <sub>19</sub> H <sub>27</sub> NO
Penthienate	Mydriatic	22064-27-3		C <sub>18</sub> H <sub>30</sub> NO <sub>3</sub> S
Penthrichloral	Sedative	5684-90-2		C <sub>7</sub> H <sub>11</sub> Cl <sub>3</sub> O <sub>4</sub>
Pentiapine Maleate	Antipsychotic	81382-51-6		C <sub>15</sub> H <sub>17</sub> N <sub>5</sub> S
Pentifylline	Vasodilator	1028-33-7		C <sub>13</sub> H <sub>20</sub> N <sub>4</sub> O <sub>2</sub>
Pentigetide	Antihistaminic	62087-72-3		C <sub>22</sub> H <sub>36</sub> N <sub>8</sub> O <sub>11</sub>
Pentisomicin	Antibiotic	55870-64-9		C <sub>19</sub> H <sub>37</sub> N <sub>5</sub> O <sub>7</sub>
Pentisomide	Antiarrhythmic	78833-03-1		C <sub>19</sub> H <sub>33</sub> N <sub>3</sub> O
Pentizidone Sodium	Antibacterial	55694-83-2		C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>
Pentobarbital	Sedative	76-74-4		C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>
Pentolinium	Antihypertensive	144-44-5		C <sub>15</sub> H <sub>32</sub> N <sub>2</sub>
Pentomone	Androgen	67102-87-8		C <sub>24</sub> H <sub>26</sub> O <sub>5</sub>
Pentopril	Antihypertensive	82924-03-6		C <sub>18</sub> H <sub>23</sub> NO <sub>5</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Pentorex	Anorexic	434-43-5		C <sub>11</sub> H <sub>17</sub> N
Pentostatin	Antineoplastic	53910-25-1		C <sub>11</sub> H <sub>16</sub> N <sub>4</sub> O <sub>4</sub>
Pentoxifylline	Anticoagulant	6493-05-6		C <sub>13</sub> H <sub>18</sub> N <sub>4</sub> O <sub>3</sub>
Pentritinol	Vasodilator	1607-17-6		C <sub>5</sub> H <sub>9</sub> N <sub>3</sub> O <sub>10</sub>
Pentylentetrazol	Nootropic	54-95-5		C <sub>6</sub> H <sub>10</sub> N <sub>4</sub>
Pepstatin	Unclassified	26305-03-3		C <sub>34</sub> H <sub>63</sub> N <sub>5</sub> O <sub>9</sub>
Peradoxime	Analgesic	67254-81-3		C <sub>22</sub> H <sub>29</sub> N <sub>3</sub> O <sub>4</sub>
Perafensine	Antiparkinsonian	72444-62-3		C <sub>19</sub> H <sub>19</sub> N <sub>3</sub>
Peralopride	Antiemetic	57083-89-3		C <sub>20</sub> H <sub>22</sub> ClN <sub>3</sub> O <sub>4</sub>
Peramivir	Antiviral	330600-85-6		C <sub>15</sub> H <sub>28</sub> N <sub>4</sub> O <sub>4</sub>
Peraquinsin	Antihypertensive	35265-50-0		C <sub>23</sub> H <sub>28</sub> N <sub>4</sub> O <sub>4</sub>
Perastine	Antineoplastic	4960-10-5		C <sub>20</sub> H <sub>25</sub> NO
Peratizole	Antiuro lithic	29952-13-4		C <sub>17</sub> H <sub>26</sub> N <sub>4</sub> S <sub>2</sub>
Perazine	Antipsychotic	84-97-9		C <sub>20</sub> H <sub>25</sub> N <sub>3</sub> S
Perbufylline	Bronchodilator	110390-84-6		C <sub>23</sub> H <sub>28</sub> FN <sub>5</sub> O <sub>3</sub>
Perflisobutane	Anesthetic	354-92-7		C <sub>4</sub> F <sub>10</sub>
Perfluamine	Cardiotonic	338-83-0		C <sub>9</sub> F <sub>21</sub> N
Perflubrodec	Cardiotonic	307-43-7		C <sub>10</sub> BrF <sub>21</sub>
Perfomedil	Vasodilator	92268-40-1		C <sub>19</sub> H <sub>29</sub> NO <sub>4</sub>
Perfosamide	Antineoplastic	62435-42-1		C <sub>7</sub> H <sub>15</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>4</sub> P
Pergolide	Antiparkinsonian	66104-22-1	Y	C <sub>19</sub> H <sub>26</sub> N <sub>2</sub> S
Perhexiline	Vasodilator	6621-47-2	Y	C <sub>19</sub> H <sub>35</sub> N
Periciazine	Antipsychotic	2622-26-6		C <sub>21</sub> H <sub>23</sub> N <sub>3</sub> OS
Perifosine	Antineoplastic	157716-52-4		C <sub>25</sub> H <sub>52</sub> NO <sub>4</sub> P
Perimetazine	Antipsychotic	13093-88-4		C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> O <sub>2</sub> S
Perindopril	Antihypertensive	82834-16-0	Y	C <sub>19</sub> H <sub>32</sub> N <sub>2</sub> O <sub>5</sub>
Perindoprilat	Antihypertensive	95153-31-4		C <sub>17</sub> H <sub>28</sub> N <sub>2</sub> O <sub>5</sub>
Perisoxal	Antiinflammatory	2055-44-9		C <sub>16</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>
Perlapine	Sedative	1977-11-3		C <sub>19</sub> H <sub>21</sub> N <sub>3</sub>
Permethrin	Dermatologic	52645-53-1		C <sub>21</sub> H <sub>20</sub> Cl <sub>2</sub> O <sub>3</sub>
Perospirone	Antipsychotic	150915-41-6	Y	C <sub>23</sub> H <sub>30</sub> N <sub>4</sub> O <sub>2</sub> S
Perphenazine	Antipsychotic	58-39-9	Y	C <sub>21</sub> H <sub>26</sub> ClN <sub>3</sub> OS
Persilic Acid	Unclassified	4444-23-9		C <sub>6</sub> H <sub>6</sub> O <sub>8</sub> S <sub>2</sub>
Perzinfotel	Analgesic	144912-63-0		C <sub>9</sub> H <sub>13</sub> N <sub>2</sub> O <sub>5</sub> P
Petrichloral	Sedative	78-12-6		C <sub>13</sub> H <sub>16</sub> Cl <sub>12</sub> O <sub>8</sub>
Pexantel	Anthelmintic	10001-13-5		C <sub>12</sub> H <sub>22</sub> N <sub>2</sub> O
Phanquone	Antiamoebic	84-12-8		C <sub>12</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>
Phenacaine	Analgesic	101-93-9		C <sub>18</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>
Phenacemide	Anticonvulsant	63-98-9		C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>
Phenacetin	Analgesic	62-44-2		C <sub>10</sub> H <sub>13</sub> NO <sub>2</sub>
Phenacridane Chloride	Antibiotic	3131-8-6		C <sub>26</sub> H <sub>28</sub> NOCl
Phenactropinium Chloride	Antihypertensive	3784-89-2		C <sub>24</sub> H <sub>28</sub> ClNO <sub>4</sub>
Phenadoxone	Analgesic	467-84-5		C <sub>23</sub> H <sub>29</sub> NO <sub>2</sub>
Phenaglycodol	Sedative	79-93-6		C <sub>11</sub> H <sub>15</sub> ClO <sub>2</sub>
Phenamazoline	Antibiotic	501-62-2		C <sub>10</sub> H <sub>13</sub> N <sub>3</sub>
Phenampramide	Analgesic	129-83-9		C <sub>17</sub> H <sub>26</sub> N <sub>2</sub> O
Phenanthrene	Antineoplastic	85-01-8		C <sub>14</sub> H <sub>10</sub>
Phenaphthazine	Analgesic	1716-22-9		C <sub>16</sub> H <sub>10</sub> N <sub>4</sub> O <sub>11</sub> S <sub>2</sub>
Phenarsones Sulfoxylate	Antibiotic	497-97-2		C <sub>7</sub> H <sub>10</sub> AsNO <sub>6</sub> S
Phenazocine Hydrobromide	Analgesic	127-35-5		C <sub>22</sub> H <sub>27</sub> NO
Phenazopyridine	Analgesic	94-78-0	Y	C <sub>11</sub> H <sub>11</sub> N <sub>5</sub>
Phenbutazone Sodium Glycerate	Antiinflammatory	798-21-0		C <sub>19</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>
Phencarbamide	Antispasmodic	3735-90-8		C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> O <sub>5</sub> S
Phencyclidine	Anesthetic	77-10-1		C <sub>17</sub> H <sub>25</sub> N
Phendimetrazine	Anorexic	634-03-7	Y	C <sub>12</sub> H <sub>17</sub> NO
Phenelzine	Antidepressant	51-71-8	Y	C <sub>8</sub> H <sub>12</sub> N <sub>2</sub>
Phenethicillin Potassium	Antibiotic	147-55-7	Y	C <sub>17</sub> H <sub>20</sub> N <sub>2</sub> O <sub>5</sub> S
Pheneturide	Anticonvulsant	90-49-3		C <sub>11</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Phenformin	Antidiabetic	114-86-3		C <sub>10</sub> H <sub>15</sub> N <sub>5</sub>
Phenglutarimide	Antiparkinsonian	1156-05-4		C <sub>17</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub>
Phenicarbazide	Antiinflammatory	103-03-7		C <sub>7</sub> H <sub>9</sub> N <sub>3</sub> O
Phenindamine	Antihistaminic	82-88-2		C <sub>19</sub> H <sub>19</sub> N
Phenindione	Anticoagulant	83-12-5		C <sub>15</sub> H <sub>10</sub> O <sub>2</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Pheniprazine	Antihypertensive	55-52-7		C <sub>9</sub> H <sub>14</sub> N <sub>2</sub>
Pheniramine	Antihistaminic	86-21-5		C <sub>16</sub> H <sub>20</sub> N <sub>2</sub>
Phenisonone Hydrobromide	Respiratory Stimulant	715646-49-4		C <sub>12</sub> H <sub>17</sub> NO <sub>3</sub>
Phenmetrazine	Anorexic	134-49-6		C <sub>11</sub> H <sub>15</sub> NO
Phenobarbital	Anticonvulsant	50-06-6	Y	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>
Phenol Camphorated	Dermatologic	108-95-2		C <sub>6</sub> H <sub>6</sub> O
Phenolphthalein	Laxative	77-09-8		C <sub>20</sub> H <sub>14</sub> O <sub>4</sub>
Phenomorphane	Analgesic	468-07-5		C <sub>24</sub> H <sub>29</sub> NO
Phenoperidine	Analgesic	562-26-5		C <sub>23</sub> H <sub>29</sub> NO <sub>3</sub>
Phenothiazine	Anthelminthic	92-84-2		C <sub>12</sub> H <sub>9</sub> NS
Phenothrin	Dermatologic	26002-80-2		C <sub>23</sub> H <sub>26</sub> O <sub>3</sub>
Phenoxyacetic Acid	Dermatologic	122-59-8		C <sub>8</sub> H <sub>8</sub> O <sub>3</sub>
Phenoxybenzamine	Antihypertensive	59-96-1	Y	C <sub>18</sub> H <sub>22</sub> ClNO
Phenoxypropazine	Antidepressant	3818-37-9		C <sub>9</sub> H <sub>14</sub> N <sub>2</sub> O
Phenprobamate	Muscle Relaxant	673-31-4		C <sub>10</sub> H <sub>13</sub> NO <sub>2</sub>
Phenprocoumon	Anticoagulant	435-97-2	Y	C <sub>18</sub> H <sub>16</sub> O <sub>3</sub>
Phenpromethamine	Adrenergic	93-88-9		C <sub>10</sub> H <sub>15</sub> N
Phensuximide	Anticonvulsant	86-34-0		C <sub>11</sub> H <sub>11</sub> NO <sub>2</sub>
Phentermine	Anorexic	122-09-8	Y	C <sub>10</sub> H <sub>15</sub> N
Phentolamine	Antihypertensive	50-60-2		C <sub>17</sub> H <sub>19</sub> N <sub>3</sub> O
Phenyl Aminosalicilate	Antibacterial	133-11-9		C <sub>13</sub> H <sub>11</sub> NO <sub>3</sub>
Phenyl Salicylate	Analgesic	118-55-8		C <sub>13</sub> H <sub>10</sub> O <sub>3</sub>
Phenylbutazone	Antiinflammatory	50-33-9		C <sub>19</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>
Phenylephrine	Mydriatic	59-42-7		C <sub>9</sub> H <sub>13</sub> NO <sub>2</sub>
Phenylpropanolamine	Decongestant	14838-15-4		C <sub>9</sub> H <sub>13</sub> NO
Phenylthilone	Laxative	115-55-9		C <sub>12</sub> H <sub>13</sub> NO <sub>2</sub> S
Phenylthioacetic Acid	Antispasmodic	949-01-9		C <sub>12</sub> H <sub>15</sub> NOS
Phenyltoloxamine	Antihistaminic	92-12-6		C <sub>17</sub> H <sub>21</sub> NO
Phenyrracillin	Antibiotic	7463-81-2		C <sub>16</sub> H <sub>18</sub> N <sub>2</sub>
Phenylramidol	Analgesic	553-69-5		C <sub>13</sub> H <sub>14</sub> N <sub>2</sub> O
Phenytoin	Anticonvulsant	57-41-0	Y	C <sub>15</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>
Phetharbital	Sedative	357-67-5		C <sub>14</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>
Phethenylate Sodium	Anticonvulsant	7772-37-4		C <sub>13</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> S
Pholcodine	Antitussive	509-67-1		C <sub>23</sub> H <sub>30</sub> N <sub>2</sub> O <sub>4</sub>
Pholedrine	Antihypotensive	370-14-9		C <sub>10</sub> H <sub>15</sub> NO
Phthalofyne	Anthelminthic	131-67-9		C <sub>14</sub> H <sub>14</sub> O <sub>4</sub>
Phthalylsulfacetamide	Antibiotic	131-69-1		C <sub>16</sub> H <sub>14</sub> N <sub>2</sub> O <sub>6</sub> S
Phthalylsulfamethizole	Antibiotic	485-24-5		C <sub>17</sub> H <sub>14</sub> N <sub>4</sub> O <sub>5</sub> S <sub>2</sub>
Phthalylsulfathiazole	Antibiotic	85-73-4		C <sub>17</sub> H <sub>13</sub> N <sub>3</sub> O <sub>5</sub> S <sub>2</sub>
Physostigmine	Cholinergic	57-47-6		C <sub>15</sub> H <sub>21</sub> N <sub>3</sub> O <sub>2</sub>
Piberaline	Antidepressant	39640-15-8		C <sub>17</sub> H <sub>19</sub> N <sub>3</sub> O
Piboserod	Gastroprokinetic	152811-62-6		C <sub>22</sub> H <sub>31</sub> N <sub>3</sub> O <sub>2</sub>
Pibrozelesin	Antineoplastic	154889-68-6		C <sub>32</sub> H <sub>40</sub> BrN <sub>5</sub> O <sub>8</sub>
Pibutidine	Antitulcerative	103922-33-4		C <sub>19</sub> H <sub>24</sub> N <sub>4</sub> O <sub>3</sub>
Picafibrate	Antihyperlipidemic	57548-79-5		C <sub>18</sub> H <sub>19</sub> ClN <sub>2</sub> O <sub>4</sub>
Picartamide	Antimigraine	76732-75-7		C <sub>11</sub> H <sub>14</sub> N <sub>2</sub> S <sub>2</sub>
Picenadol	Analgesic	79201-85-7		C <sub>16</sub> H <sub>25</sub> NO
Picilorex	Anorexic	62510-56-9		C <sub>14</sub> H <sub>18</sub> ClN
Piclamilast	Antiinflammatory	144035-83-6		C <sub>18</sub> H <sub>18</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>3</sub>
Piclonidine	Antihypertensive	72467-44-8		C <sub>14</sub> H <sub>17</sub> Cl <sub>2</sub> N <sub>3</sub> O
Piclopastine	Antineoplastic	55837-13-3		C <sub>20</sub> H <sub>26</sub> ClN <sub>3</sub> O <sub>2</sub>
Picloxydine	Antibacterial	5636-92-0		C <sub>20</sub> H <sub>24</sub> Cl <sub>2</sub> N <sub>10</sub>
Piclozotan	Nootropic	182415-09-4		C <sub>23</sub> H <sub>24</sub> ClN <sub>3</sub> O <sub>2</sub>
Picobenzide	Antipsychotic	51832-87-2		C <sub>15</sub> H <sub>16</sub> N <sub>2</sub> O
Picodralazine	Diuretic	17692-43-2		C <sub>14</sub> H <sub>13</sub> N <sub>5</sub>
Picolamine	Dermatologic	3731-52-0		C <sub>6</sub> H <sub>8</sub> N <sub>2</sub>
Piconol	Decongestant	586-98-1		C <sub>6</sub> H <sub>7</sub> NO
Picoperine	Antitussive	21755-66-8		C <sub>19</sub> H <sub>25</sub> N <sub>3</sub>
Picoprazole	Antitulcerative	78090-11-6		C <sub>17</sub> H <sub>17</sub> N <sub>3</sub> O <sub>3</sub> S
Picotamide	Antithrombotic	32828-81-2		C <sub>21</sub> H <sub>20</sub> N <sub>4</sub> O <sub>3</sub>
Picotrin Diolamine	Hepatic Protectant	64063-57-6		C <sub>25</sub> H <sub>19</sub> NO <sub>2</sub>
Picric Acid	Dermatologic	88-89-1		C <sub>6</sub> H <sub>3</sub> N <sub>3</sub> O <sub>7</sub>
Picrotoxin	Nootropic	21416-53-5		C <sub>15</sub> H <sub>18</sub> O <sub>7</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Picrotoxin	Nootropic	17617-45-7		C <sub>15</sub> H <sub>16</sub> O <sub>6</sub>
Picumast	Antihistaminic	39577-19-0		C <sub>25</sub> H <sub>29</sub> ClN <sub>2</sub> O <sub>3</sub>
Picumeterol Fumarate	Bronchodilator	130641-36-0		C <sub>21</sub> H <sub>29</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>2</sub>
Pidobenzone	Dermatologic	138506-45-3		C <sub>11</sub> H <sub>11</sub> NO <sub>4</sub>
Pidolacetamol	Analgesic	114485-92-6		C <sub>13</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub>
Pidolic Acid	Unclassified	98-79-3		C <sub>5</sub> H <sub>7</sub> NO <sub>3</sub>
Pidotimod	Immunomodulator	121808-62-6		C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub> S
Pifarnine	Antitulcerative	56208-01-6		C <sub>27</sub> H <sub>40</sub> N <sub>2</sub> O <sub>2</sub>
Pifenate	Uricosuric	15686-87-0		C <sub>22</sub> H <sub>27</sub> NO <sub>2</sub>
Pifexole	Antiparkinsonian	27199-40-2		C <sub>13</sub> H <sub>8</sub> ClN <sub>3</sub> O
Piflutixol	Antipsychotic	54341-02-5		C <sub>24</sub> H <sub>25</sub> F <sub>4</sub> NOS
Pifoxime	Analgesic	31224-92-7		C <sub>15</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub>
Piketopufen	Antiinflammatory	60576-13-8		C <sub>22</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>
Pildralazine	Vasodilator	64000-73-3		C <sub>8</sub> H <sub>15</sub> N <sub>5</sub> O
Pilocarpine	Antiglaucoma	92-13-7	Y	C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>
Pilsicainide	Antiarrhythmic	88069-67-4	Y	C <sub>17</sub> H <sub>24</sub> N <sub>2</sub> O
Pimagedine	Antidiabetic	79-17-4		CH <sub>6</sub> N <sub>4</sub>
Pimeclone	Respiratory Stimulant	534-84-9		C <sub>12</sub> H <sub>21</sub> NO
Pimecrolimus	Immunosuppressant	137071-32-0		C <sub>43</sub> H <sub>68</sub> ClNO <sub>11</sub>
Pimefylline	Vasodilator	10001-43-1		C <sub>15</sub> H <sub>18</sub> N <sub>6</sub> O <sub>2</sub>
Pimelautide	Immunomodulator	78512-63-7		C <sub>29</sub> H <sub>52</sub> N <sub>6</sub> O <sub>9</sub>
Pimetacin	Analgesic	79992-71-5		C <sub>25</sub> H <sub>21</sub> ClN <sub>2</sub> O <sub>3</sub> S
Pimethixene	Antipsychotic	314-03-4		C <sub>19</sub> H <sub>19</sub> NS
Pimetine	Antihyperlipidemic	3565-03-5		C <sub>16</sub> H <sub>26</sub> N <sub>2</sub>
Pimetremide	Anticonvulsant	578-89-2		C <sub>16</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>
Pimilprost	Prostaglandin	139403-31-9		C <sub>23</sub> H <sub>40</sub> O <sub>5</sub>
Piminodine Esylate	Analgesic	13495-09-5		C <sub>23</sub> H <sub>30</sub> N <sub>2</sub> O <sub>2</sub>
Pimobendan	Cardiotonic	74150-27-9	Y	C <sub>19</sub> H <sub>18</sub> N <sub>4</sub> O <sub>2</sub>
Pimonidazole	Antiprotozoal	70132-50-2		C <sub>11</sub> H <sub>18</sub> N <sub>4</sub> O <sub>3</sub>
Pimozide	Antipsychotic	2062-78-4	Y	C <sub>28</sub> H <sub>29</sub> F <sub>2</sub> N <sub>3</sub> O
Pinacidil	Antihypertensive	60560-33-0		C <sub>13</sub> H <sub>19</sub> N <sub>5</sub>
Pinadoline	Analgesic	38955-22-5		C <sub>19</sub> H <sub>19</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>3</sub>
Pinafide	Antineoplastic	54824-20-3		C <sub>18</sub> H <sub>17</sub> N <sub>3</sub> O <sub>4</sub>
Pinaverium Bromide	Antispasmodic	53251-94-8	Y	C <sub>26</sub> H <sub>41</sub> B <sub>2</sub> N <sub>4</sub> O <sub>4</sub>
Pinazepam	Anxiolytic	52463-83-9		C <sub>18</sub> H <sub>13</sub> ClN <sub>2</sub> O
Pinainide	Antiarrhythmic	83471-41-4		C <sub>16</sub> H <sub>24</sub> N <sub>2</sub> O
Pindolol	Antihypertensive	13523-86-9	Y	C <sub>14</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>
Pinokalant	Antiarrhythmic	149759-26-2		C <sub>41</sub> H <sub>48</sub> N <sub>2</sub> O <sub>9</sub>
Pinolcaine	Anesthetic	28240-18-8		C <sub>23</sub> H <sub>29</sub> NO <sub>2</sub>
Pinoxepin	Antipsychotic	14008-66-3		C <sub>23</sub> H <sub>27</sub> ClN <sub>2</sub> O <sub>2</sub>
Pioglitazone	Antidiabetic	111025-46-8	Y	C <sub>19</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> S
Pipacycline	Antibiotic	1110-80-1		C <sub>29</sub> H <sub>38</sub> N <sub>4</sub> O <sub>9</sub>
Pipamazine	Antiemetic	84-04-8		C <sub>21</sub> H <sub>24</sub> ClN <sub>3</sub> OS
Pipamperone	Antipsychotic	1893-33-0		C <sub>21</sub> H <sub>30</sub> FN <sub>3</sub> O <sub>2</sub>
Pipazethate	Antitussive	2167-85-3		C <sub>21</sub> H <sub>25</sub> N <sub>3</sub> O <sub>3</sub> S
Pipebuzone	Antiinflammatory	27315-91-9		C <sub>25</sub> H <sub>32</sub> N <sub>4</sub> O <sub>2</sub>
Pipecuronium Bromide	Muscle Relaxant	52212-02-9		C <sub>35</sub> H <sub>62</sub> Br <sub>2</sub> N <sub>4</sub> O <sub>4</sub>
Pipemidic Acid	Antibiotic	51940-44-4		C <sub>14</sub> H <sub>17</sub> N <sub>5</sub> O <sub>3</sub>
Pipendoxifene	Progestogen	198480-55-6		C <sub>29</sub> H <sub>32</sub> N <sub>2</sub> O <sub>3</sub>
Pipenzolate Bromide	Antispasmodic	125-51-9		C <sub>22</sub> H <sub>28</sub> BrNO <sub>3</sub>
Pipequaline	Anxiolytic	77472-98-1		C <sub>22</sub> H <sub>24</sub> N <sub>2</sub>
Piperacetazine	Antipsychotic	3819-00-9		C <sub>24</sub> H <sub>30</sub> N <sub>2</sub> O <sub>2</sub> S
Piperacillin	Antibiotic	61477-96-1		C <sub>23</sub> H <sub>27</sub> N <sub>5</sub> O <sub>7</sub> S
Piperamide Maleate	Anthelminthic	299-48-9		C <sub>17</sub> H <sub>28</sub> N <sub>4</sub> O
Piperazine	Anthelminthic	110-85-0		C <sub>4</sub> H <sub>10</sub> N <sub>2</sub>
Piperidine Phosphate	Unclassified	110-89-4		C <sub>5</sub> H <sub>11</sub> N
Piperidione	Antitussive	77-03-2		C <sub>9</sub> H <sub>15</sub> NO <sub>2</sub>
Piperidolate	Antispasmodic	82-98-4		C <sub>21</sub> H <sub>25</sub> NO <sub>2</sub>
Piperilate	Antispasmodic	4546-39-8		C <sub>21</sub> H <sub>25</sub> NO <sub>3</sub>
Piperine	Antibacterial	94-62-2		C <sub>17</sub> H <sub>19</sub> NO <sub>3</sub>
Piperocaine	Anesthetic	136-82-3		C <sub>16</sub> H <sub>23</sub> NO <sub>2</sub>
Piperonyl Butoxide	Anthelminthic	51-03-6		C <sub>19</sub> H <sub>30</sub> O <sub>5</sub>
Piperoxan	Antihypertensive	59-39-2		C <sub>14</sub> H <sub>19</sub> NO <sub>2</sub>



Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Piperphenidol	Antiemetic	90-23-3		C <sub>18</sub> H <sub>29</sub> NO
Piperylone	Analgesic	2531-04-6		C <sub>17</sub> H <sub>23</sub> N <sub>3</sub> O
Pipobroman	Antineoplastic	54-91-1		C <sub>10</sub> H <sub>16</sub> Br <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Pipoctanone	Bone Resorption Inhibitor	18841-58-2		C <sub>22</sub> H <sub>35</sub> NO
Pipofezine	Unclassified	24886-52-0		C <sub>16</sub> H <sub>19</sub> N <sub>5</sub> O
Piposulfan	Antineoplastic	2608-24-4		C <sub>12</sub> H <sub>22</sub> N <sub>2</sub> O <sub>8</sub> S <sub>2</sub>
Pipotiazine Palmitate	Antipsychotic	37517-26-3		C <sub>40</sub> H <sub>63</sub> N <sub>3</sub> O <sub>4</sub> S <sub>2</sub>
Pipoxizine	Sedative	55837-21-3		C <sub>24</sub> H <sub>31</sub> NO <sub>3</sub>
Pipoxolan	Muscle Relaxant	23744-24-3		C <sub>22</sub> H <sub>25</sub> NO <sub>3</sub>
Pipradimadol	Analgesic	68797-29-5		C <sub>24</sub> H <sub>37</sub> ClN <sub>2</sub> O <sub>2</sub>
Pipradrol	Nootropic	467-60-7		C <sub>18</sub> H <sub>21</sub> NO
Pipramadol	Analgesic	55313-67-2		C <sub>23</sub> H <sub>35</sub> ClN <sub>2</sub> O <sub>2</sub>
Pipratecol	Antitulcerative	15534-05-1		C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> O <sub>4</sub>
Piprocuarium Iodide	Neuromuscular Blocking Agent	3562-55-8		C <sub>23</sub> H <sub>40</sub> I <sub>2</sub> N <sub>2</sub> O <sub>3</sub>
Piprofurol	Antiarrhythmic	40680-87-3		C <sub>26</sub> H <sub>33</sub> NO <sub>6</sub>
Piprozolin	Choleretic	17243-64-0		C <sub>14</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub> S
Piquindone	Antipsychotic	78541-97-6		C <sub>15</sub> H <sub>22</sub> N <sub>2</sub> O
Piquizil	Bronchodilator	21560-58-7		C <sub>19</sub> H <sub>26</sub> N <sub>4</sub> O <sub>4</sub>
Piracetam	Nootropic	7491-74-9	Y	C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>
Pirandamine	Antidepressant	42408-79-7		C <sub>17</sub> H <sub>23</sub> NO
Pirarubicin	Antineoplastic	72496-41-4		C <sub>32</sub> H <sub>37</sub> NO <sub>12</sub>
Piraxelate	Unclassified	82209-39-0		C <sub>15</sub> H <sub>25</sub> NO <sub>3</sub>
Pirazmonam Sodium	Antibiotic	108319-07-9		C <sub>22</sub> H <sub>24</sub> N <sub>10</sub> O <sub>12</sub> S <sub>2</sub>
Pirazolac	Antirheumatic	71002-09-0		C <sub>17</sub> H <sub>12</sub> ClFN <sub>2</sub> O <sub>2</sub>
Pirbenicillin Sodium	Antibacterial	55975-92-3		C <sub>24</sub> H <sub>26</sub> N <sub>6</sub> O <sub>5</sub> S
Pirbuterol	Bronchodilator	38677-81-5		C <sub>12</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub>
Pirdonium Bromide	Antihistaminic	35620-67-8		C <sub>22</sub> H <sub>30</sub> NOBr
Pirenoxine	Ophthalmic	1043-21-6		C <sub>16</sub> H <sub>8</sub> N <sub>2</sub> O <sub>5</sub>
Pirenperone	Antidote	75444-65-4		C <sub>23</sub> H <sub>24</sub> FN <sub>3</sub> O <sub>2</sub>
Pirenzepine	Antitulcerative	28797-61-7	Y	C <sub>19</sub> H <sub>21</sub> N <sub>5</sub> O <sub>2</sub>
Pirepolol	Antihypertensive	69479-26-1		C <sub>21</sub> H <sub>32</sub> N <sub>4</sub> O <sub>5</sub>
Piretanide	Diuretic	55837-27-9	Y	C <sub>17</sub> H <sub>18</sub> N <sub>2</sub> O <sub>5</sub> S
Pirfenidone	Analgesic	53179-13-8	Y	C <sub>12</sub> H <sub>11</sub> NO
Piribedil	Vasodilator	3605-01-4	Y	C <sub>16</sub> H <sub>18</sub> N <sub>4</sub> O <sub>2</sub>
Piridicillin Sodium	Antibacterial	69414-41-1		C <sub>32</sub> H <sub>35</sub> N <sub>5</sub> O <sub>11</sub> S <sub>2</sub> Na
Piridocaine	Analgesic	87-21-8		C <sub>14</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>
Piridoxilate	Nootropic	46794-57-4		C <sub>10</sub> H <sub>13</sub> NO <sub>6</sub>
Piridoxilate	Nootropic	17692-44-3		C <sub>10</sub> H <sub>13</sub> NO <sub>6</sub>
Piridronic Acid	Bone Resorption Inhibitor	75755-07-6		C <sub>7</sub> H <sub>11</sub> NO <sub>6</sub> P <sub>2</sub>
Pirifibrate	Antihyperlipidemic	55285-45-5		C <sub>17</sub> H <sub>18</sub> ClNO <sub>4</sub>
Pirinidazole	Antiprotozoal	55432-15-0		C <sub>10</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub> S
Pirinixic Acid	Antihyperlipidemic	50892-23-4		C <sub>14</sub> H <sub>14</sub> ClN <sub>3</sub> O <sub>2</sub> S
Pirinixil	Antihyperlipidemic	65089-17-0		C <sub>16</sub> H <sub>19</sub> ClN <sub>4</sub> O <sub>2</sub> S
Piriprost	Bronchodilator	79672-88-1		C <sub>26</sub> H <sub>35</sub> NO <sub>4</sub>
Piriqualone	Muscle Relaxant	1897-89-8		C <sub>22</sub> H <sub>17</sub> N <sub>3</sub> O
Pirisudanol	Antidepressant	33605-94-6		C <sub>16</sub> H <sub>24</sub> N <sub>2</sub> O <sub>6</sub>
Piritramide	Analgesic	302-41-0		C <sub>27</sub> H <sub>34</sub> N <sub>4</sub> O
Piritrexim Isethionate	Antineoplastic	72732-56-0		C <sub>17</sub> H <sub>19</sub> N <sub>5</sub> O <sub>2</sub>
Pirlimycin	Antibacterial	79548-73-5		C <sub>17</sub> H <sub>31</sub> ClN <sub>2</sub> O <sub>5</sub> S
Pirlindole	Antidepressant	60762-57-4		C <sub>15</sub> H <sub>18</sub> N <sub>2</sub>
Pirmagrel	Antithrombotic	85691-74-3		C <sub>13</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>
Pirmenol	Antiarrhythmic	68252-19-7		C <sub>22</sub> H <sub>30</sub> N <sub>2</sub> O
Pirnabine	Antiglaucoma	19825-63-9	Y	C <sub>19</sub> H <sub>24</sub> O <sub>3</sub>
Piroctone	Dermatologic	50650-76-5		C <sub>14</sub> H <sub>23</sub> NO <sub>2</sub>
Pirodavir	Antiviral	124436-59-5		C <sub>21</sub> H <sub>27</sub> N <sub>3</sub> O <sub>3</sub>
Pirodomast	Antihistamine	108310-20-9		C <sub>18</sub> H <sub>17</sub> N <sub>3</sub> O <sub>2</sub>
Pirogliride Tartrate	Antidiabetic	62625-18-7		C <sub>16</sub> H <sub>22</sub> N <sub>4</sub>
Piroheptine	Antiparkinsonian	16378-21-5		C <sub>22</sub> H <sub>25</sub> N
Pirolate	Bronchodilator	55149-05-8		C <sub>16</sub> H <sub>15</sub> N <sub>3</sub> O <sub>5</sub>
Pirolazamide	Antiarrhythmic	39186-49-7		C <sub>23</sub> H <sub>29</sub> N <sub>3</sub> O
Piromidic Acid	Antibacterial	19562-30-2		C <sub>14</sub> H <sub>16</sub> N <sub>4</sub> O <sub>3</sub>
Piroxantrone	Antineoplastic	91441-23-5		C <sub>21</sub> H <sub>25</sub> N <sub>5</sub> O <sub>4</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Piroxicam	Antiinflammatory	36322-90-4	Y	C <sub>15</sub> H <sub>13</sub> N <sub>3</sub> O <sub>4</sub> S
Piroxicam Cinnamate	Antiinflammatory	87234-24-0		C <sub>24</sub> H <sub>19</sub> N <sub>3</sub> O <sub>5</sub> S
Piroxicillin	Antibiotic	82509-56-6		C <sub>27</sub> H <sub>28</sub> N <sub>8</sub> O <sub>9</sub> S <sub>2</sub>
Piroximone	Cardiotonic	84490-12-0		C <sub>11</sub> H <sub>11</sub> N <sub>3</sub> O <sub>2</sub>
Pirozadil	Antihyperlipidemic	54110-25-7		C <sub>27</sub> H <sub>29</sub> NO <sub>10</sub>
Pirprofen	Antiinflammatory	31793-07-4		C <sub>13</sub> H <sub>14</sub> ClNO <sub>2</sub>
Pirquinozol	Antihistaminic	65950-99-4		C <sub>11</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub>
Pirsidomine	Vasodilator	132722-74-8		C <sub>17</sub> H <sub>22</sub> N <sub>4</sub> O <sub>3</sub>
Pirtenidine	Antibacterial	103923-27-9		C <sub>21</sub> H <sub>38</sub> N <sub>2</sub>
Pitavastatin	Antihyperlipidemic	147511-69-1	Y	C <sub>25</sub> H <sub>24</sub> FNO <sub>4</sub>
Pitenodil	Cardiotonic	59840-71-0		C <sub>17</sub> H <sub>27</sub> N <sub>3</sub> O <sub>3</sub> S
Pitofenone	Antispasmodic	54063-52-4		C <sub>22</sub> H <sub>25</sub> NO <sub>4</sub>
Pituxate	Antilucerative	39123-11-0		C <sub>23</sub> H <sub>27</sub> NO <sub>2</sub>
Pivagabine	Anticonvulsant	69542-93-4		C <sub>9</sub> H <sub>17</sub> NO <sub>3</sub>
Pivampicillin	Antibacterial	33817-20-8		C <sub>22</sub> H <sub>29</sub> N <sub>3</sub> O <sub>6</sub> S
Pivenfrine	Unclassified	71206-88-7		C <sub>14</sub> H <sub>21</sub> NO <sub>3</sub>
Pivhydrazine	Antidepressant	306-19-4		C <sub>12</sub> H <sub>18</sub> N <sub>2</sub> O
Pivopril	Antihypertensive	81045-50-3		C <sub>16</sub> H <sub>27</sub> NO <sub>4</sub> S
Pivoxazepam	Anxiolytic	55299-10-0		C <sub>20</sub> H <sub>19</sub> ClN <sub>2</sub> O <sub>3</sub>
Pixantrone	Antineoplastic	144510-96-3		C <sub>17</sub> H <sub>19</sub> N <sub>5</sub> O <sub>2</sub>
Pizotyline	Antidepressant	15574-96-6		C <sub>19</sub> H <sub>21</sub> NS
Plafibrade	Antithrombotic	63394-05-8		C <sub>16</sub> H <sub>22</sub> ClN <sub>3</sub> O <sub>4</sub>
Platonin	Immunomodulator	6009-02-5		C <sub>38</sub> H <sub>61</sub> N <sub>3</sub> S <sub>3</sub> .2Cl
Planutol	Antilucerative	64218-02-6	Y	C <sub>20</sub> H <sub>34</sub> O <sub>2</sub>
Pleconaril	Antiviral	153168-05-9		C <sub>18</sub> H <sub>18</sub> F <sub>3</sub> N <sub>3</sub> O <sub>3</sub>
Plerixafor	Antineoplastic	110078-46-1		C <sub>28</sub> H <sub>54</sub> N <sub>8</sub>
Pleuromulin	Antibiotic	125-65-5		C <sub>22</sub> H <sub>34</sub> O <sub>5</sub>
Plevitrexed	Antineoplastic	153537-73-6		C <sub>26</sub> H <sub>25</sub> FN <sub>8</sub> O <sub>4</sub>
Plomestane	Antineoplastic	77016-85-4		C <sub>21</sub> H <sub>26</sub> O <sub>2</sub>
P Nitrophenyl O Ethyl Ethylphosphonate	Unclassified	546-71-4		C <sub>10</sub> H <sub>14</sub> NO <sub>5</sub> P
Pobilukast Edamine	Bronchodilator	107023-41-6		C <sub>26</sub> H <sub>34</sub> O <sub>5</sub> S
Podilfen	Unclassified	13409-53-5		C <sub>18</sub> H <sub>23</sub> N <sub>3</sub> O <sub>2</sub> S
Podofilox	Antiviral	518-28-5		C <sub>22</sub> H <sub>22</sub> O <sub>8</sub>
Polaprezinc	Antilucerative	107667-60-7	Y	C <sub>9</sub> H <sub>12</sub> N <sub>4</sub> O <sub>3</sub> Zn
Poldine	Mydriatic	596-50-9		C <sub>21</sub> H <sub>26</sub> NO <sub>3</sub>
Polythiazide	Diuretic	346-18-9	Y	C <sub>11</sub> H <sub>13</sub> ClF <sub>3</sub> N <sub>3</sub> O <sub>4</sub> S <sub>3</sub>
Pomisartan	Antihypertensive	144702-17-0		C <sub>31</sub> H <sub>30</sub> N <sub>4</sub> O <sub>2</sub>
Ponalrestat	Antidiabetic	72702-95-5		C <sub>17</sub> H <sub>12</sub> BrFN <sub>2</sub> O <sub>3</sub>
Ponazuril	Antibiotic	69004-04-2		C <sub>18</sub> H <sub>14</sub> F <sub>3</sub> N <sub>3</sub> O <sub>6</sub> S
Ponfibrate	Antihyperlipidemic	53341-49-4		C <sub>18</sub> H <sub>16</sub> Cl <sub>2</sub> O <sub>4</sub>
Porfiromycin	Antibacterial	801-52-5		C <sub>16</sub> H <sub>20</sub> N <sub>4</sub> O <sub>5</sub>
Posaconazole	Antifungal	171228-49-2	Y	C <sub>37</sub> H <sub>42</sub> F <sub>2</sub> N <sub>8</sub> O <sub>4</sub>
Posatirelin	Pituitary	78664-73-0		C <sub>17</sub> H <sub>28</sub> N <sub>4</sub> O <sub>4</sub>
Posizolid	Antibiotic	252260-02-9	Y	C <sub>21</sub> H <sub>21</sub> F <sub>2</sub> N <sub>3</sub> O <sub>7</sub>
Poskine	Anxiolytic	585-14-8		C <sub>20</sub> H <sub>25</sub> NO <sub>5</sub>
Nitrazepate	Anxiolytic	60676-80-4		C <sub>16</sub> H <sub>11</sub> N <sub>3</sub> O <sub>5</sub>
Thiocyanate	Unclassified	302-04-5		CNS
Practolol	Antiarrhythmic	6673-35-4		C <sub>14</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub>
Pradefovir Mesylate	Antiviral	625095-60-5	Y	C <sub>17</sub> H <sub>19</sub> ClN <sub>5</sub> O <sub>4</sub> P
Pradofloxacin	Antibiotic	195532-12-8		C <sub>21</sub> H <sub>21</sub> FN <sub>4</sub> O <sub>3</sub>
Prajmalium Bitartrate	Antiarrhythmic	2589-47-1	Y	C <sub>27</sub> H <sub>38</sub> N <sub>2</sub> O <sub>8</sub>
Pralatrexate	Antineoplastic	146464-95-1		C <sub>23</sub> H <sub>23</sub> N <sub>7</sub> O <sub>5</sub>
Pralidoxime	Antidote	6735-59-7		C <sub>7</sub> H <sub>9</sub> N <sub>2</sub> O
Pralmorelin Dihydrochloride	Pituitary	158861-67-7		C <sub>45</sub> H <sub>55</sub> N <sub>9</sub> O <sub>6</sub>
Pralnacasan	Antirheumatic	192755-52-5		C <sub>26</sub> H <sub>29</sub> N <sub>5</sub> O <sub>7</sub>
Pramipexole	Antiparkinsonian	104632-26-0	Y	C <sub>10</sub> H <sub>17</sub> N <sub>3</sub> S
Pramiracetam	Nootropic	68497-62-1	Y	C <sub>14</sub> H <sub>27</sub> N <sub>3</sub> O <sub>2</sub>
Pramiverine	Antispasmodic	14334-40-8		C <sub>21</sub> H <sub>27</sub> N
Pramoxine	Anesthetic	140-65-8		C <sub>17</sub> H <sub>27</sub> NO <sub>3</sub>
Prampine	Unclassified	7009-65-6		C <sub>20</sub> H <sub>27</sub> NO <sub>4</sub>
Pranazepide	Antispasmodic	150408-73-4		C <sub>26</sub> H <sub>19</sub> FN <sub>4</sub> O <sub>2</sub>
Pranidipine	Antihypertensive	99522-79-9		C <sub>25</sub> H <sub>24</sub> N <sub>2</sub> O <sub>6</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Pranlukast	Bronchodilator	103177-37-3	Y	C <sub>27</sub> H <sub>23</sub> N <sub>5</sub> O <sub>4</sub>
Pranolium Chloride	Antiarrhythmic	42879-47-0		C <sub>18</sub> H <sub>26</sub> ClNO <sub>2</sub>
Pranoprofen	Antiinflammatory	52549-17-4		C <sub>15</sub> H <sub>13</sub> NO <sub>3</sub>
Pranosal	Unclassified	17716-89-1		C <sub>16</sub> H <sub>23</sub> NO <sub>3</sub>
Prasterone	Steroid	53-43-0	Y	C <sub>19</sub> H <sub>28</sub> O <sub>2</sub>
Prasugrel	Anticoagulant	150322-43-3	Y	C <sub>20</sub> H <sub>20</sub> FNO <sub>3</sub> S
Pratosartan	Antihypertensive	153804-05-8	Y	C <sub>25</sub> H <sub>26</sub> N <sub>6</sub> O
Pravadoline	Analgesic	92623-83-1		C <sub>23</sub> H <sub>26</sub> N <sub>2</sub> O <sub>3</sub>
Pravastatin Sodium	Antihyperlipidemic	81093-37-0	Y	C <sub>23</sub> H <sub>36</sub> O <sub>7</sub>
Praxadine	Antibiotic	4023-00-1		C <sub>4</sub> H <sub>6</sub> N <sub>4</sub>
Prazepam	Sedative	2955-38-6	Y	C <sub>19</sub> H <sub>17</sub> ClN <sub>2</sub> O
Prazepine	Anticonvulsant	50-49-7		C <sub>19</sub> H <sub>24</sub> N <sub>2</sub>
Praziquantel	Anthelminthic	55268-74-1	Y	C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub>
Prazitone	Antipsychotic	2409-26-9		C <sub>16</sub> H <sub>19</sub> N <sub>3</sub> O <sub>3</sub>
Prazocillin	Antibiotic	15949-72-1		C <sub>19</sub> H <sub>18</sub> Cl <sub>2</sub> N <sub>4</sub> O <sub>4</sub> S
Prazosin	Antihypertensive	19216-56-9	Y	C <sub>19</sub> H <sub>21</sub> N <sub>5</sub> O <sub>4</sub>
Preclamol	Antipsychotic	85966-89-8		C <sub>14</sub> H <sub>21</sub> NO
Prednazoline	Antiinflammatory	4846-91-7		C <sub>13</sub> H <sub>18</sub> N <sub>2</sub> O
Prednicarbate	Glucocorticoid	73771-04-7		C <sub>27</sub> H <sub>36</sub> O <sub>8</sub>
Prednimustine	Antineoplastic	29069-24-7		C <sub>35</sub> H <sub>45</sub> Cl <sub>2</sub> NO <sub>6</sub>
Prednisolamate	Glucocorticoid	5626-34-6		C <sub>27</sub> H <sub>39</sub> NO <sub>6</sub>
Prednisolone	Glucocorticoid	50-24-8	Y	C <sub>21</sub> H <sub>28</sub> O <sub>5</sub>
Prednisolone Acetate	Glucocorticoid	52-21-1	Y	C <sub>23</sub> H <sub>30</sub> O <sub>6</sub>
Prednisolone Hemisuccinate	Glucocorticoid	2920-86-7		C <sub>25</sub> H <sub>32</sub> O <sub>8</sub>
Prednisolone Pivalate	Glucocorticoid	1107-99-9		C <sub>26</sub> H <sub>36</sub> O <sub>6</sub>
Prednisolone Sodium Phosphate	Glucocorticoid	302-25-0		C <sub>21</sub> H <sub>29</sub> O <sub>8</sub> P
Prednisolone Steaglate	Glucocorticoid	5060-55-9		C <sub>41</sub> H <sub>64</sub> O <sub>8</sub>
Prednisolone Tebutate	Glucocorticoid	7681-14-3		C <sub>27</sub> H <sub>38</sub> O <sub>6</sub>
Prednisolone Valerate Acetate	Glucocorticoid	72064-79-0		C <sub>28</sub> H <sub>38</sub> O <sub>7</sub>
Prednisone	Glucocorticoid	53-03-2	Y	C <sub>21</sub> H <sub>26</sub> O <sub>5</sub>
Prednival	Glucocorticoid	15180-00-4		C <sub>26</sub> H <sub>36</sub> O <sub>6</sub>
Prednylidene	Glucocorticoid	599-33-7		C <sub>22</sub> H <sub>28</sub> O <sub>5</sub>
Prefenamate	Antiinflammatory	57775-28-7		C <sub>19</sub> H <sub>18</sub> F <sub>3</sub> NO <sub>2</sub>
Pregabalin	Anticonvulsant	148553-50-8	Y	C <sub>8</sub> H <sub>17</sub> NO <sub>2</sub>
Pregnandiol	Progestogen	25908-35-4		C <sub>21</sub> H <sub>36</sub> O <sub>2</sub>
Pregnenolone	Progestogen	145-13-1		C <sub>21</sub> H <sub>32</sub> O <sub>2</sub>
Pregnenolone Acetate	Progestogen	1778-02-5		C <sub>23</sub> H <sub>34</sub> O <sub>3</sub>
Pregnenolone Succinate	Progestogen	4598-67-8		C <sub>25</sub> H <sub>36</sub> O <sub>5</sub>
Premafloxacin	Antibacterial	143383-65-7		C <sub>21</sub> H <sub>26</sub> FN <sub>3</sub> O <sub>4</sub>
Premazepam	Anxiolytic	57435-86-6		C <sub>15</sub> H <sub>15</sub> N <sub>3</sub> O
Prenalterol	Adrenergic	57526-81-5		C <sub>12</sub> H <sub>19</sub> NO <sub>3</sub>
Prenderol	Unclassified	115-76-4		C <sub>7</sub> H <sub>16</sub> O <sub>2</sub>
Prenisteine	Antitussive	5287-46-7		C <sub>8</sub> H <sub>15</sub> NO <sub>2</sub> S
Prenoverine	Mucolytic	66022-25-1		C <sub>25</sub> H <sub>29</sub> NO <sub>2</sub>
Prenoxdiazine	Antitussive	47543-65-7		C <sub>23</sub> H <sub>27</sub> N <sub>3</sub> O
Prenylamine	Vasodilator	390-64-7		C <sub>24</sub> H <sub>27</sub> N
Pretamazium Iodide	Unclassified	24840-59-3		C <sub>29</sub> H <sub>29</sub> N <sub>2</sub> SI
Pretiadil	Antianginal	30840-27-8		C <sub>26</sub> H <sub>31</sub> N <sub>3</sub> O <sub>2</sub> S
Pribecaine	Anesthetic	55837-22-4		C <sub>16</sub> H <sub>23</sub> NO <sub>3</sub>
Pridefine	Antidepressant	5370-41-2		C <sub>19</sub> H <sub>21</sub> N
Prideperone	Antipsychotic	95374-52-0		C <sub>23</sub> H <sub>24</sub> FN <sub>3</sub> O <sub>3</sub>
Pridinol	Antiparkinsonian	511-45-5		C <sub>20</sub> H <sub>25</sub> NO
Prifelone	Antiinflammatory	69425-13-4		C <sub>19</sub> H <sub>24</sub> O <sub>2</sub> S
Prifinium Bromide	Antispasmodic	4630-95-9		C <sub>22</sub> H <sub>28</sub> BrN
Prifuroline	Antipsychotic	70833-07-7		C <sub>14</sub> H <sub>16</sub> N <sub>2</sub> O
Prilocaine	Anesthetic	721-50-6		C <sub>13</sub> H <sub>20</sub> N <sub>2</sub> O
Primaperone	Antipsychotic	1219-35-8		C <sub>15</sub> H <sub>20</sub> FNO
Primaquine	Antimalarial	90-34-6	Y	C <sub>15</sub> H <sub>21</sub> N <sub>3</sub> O
Primidolol	Antihypertensive	67227-55-8		C <sub>17</sub> H <sub>23</sub> N <sub>3</sub> O <sub>4</sub>
Prinomastat	Antineoplastic	192329-42-3		C <sub>18</sub> H <sub>21</sub> N <sub>3</sub> O <sub>5</sub> S <sub>2</sub>
Prinomide Tromethamine	Antirheumatic	77639-66-8		C <sub>15</sub> H <sub>13</sub> N <sub>3</sub> O <sub>2</sub>
Prinoxodan	Cardiotonic	111786-07-3		C <sub>13</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub>
Prisotinol	Nootropic	76906-79-1		C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> O

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Prizidilol	Antihypertensive	59010-44-5		C <sub>17</sub> H <sub>25</sub> N <sub>5</sub> O <sub>2</sub>
Proadifen	Antidiabetic	302-33-0		C <sub>23</sub> H <sub>31</sub> NO <sub>2</sub>
Probarbital Sodium	Sedative	76-76-6		C <sub>9</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>
Probenecid	Uricosuric	57-66-9	Y	C <sub>13</sub> H <sub>19</sub> NO <sub>4</sub> S
Probicromil Calcium	Antihistaminic	58805-38-2		C <sub>17</sub> H <sub>12</sub> O <sub>8</sub>
Probucof	Antihyperlipidemic	23288-49-5		C <sub>31</sub> H <sub>48</sub> O <sub>2</sub> S <sub>2</sub>
Procainamide	Antiarrhythmic	51-06-9	Y	C <sub>13</sub> H <sub>21</sub> N <sub>3</sub> O
Procaine	Anesthetic	59-46-1	Y	C <sub>13</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>
Procarbazine	Antineoplastic	671-16-9	Y	C <sub>12</sub> H <sub>19</sub> N <sub>3</sub> O
Procaterol	Bronchodilator	72332-33-3		C <sub>16</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub>
Prochlorperazine	Antiemetic	58-38-8	Y	C <sub>20</sub> H <sub>24</sub> ClN <sub>3</sub> S
Procinolol	Antihypertensive	27325-36-6		C <sub>15</sub> H <sub>23</sub> NO <sub>2</sub>
Procinonide	Steroid	58497-00-0		C <sub>27</sub> H <sub>34</sub> F <sub>2</sub> O <sub>7</sub>
Proclonol	Anthelminthic	14088-71-2		C <sub>16</sub> H <sub>14</sub> Cl <sub>2</sub> O
Procodazole	Immunomodulator	23249-97-0		C <sub>10</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>
Procyclidine	Antiparkinsonian	77-37-2	Y	C <sub>19</sub> H <sub>29</sub> NO
Procymate	Anxiolytic	13931-64-1		C <sub>10</sub> H <sub>19</sub> NO <sub>2</sub>
Prodeconium Bromide	Antifungal	3690-61-7		C <sub>28</sub> H <sub>58</sub> Br <sub>2</sub> N <sub>2</sub> O <sub>6</sub>
Prodilidine	Analgesic	3734-17-6		C <sub>15</sub> H <sub>21</sub> NO <sub>2</sub>
Prodipine	Antiparkinsonian	31314-38-2		C <sub>20</sub> H <sub>25</sub> N
Prodolic Acid	Antiinflammatory	36505-82-5		C <sub>16</sub> H <sub>19</sub> NO <sub>3</sub>
Profadol	Analgesic	428-37-5		C <sub>14</sub> H <sub>21</sub> NO
Profexalone	Sedative	34740-13-1		C <sub>13</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>
Proflazepam	Anxiolytic	52829-30-8		C <sub>18</sub> H <sub>16</sub> ClFN <sub>2</sub> O <sub>3</sub>
Progabide	Anticonvulsant	62666-20-0		C <sub>17</sub> H <sub>16</sub> ClFN <sub>2</sub> O <sub>2</sub>
Progesterone	Progestogen	57-83-0	Y	C <sub>21</sub> H <sub>30</sub> O <sub>2</sub>
Proglumetacin	Antiinflammatory	57132-53-3	Y	C <sub>46</sub> H <sub>58</sub> ClN <sub>5</sub> O <sub>8</sub>
Proglumide	Antiulcerative	6620-60-6	Y	C <sub>18</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub>
Proheptazine	Analgesic	77-14-5		C <sub>17</sub> H <sub>25</sub> NO <sub>2</sub>
Proligestone	Progestogen	23873-85-0		C <sub>24</sub> H <sub>34</sub> O <sub>4</sub>
Prolintane	Antidepressant	493-92-5		C <sub>15</sub> H <sub>23</sub> N
Promazine	Antipsychotic	58-40-2		C <sub>17</sub> H <sub>20</sub> N <sub>2</sub> S
Promegestone	Progestogen	34184-77-5	Y	C <sub>22</sub> H <sub>30</sub> O <sub>2</sub>
Promestriene	Dermatologic	39219-28-8		C <sub>22</sub> H <sub>32</sub> O <sub>2</sub>
Promethazine	Antihistaminic	60-87-7	Y	C <sub>17</sub> H <sub>20</sub> N <sub>2</sub> S
Promethestrol Dipropionate	Estrogen	84-13-9		C <sub>26</sub> H <sub>34</sub> O <sub>4</sub>
Promolate	Antitussive	3615-74-5		C <sub>16</sub> H <sub>23</sub> NO <sub>4</sub>
Promoxolane	Unclassified	470-43-9		C <sub>10</sub> H <sub>20</sub> O <sub>3</sub>
Pronetalol	Antianginal	54-80-8		C <sub>15</sub> H <sub>19</sub> NO
Propacetamol	Analgesic	66532-85-2		C <sub>14</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub>
Propafenone	Antiarrhythmic	54063-53-5	Y	C <sub>21</sub> H <sub>27</sub> NO <sub>3</sub>
Propamidine	Antiprotozoal	104-32-5		C <sub>17</sub> H <sub>20</sub> N <sub>4</sub> O <sub>2</sub>
Propanidid	Anesthetic	1421-14-3		C <sub>18</sub> H <sub>27</sub> NO <sub>5</sub>
Propanocaine	Anesthetic	493-76-5		C <sub>20</sub> H <sub>25</sub> NO <sub>2</sub>
Propantheline	Antispasmodic	298-50-0	Y	C <sub>23</sub> H <sub>30</sub> NO <sub>3</sub>
Proparacaine	Anesthetic	499-67-2		C <sub>16</sub> H <sub>26</sub> N <sub>2</sub> O <sub>3</sub>
Propatyl Nitrate	Vasodilator	2921-92-8		C <sub>6</sub> H <sub>11</sub> N <sub>3</sub> O <sub>9</sub>
Propentofylline	Nootropic	55242-55-2		C <sub>15</sub> H <sub>22</sub> N <sub>4</sub> O <sub>3</sub>
Propenzolate	Mydriatic	4354-45-4		C <sub>25</sub> H <sub>29</sub> NO <sub>3</sub>
Propetidine	Analgesic	561-76-2		C <sub>16</sub> H <sub>23</sub> NO <sub>2</sub>
Propetamide	Antidiabetic	730-07-4		C <sub>14</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>
Propetandrol	Steroid	3638-82-2		C <sub>23</sub> H <sub>36</sub> O <sub>3</sub>
Propicillin	Antibiotic	551-27-9		C <sub>18</sub> H <sub>22</sub> N <sub>2</sub> O <sub>5</sub> S
Propikacin	Antibacterial	66887-96-5		C <sub>21</sub> H <sub>43</sub> N <sub>5</sub> O <sub>12</sub>
Propinetidine	Antiulcerative	3811-53-8		C <sub>19</sub> H <sub>25</sub> NO <sub>2</sub>
Propiomazine	Sedative	362-29-8		C <sub>20</sub> H <sub>24</sub> N <sub>2</sub> OS
Propionic Acid	Antifungal	79-09-4		C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>
Propipocaine	Anesthetic	3670-68-6		C <sub>17</sub> H <sub>25</sub> NO <sub>2</sub>
Propiram Fumarate	Analgesic	15686-91-6		C <sub>16</sub> H <sub>25</sub> N <sub>3</sub> O
Propisergide	Antimigraine	5793-04-4		C <sub>20</sub> H <sub>25</sub> N <sub>3</sub> O <sub>2</sub>
Propiverine	Antispasmodic	60569-19-9	Y	C <sub>23</sub> H <sub>29</sub> NO <sub>3</sub>
Propizepine	Antidepressant	10321-12-7		C <sub>17</sub> H <sub>20</sub> N <sub>4</sub> O
Propofol	Anesthetic	2078-54-8		C <sub>12</sub> H <sub>18</sub> O

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Propoxate	Antidepressant	7036-58-0		C <sub>15</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>
Propoxycaïne	Anesthetic	86-43-1		C <sub>16</sub> H <sub>26</sub> N <sub>2</sub> O <sub>3</sub>
Propoxyphene	Analgesic	469-62-5		C <sub>22</sub> H <sub>29</sub> NO <sub>2</sub>
Propranolol	Antihypertensive	525-66-6	Y	C <sub>16</sub> H <sub>21</sub> NO <sub>2</sub>
Propylhexedrine	Adrenergic	101-40-6		C <sub>10</sub> H <sub>21</sub> N
Propylthiouracil	Thyroid	51-52-5	Y	C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> OS
Propyperone	Antipsychotic	3781-28-0		C <sub>23</sub> H <sub>33</sub> FN <sub>2</sub> O <sub>2</sub>
Propyphenazone	Analgesic	479-92-5		C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O
Propyromazine Bromide	Antispasmodic	145-54-0		C <sub>20</sub> H <sub>23</sub> BrN <sub>2</sub> O <sub>5</sub>
Proquazone	Antiinflammatory	22760-18-5		C <sub>18</sub> H <sub>18</sub> N <sub>2</sub> O
Proquinolate	Antibacterial	1698-95-9		C <sub>17</sub> H <sub>21</sub> NO <sub>5</sub>
Prorenoate Potassium	Antihypertensive	49848-01-3		C <sub>23</sub> H <sub>32</sub> O <sub>4</sub>
Proroxan	Antihypertensive	33743-96-3		C <sub>21</sub> H <sub>23</sub> NO <sub>3</sub>
Proscillaridin	Cardiotonic	466-06-8		C <sub>30</sub> H <sub>42</sub> O <sub>8</sub>
Prospidium Chloride	Antineoplastic	23476-83-7		C <sub>18</sub> H <sub>36</sub> Cl <sub>4</sub> N <sub>4</sub> O <sub>2</sub>
Prostalene	Prostaglandin	54120-61-5		C <sub>22</sub> H <sub>36</sub> O <sub>5</sub>
Prosulpride	Antipsychotic	68556-59-2		C <sub>16</sub> H <sub>25</sub> N <sub>3</sub> O <sub>4</sub> S
Protein Hydrolysate	Plasma Volume Expander	852812-98-7		C <sub>35</sub> H <sub>47</sub> N <sub>7</sub> O <sub>10</sub>
Proterguride	Antipsychotic	77650-95-4		C <sub>22</sub> H <sub>32</sub> N <sub>4</sub> O
Protheobromine	Diuretic	50-39-5		C <sub>10</sub> H <sub>14</sub> N <sub>4</sub> O <sub>3</sub>
Prothipendyl	Antipsychotic	303-69-5		C <sub>16</sub> H <sub>19</sub> N <sub>3</sub> S
Prothixene	Antipsychotic	2622-24-4		C <sub>18</sub> H <sub>19</sub> NS
Protiofate	Antibiotic	58416-00-5		C <sub>12</sub> H <sub>16</sub> O <sub>6</sub> S
Protionamide	Antibacterial	14222-60-7		C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> S
Protirelin	Pituitary	24305-27-9		C <sub>16</sub> H <sub>22</sub> N <sub>6</sub> O <sub>4</sub>
Protizinic Acid	Antiinflammatory	13799-03-6		C <sub>17</sub> H <sub>17</sub> NO <sub>3</sub> S
Protokylol	Bronchodilator	136-70-9		C <sub>18</sub> H <sub>21</sub> NO <sub>5</sub>
Protoporphyrin IX	Hepatic Protectant	553-12-8		C <sub>34</sub> H <sub>34</sub> N <sub>4</sub> O <sub>4</sub>
Protoveratrine A	Antihypertensive	143-57-7		C <sub>41</sub> H <sub>63</sub> NO <sub>14</sub>
Protoveratrine B	Antihypertensive	124-97-0		C <sub>41</sub> H <sub>63</sub> NO <sub>15</sub>
Protriptyline	Antidepressant	438-60-8	Y	C <sub>19</sub> H <sub>21</sub> N
Proxazole	Muscle Relaxant	5696-09-3		C <sub>17</sub> H <sub>25</sub> N <sub>3</sub> O
Proxibarbal	Sedative	2537-29-3		C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub>
Proxibutene	Analgesic	14089-84-0		C <sub>22</sub> H <sub>27</sub> NO <sub>2</sub>
Proxicromil	Antihistaminic	60400-92-2		C <sub>17</sub> H <sub>18</sub> O <sub>5</sub>
Proxorphan Tartrate	Analgesic	69815-38-9		C <sub>19</sub> H <sub>25</sub> NO <sub>2</sub>
Proxyphylline	Bronchodilator	603-00-9		C <sub>10</sub> H <sub>14</sub> N <sub>4</sub> O <sub>3</sub>
Prozapine	Antispasmodic	3426-08-2		C <sub>21</sub> H <sub>27</sub> N
Prucalopride	Gastroprokinetic	179474-81-8	Y	C <sub>18</sub> H <sub>26</sub> ClN <sub>3</sub> O <sub>3</sub>
Prulifloxacin	Antibacterial	123447-62-1	Y	C <sub>21</sub> H <sub>20</sub> FN <sub>3</sub> O <sub>6</sub> S
Pruvanserin	Antidepressant	443144-26-1		C <sub>22</sub> H <sub>21</sub> FN <sub>4</sub> O
Pseudoephedrine	Decongestant	90-82-4	Y	C <sub>10</sub> H <sub>15</sub> NO
Psilocybine	Antipsychotic	520-52-5		C <sub>12</sub> H <sub>17</sub> N <sub>2</sub> O <sub>4</sub> P
Pteropterin	Unclassified	89-38-3		C <sub>29</sub> H <sub>33</sub> N <sub>9</sub> O <sub>12</sub>
Pumafentrine	Antimalarial	207993-12-2		C <sub>29</sub> H <sub>39</sub> N <sub>3</sub> O <sub>3</sub>
Pumaprazole	Antiulcerative	158364-59-1		C <sub>19</sub> H <sub>22</sub> N <sub>4</sub> O <sub>2</sub>
Pumitepa	Antineoplastic	42061-52-9		C <sub>12</sub> H <sub>19</sub> N <sub>8</sub> OP
Pumosetrag	Gastroprokinetic	153062-94-3		C <sub>15</sub> H <sub>17</sub> N <sub>3</sub> O <sub>2</sub> S
Puromycin	Antineoplastic	53-79-2		C <sub>22</sub> H <sub>29</sub> N <sub>7</sub> O <sub>5</sub>
Pyrabrom	Antihistaminic	606-05-3		C <sub>24</sub> H <sub>30</sub> BrN <sub>7</sub> O <sub>3</sub>
Pyrantel	Anthelmintic	15686-83-6	Y	C <sub>11</sub> H <sub>14</sub> N <sub>2</sub> S
Pyraethiazine	Anthelmintic	84-08-2		C <sub>18</sub> H <sub>20</sub> N <sub>2</sub> S
Pyrazinamide	Antibacterial	98-96-4	Y	C <sub>5</sub> H <sub>5</sub> N <sub>3</sub> O
Pyrazofurin	Antineoplastic	30868-30-5		C <sub>9</sub> H <sub>13</sub> N <sub>3</sub> O <sub>6</sub>
Pyricarbate	Glucocorticoid	1882-26-4		C <sub>11</sub> H <sub>15</sub> N <sub>3</sub> O <sub>4</sub>
Pyridarone	Antiarrhythmic	7035-04-3		C <sub>13</sub> H <sub>9</sub> NO
Pyridofylline	Vasodilator	53403-96-6		C <sub>9</sub> H <sub>12</sub> N <sub>4</sub> O <sub>6</sub> S
Pyridofylline	Vasodilator	65-23-6		C <sub>8</sub> H <sub>11</sub> NO <sub>3</sub>
Pyridostigmine	Cholinergic	155-97-5	Y	C <sub>9</sub> H <sub>13</sub> N <sub>2</sub> O <sub>2</sub>
Pyrilamine	Antihistaminic	91-84-9		C <sub>17</sub> H <sub>23</sub> N <sub>3</sub> O
Pyrimethamine	Antimalarial	58-14-0	Y	C <sub>12</sub> H <sub>13</sub> ClN <sub>4</sub>
Pyrinoline	Antiarrhythmic	1740-22-3		C <sub>27</sub> H <sub>20</sub> N <sub>4</sub> O
Pyrrithione	Antibacterial	1121-30-8		C <sub>5</sub> H <sub>5</sub> NOS

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Pyrithoxin	Nootropic	1098-97-1		C <sub>16</sub> H <sub>20</sub> N <sub>2</sub> O <sub>4</sub> S <sub>2</sub>
Pyrithyldione	Sedative	77-04-3		C <sub>9</sub> H <sub>13</sub> NO <sub>2</sub>
Pyritidium	Antiprotozoal	3616-05-5		C <sub>25</sub> H <sub>24</sub> N <sub>7</sub>
Pyrogallol	Neuromuscular Blocking Agent	87-66-1		C <sub>6</sub> H <sub>6</sub> O <sub>3</sub>
Pyrovalerone	Nootropic	3563-49-3		C <sub>16</sub> H <sub>23</sub> NO
Pyroxamine Maleate	Antihistaminic	7009-68-9		C <sub>18</sub> H <sub>20</sub> ClNO
Pyrobutamine Phosphate	Antihistaminic	91-82-7		C <sub>20</sub> H <sub>22</sub> ClN
Pyrocaine	Anesthetic	2210-77-7		C <sub>14</sub> H <sub>20</sub> N <sub>2</sub> O
Pyrrroliphen	Analgesic	15686-97-2		C <sub>23</sub> H <sub>29</sub> NO <sub>2</sub>
Pyrrrolnitrin	Antifungal	1018-71-9		C <sub>10</sub> H <sub>6</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Pytamine	Antidepressant	15301-88-9		C <sub>20</sub> H <sub>28</sub> N <sub>2</sub> O
Quadazocine Mesylate	Analgesic	71276-43-2		C <sub>25</sub> H <sub>37</sub> NO <sub>2</sub>
Quadrosilan	Unclassified	33204-76-1		C <sub>18</sub> H <sub>28</sub> O <sub>4</sub> Si <sub>4</sub>
Quatacaine	Anesthetic	17692-45-4		C <sub>14</sub> H <sub>22</sub> N <sub>2</sub> O
Quazepam	Sedative	36735-22-5	Y	C <sub>17</sub> H <sub>11</sub> ClF <sub>4</sub> N <sub>2</sub> S
Quazinone	Cardiotonic	70018-51-8		C <sub>11</sub> H <sub>10</sub> ClN <sub>3</sub> O
Quazodine	Cardiotonic	4015-32-1		C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Quazolast	Bronchodilator	86048-40-0		C <sub>12</sub> H <sub>7</sub> ClN <sub>2</sub> O <sub>3</sub>
Quercetin	Capillary Protectant	117-39-5	Y	C <sub>15</sub> H <sub>10</sub> O <sub>7</sub>
Quetiapine	Antipsychotic	111974-69-7	Y	C <sub>21</sub> H <sub>25</sub> N <sub>3</sub> O <sub>2</sub> S
Quifenadine	Antihistaminic	10447-39-9		C <sub>20</sub> H <sub>23</sub> NO
Quiflapon Sodium	Antiinflammatory	136668-42-3		C <sub>34</sub> H <sub>35</sub> ClN <sub>2</sub> O <sub>5</sub> S
Quillifoline	Antibacterial	15301-89-0		C <sub>21</sub> H <sub>24</sub> ClNO <sub>2</sub>
Quilostigmine	Cholinergic	139314-01-5		C <sub>23</sub> H <sub>27</sub> N <sub>3</sub> O <sub>2</sub>
Quinacainol	Antiarrhythmic	86073-85-0		C <sub>21</sub> H <sub>30</sub> N <sub>2</sub> O
Quinacillin	Antibiotic	1596-63-0		C <sub>18</sub> H <sub>16</sub> N <sub>4</sub> O <sub>6</sub> S
Quinacrine	Antimalarial	83-89-6	Y	C <sub>23</sub> H <sub>30</sub> ClN <sub>3</sub> O
Quinagolide	Antipsychotic	87056-78-8	Y	C <sub>20</sub> H <sub>33</sub> N <sub>3</sub> O <sub>3</sub> S
Quinaldine Blue	Antineoplastic	2768-90-3		C <sub>25</sub> H <sub>25</sub> N <sub>2</sub> Cl
Quinapril	Antihypertensive	85441-61-8	Y	C <sub>25</sub> H <sub>30</sub> N <sub>2</sub> O <sub>5</sub>
Quinaprilat	Antihypertensive	82768-85-2	Y	C <sub>23</sub> H <sub>26</sub> N <sub>2</sub> O <sub>5</sub>
Quinazosin	Antihypertensive	15793-38-1		C <sub>17</sub> H <sub>23</sub> N <sub>5</sub> O <sub>2</sub>
Quinbolone	Steroid	2487-63-0		C <sub>24</sub> H <sub>32</sub> O <sub>2</sub>
Quincarbonate	Urologic	54340-59-9		C <sub>17</sub> H <sub>18</sub> ClNO <sub>6</sub>
Quindecamine Acetate	Antibacterial	19056-26-9		C <sub>30</sub> H <sub>38</sub> N <sub>4</sub>
Quindonium Bromide	Antiarrhythmic	130-81-4		C <sub>16</sub> H <sub>20</sub> NO.Br
Quindoxin	Antibacterial	2423-66-7		C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>
Quinelorane	Antihypertensive	97466-90-5		C <sub>14</sub> H <sub>22</sub> N <sub>4</sub>
Quinestradol	Estrogen	1169-79-5		C <sub>23</sub> H <sub>32</sub> O <sub>3</sub>
Quinestrol	Estrogen	152-43-2		C <sub>25</sub> H <sub>32</sub> O <sub>2</sub>
Quinethazone	Diuretic	73-49-4		C <sub>10</sub> H <sub>12</sub> ClN <sub>3</sub> O <sub>3</sub> S
Quinetolate	Muscle Relaxant	27166-18-3		C <sub>14</sub> H <sub>19</sub> N <sub>3</sub> O
Quinetolate	Muscle Relaxant	131-64-6		C <sub>12</sub> H <sub>19</sub> NO <sub>3</sub>
Quinezamide	Antidiabetic	77197-48-9		C <sub>13</sub> H <sub>12</sub> N <sub>4</sub> O
Quinfamide	Antiamebic	62265-68-3		C <sub>16</sub> H <sub>13</sub> Cl <sub>2</sub> NO <sub>4</sub>
Quingestanol Acetate	Progestogen	3000-39-3		C <sub>27</sub> H <sub>36</sub> O <sub>3</sub>
Quingestrone	Progestogen	67-95-8		C <sub>26</sub> H <sub>38</sub> O <sub>2</sub>
Quinidine	Antimalarial	56-54-2	Y	C <sub>20</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub>
Quinine	Antimalarial	130-95-0	Y	C <sub>20</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub>
Quinocide	Antimalarial	525-61-1		C <sub>15</sub> H <sub>21</sub> N <sub>3</sub> O
Quinpirole	Antihypertensive	80373-22-4		C <sub>13</sub> H <sub>21</sub> N <sub>3</sub>
Quinterenol Sulfate	Bronchodilator	13757-97-6		C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>
Quintiofos	Ectoparasiticide	1776-83-6		C <sub>17</sub> H <sub>16</sub> NO <sub>2</sub> PS
Quinuclium Bromide	Antihypertensive	35425-83-3		C <sub>14</sub> H <sub>18</sub> BrNO
Quinupramine	Antidepressant	31721-17-2		C <sub>21</sub> H <sub>24</sub> N <sub>2</sub>
Quipazine Maleate	Antidepressant	4774-24-7		C <sub>13</sub> H <sub>15</sub> N <sub>3</sub>
Qisultazine	Antidepressant	64099-44-1		C <sub>21</sub> H <sub>25</sub> N <sub>3</sub> O <sub>2</sub> S <sub>2</sub>
Rabeprazole	Antilucerative	117976-89-3	Y	C <sub>18</sub> H <sub>21</sub> N <sub>3</sub> O <sub>3</sub> S
Racecadotril	Antidiarrheal	81110-73-8	Y	C <sub>21</sub> H <sub>23</sub> NO <sub>4</sub> S
Racefemine	Antispasmodic	22232-57-1		C <sub>18</sub> H <sub>23</sub> NO
Racemethol	Decongestant	89-78-1		C <sub>10</sub> H <sub>20</sub> O
Racemethorphan	Antitussive	510-53-2		C <sub>18</sub> H <sub>25</sub> NO

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Racemetirosine	Unclassified	658-48-0		C <sub>10</sub> H <sub>13</sub> NO <sub>3</sub>
Racemoramide	Analgesic	545-59-5		C <sub>25</sub> H <sub>32</sub> N <sub>2</sub> O <sub>2</sub>
Racemorphan	Analgesic	297-90-5		C <sub>17</sub> H <sub>23</sub> NO
Racephedrine	Bronchodilator	90-81-3		C <sub>10</sub> H <sub>15</sub> NO
Racephenicol	Antibacterial	847-25-6		C <sub>12</sub> H <sub>15</sub> Cl <sub>2</sub> NO <sub>5</sub> S
Racepinephrine	Bronchodilator	329-65-7		C <sub>9</sub> H <sub>13</sub> NO <sub>3</sub>
Ractopamine	Steroid	97825-25-7		C <sub>18</sub> H <sub>23</sub> NO <sub>3</sub>
Radafaxine	Antidepressant	192374-14-4		C <sub>13</sub> H <sub>18</sub> ClNO <sub>2</sub>
Rafabegron	Antidiabetic	244081-42-3		C <sub>21</sub> H <sub>23</sub> ClN <sub>2</sub> O <sub>4</sub>
Rafoxanide	Anthelminthic	22662-39-1		C <sub>19</sub> H <sub>11</sub> Cl <sub>2</sub> I <sub>2</sub> NO <sub>3</sub>
Ragaglitazar	Antidiabetic	222834-30-2		C <sub>25</sub> H <sub>25</sub> NO <sub>5</sub>
Ralitoline	Anticonvulsant	93738-40-0		C <sub>13</sub> H <sub>13</sub> ClN <sub>2</sub> O <sub>2</sub> S
Raloxifene	Bone Resorption Inhibitor	84449-90-1	Y	C <sub>28</sub> H <sub>27</sub> NO <sub>4</sub> S
Raltitrexed	Antineoplastic	112887-68-0		C <sub>21</sub> H <sub>22</sub> N <sub>4</sub> O <sub>6</sub> S
Raluridine	Antiviral	119644-22-3		C <sub>9</sub> H <sub>10</sub> ClFN <sub>2</sub> O <sub>4</sub>
Ramatroban	Antithrombotic	116649-85-5	Y	C <sub>21</sub> H <sub>21</sub> FN <sub>2</sub> O <sub>4</sub> S
Ramciclane	Antihypotensive	96743-96-3		C <sub>21</sub> H <sub>33</sub> NO
Ramelteon	Anxiolytic	196597-26-9	Y	C <sub>16</sub> H <sub>21</sub> NO <sub>2</sub>
Ramifenazone	Analgesic	3615-24-5		C <sub>14</sub> H <sub>19</sub> N <sub>3</sub> O
Ramipril	Antihypertensive	87333-19-5	Y	C <sub>23</sub> H <sub>32</sub> N <sub>2</sub> O <sub>5</sub>
Ramiprilat	Antihypertensive	87269-97-4	Y	C <sub>21</sub> H <sub>28</sub> N <sub>2</sub> O <sub>5</sub>
Ramixotidine	Antilucerative	84071-15-8		C <sub>16</sub> H <sub>21</sub> N <sub>3</sub> O <sub>3</sub> S
Ramnodigin	Cardiotonic	33156-28-4		C <sub>29</sub> H <sub>44</sub> O <sub>6</sub>
Ramosetron	Antidepressant	132036-88-5	Y	C <sub>17</sub> H <sub>17</sub> N <sub>3</sub> O
Ranelic Acid	Bone Resorption Inhibitor	135459-90-4		C <sub>12</sub> H <sub>10</sub> N <sub>2</sub> O <sub>8</sub> S
Ranimustine	Antineoplastic	58994-96-0		C <sub>10</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>7</sub>
Ranirestat	Antidiabetic	147254-64-6	Y	C <sub>17</sub> H <sub>11</sub> BrFN <sub>3</sub> O <sub>4</sub>
Ranitidine	Antilucerative	66357-35-5	Y	C <sub>13</sub> H <sub>22</sub> N <sub>4</sub> O <sub>3</sub> S
Ranolazine	Antianginal	95635-55-5	Y	C <sub>24</sub> H <sub>33</sub> N <sub>3</sub> O <sub>4</sub>
Rapacuronium	Neuromuscular Blocking Agent	465499-11-0		C <sub>37</sub> H <sub>61</sub> N <sub>2</sub> O <sub>4</sub>
Rasagiline Mesylate	Antiparkinsonian	136236-51-6	Y	C <sub>12</sub> H <sub>13</sub> N
Rathyronine	Thyroid	3130-96-9		C <sub>15</sub> H <sub>12</sub> I <sub>3</sub> NO <sub>4</sub>
Ravuconazole	Antifungal	182760-06-1		C <sub>22</sub> H <sub>17</sub> F <sub>2</sub> N <sub>5</sub> OS
Raxofelast	Hepatic Protectant	128232-14-4		C <sub>15</sub> H <sub>18</sub> O <sub>5</sub>
Razaxaban	Anticoagulant	218298-21-6		C <sub>24</sub> H <sub>20</sub> F <sub>4</sub> N <sub>8</sub> O <sub>2</sub>
Razindolil	Cardiotonic	30271-85-3		C <sub>27</sub> H <sub>34</sub> N <sub>4</sub> O <sub>10</sub>
Razobazam	Anxiolytic	78466-98-5		C <sub>14</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub>
Razoxane	Antianginal	21416-67-1		C <sub>11</sub> H <sub>16</sub> N <sub>4</sub> O <sub>4</sub>
Rebamipide	Antilucerative	90098-04-7	Y	C <sub>19</sub> H <sub>15</sub> ClN <sub>2</sub> O <sub>4</sub>
Rebimastat	Antineoplastic	259188-38-0		C <sub>23</sub> H <sub>41</sub> N <sub>5</sub> O <sub>5</sub> S
Reboxetine	Antidepressant	71620-89-8	Y	C <sub>19</sub> H <sub>23</sub> NO <sub>3</sub>
Recainam	Antiarrhythmic	74738-24-2		C <sub>15</sub> H <sub>25</sub> N <sub>3</sub> O
Reclazepam	Sedative	76053-16-2		C <sub>18</sub> H <sub>13</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>2</sub>
Regadenoson	Vasodilator	313348-27-5		C <sub>15</sub> H <sub>18</sub> N <sub>8</sub> O <sub>5</sub>
Reglitazar	Antidiabetic	170861-63-9		C <sub>22</sub> H <sub>20</sub> N <sub>2</sub> O <sub>5</sub>
Relcovaptan	Antihypertensive	150375-75-0		C <sub>28</sub> H <sub>27</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>7</sub> S
Relomycin	Antibacterial	1404-48-4		C <sub>46</sub> H <sub>79</sub> NO <sub>17</sub>
Remacemide	Anticonvulsant	128298-28-2		C <sub>17</sub> H <sub>20</sub> N <sub>2</sub> O
Remifentanyl	Analgesic	132875-61-7		C <sub>20</sub> H <sub>28</sub> N <sub>2</sub> O <sub>5</sub>
Remikiren	Antihypertensive	126222-34-2		C <sub>33</sub> H <sub>50</sub> N <sub>4</sub> O <sub>6</sub> S
Remiprostol	Antilucerative	110845-89-1		C <sub>25</sub> H <sub>36</sub> O <sub>5</sub>
Remoxipride	Antipsychotic	80125-14-0	Y	C <sub>16</sub> H <sub>23</sub> BrN <sub>2</sub> O <sub>3</sub>
Renanolone	Antiinflammatory	565-99-1		C <sub>21</sub> H <sub>32</sub> O <sub>3</sub>
Rentiapril	Antihypertensive	80830-42-8		C <sub>13</sub> H <sub>15</sub> NO <sub>4</sub> S <sub>2</sub>
Renzapride	Gastroprokinetic	112727-80-7		C <sub>16</sub> H <sub>22</sub> ClN <sub>3</sub> O <sub>2</sub>
Repagermanium	Immunomodulator	12758-40-6		C <sub>6</sub> H <sub>10</sub> Ge <sub>2</sub> O <sub>7</sub>
Repaglinide	Antidiabetic	135062-02-1	Y	C <sub>27</sub> H <sub>36</sub> N <sub>2</sub> O <sub>4</sub>
Reparixin	Analgesic	266359-83-5	Y	C <sub>14</sub> H <sub>21</sub> NO <sub>3</sub> S
Repinotan	Nootropic	144980-29-0		C <sub>21</sub> H <sub>24</sub> N <sub>2</sub> O <sub>4</sub> S
Repirinast	Antihistaminic	73080-51-0		C <sub>20</sub> H <sub>21</sub> NO <sub>5</sub>
Repromicin	Antibacterial	56689-42-0		C <sub>31</sub> H <sub>51</sub> NO <sub>8</sub>
Reproterol	Bronchodilator	54063-54-6		C <sub>18</sub> H <sub>23</sub> N <sub>5</sub> O <sub>5</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Rescimetol	Antihypertensive	73573-42-9		C <sub>33</sub> H <sub>38</sub> N <sub>2</sub> O <sub>8</sub>
Rescinamine	Antihypertensive	24815-24-5		C <sub>35</sub> H <sub>42</sub> N <sub>2</sub> O <sub>9</sub>
Reserpine	Antihypertensive	50-55-5		C <sub>33</sub> H <sub>40</sub> N <sub>2</sub> O <sub>9</sub>
Resiquimod	Antiviral	144875-48-9		C <sub>17</sub> H <sub>22</sub> N <sub>4</sub> O <sub>2</sub>
Resocortol Butyrate	Antiinflammatory	76738-96-0		C <sub>26</sub> H <sub>38</sub> O <sub>5</sub>
Resorantel	Anthelmintic	20788-07-2		C <sub>13</sub> H <sub>10</sub> BrNO <sub>3</sub>
Resorcin Brown	Anthelmintic	30282-44-1		C <sub>20</sub> H <sub>18</sub> N <sub>4</sub> O <sub>5</sub> S
Retapamulin	Antibiotic	224452-66-8		C <sub>30</sub> H <sub>47</sub> NO <sub>4</sub> S
Retelliptine	Antineoplastic	72238-02-9		C <sub>25</sub> H <sub>32</sub> N <sub>4</sub> O
Retigabine	Anticonvulsant	150812-12-7	Y	C <sub>16</sub> H <sub>18</sub> FN <sub>3</sub> O <sub>2</sub>
Revaprazan	Antiulcerative	199463-33-7	Y	C <sub>22</sub> H <sub>23</sub> FN <sub>4</sub>
Revatropate	Bronchodilator	149926-91-0		C <sub>19</sub> H <sub>27</sub> NO <sub>4</sub> S
Revenast	Bronchodilator	85673-87-6		C <sub>27</sub> H <sub>29</sub> N <sub>5</sub> O
Revizinone	Cardiotonic	133718-29-3		C <sub>26</sub> H <sub>29</sub> N <sub>5</sub> O <sub>3</sub>
Revospirone	Anxiolytic	95847-87-3		C <sub>18</sub> H <sub>21</sub> N <sub>5</sub> O <sub>3</sub> S
Ribavirin	Antiviral	36791-04-5	Y	C <sub>8</sub> H <sub>12</sub> N <sub>4</sub> O <sub>5</sub>
Riboprine	Antineoplastic	7724-76-7		C <sub>15</sub> H <sub>21</sub> N <sub>5</sub> O <sub>4</sub>
Ribostamycin	Antibiotic	25546-65-0		C <sub>17</sub> H <sub>34</sub> N <sub>4</sub> O <sub>10</sub>
Ricasetron	Antiemetic	117086-68-7		C <sub>19</sub> H <sub>27</sub> N <sub>3</sub> O
Ricinolsulfuric Acid	Unclassified	36634-48-7		C <sub>18</sub> H <sub>34</sub> O <sub>6</sub> S
Ridazolol	Antihypertensive	83395-21-5		C <sub>15</sub> H <sub>18</sub> Cl <sub>2</sub> N <sub>4</sub> O <sub>3</sub>
Ridogrel	Antithrombotic	110140-89-1		C <sub>18</sub> H <sub>17</sub> F <sub>3</sub> N <sub>2</sub> O <sub>3</sub>
Rifabutin	Antibacterial	72559-06-9	Y	C <sub>46</sub> H <sub>62</sub> N <sub>4</sub> O <sub>11</sub>
Rifalazil	Antibacterial	129791-92-0	Y	C <sub>51</sub> H <sub>64</sub> N <sub>4</sub> O <sub>13</sub>
Rifametane	Antibacterial	94168-98-6		C <sub>44</sub> H <sub>60</sub> N <sub>4</sub> O <sub>12</sub>
Rifamexil	Antibacterial	113102-19-5		C <sub>42</sub> H <sub>55</sub> N <sub>3</sub> O <sub>11</sub> S
Rifamide	Antibacterial	2750-76-7		C <sub>43</sub> H <sub>58</sub> N <sub>2</sub> O <sub>13</sub>
Rifampin	Antibacterial	13292-46-1		C <sub>43</sub> H <sub>58</sub> N <sub>4</sub> O <sub>12</sub>
Rifamycin	Antibiotic	6998-60-3	Y	C <sub>37</sub> H <sub>47</sub> NO <sub>12</sub>
Rifapentine	Antibacterial	61379-65-5	Y	C <sub>47</sub> H <sub>64</sub> N <sub>4</sub> O <sub>12</sub>
Rifaximin	Antibacterial	80621-81-4	Y	C <sub>43</sub> H <sub>51</sub> N <sub>3</sub> O <sub>11</sub>
Rilapine	Antipsychotic	79781-95-6		C <sub>22</sub> H <sub>20</sub> ClN <sub>3</sub>
Rilapladib	Antihyperlipidemic	412950-08-4	Y	C <sub>40</sub> H <sub>38</sub> F <sub>5</sub> N <sub>3</sub> O <sub>5</sub> S
Rilmakalim	Antihypertensive	132014-21-2		C <sub>21</sub> H <sub>23</sub> NO <sub>5</sub> S
Rilmazafone	Sedative	99593-25-6	Y	C <sub>21</sub> H <sub>20</sub> Cl <sub>2</sub> N <sub>6</sub> O <sub>3</sub>
Rilmenidine	Antihypertensive	54187-04-1	Y	C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O
Rilopirox	Antifungal	104153-37-9		C <sub>19</sub> H <sub>16</sub> ClNO <sub>4</sub>
Rilozarone	Antiarrhythmic	79282-39-6		C <sub>32</sub> H <sub>36</sub> BrClN <sub>2</sub> O <sub>2</sub>
Rilpivirine	Antiviral	500287-72-9	Y	C <sub>22</sub> H <sub>18</sub> N <sub>6</sub>
Riluzole	Nootropic	1744-22-5	Y	C <sub>8</sub> H <sub>5</sub> F <sub>3</sub> N <sub>2</sub> OS
Rimacalib	Unclassified	215174-50-8		C <sub>22</sub> H <sub>23</sub> FN <sub>4</sub> O <sub>2</sub>
Rimantadine	Antiviral	13392-28-4	Y	C <sub>12</sub> H <sub>21</sub> N
Rimazolium Metilsulfate	Analgesic	28610-84-6		C <sub>13</sub> H <sub>19</sub> N <sub>2</sub> O <sub>3</sub> ·CH <sub>3</sub> O <sub>4</sub> S
Rimcazole	Antipsychotic	75859-04-0		C <sub>21</sub> H <sub>27</sub> N <sub>3</sub>
Rimeporide	Cardiotonic	187870-78-6		C <sub>11</sub> H <sub>15</sub> N <sub>3</sub> O <sub>5</sub> S <sub>2</sub>
Rimexolone	Antiinflammatory	49697-38-3		C <sub>24</sub> H <sub>34</sub> O <sub>3</sub>
Rimiterol	Bronchodilator	32953-89-2		C <sub>12</sub> H <sub>17</sub> NO <sub>3</sub>
Rimonabant	Antiobesity	168273-06-1		C <sub>22</sub> H <sub>21</sub> Cl <sub>3</sub> N <sub>4</sub> O
Rimoprogin	Antibiotic	37750-83-7		C <sub>8</sub> H <sub>7</sub> IN <sub>2</sub> OS
Riodipine	Antiarrhythmic	71653-63-9		C <sub>18</sub> H <sub>19</sub> F <sub>2</sub> NO <sub>5</sub>
Rioprostil	Antiulcerative	77287-05-9		C <sub>21</sub> H <sub>38</sub> O <sub>4</sub>
Ripazepam	Anxiolytic	26308-28-1		C <sub>15</sub> H <sub>16</sub> N <sub>4</sub> O
Ripisartan	Antihypertensive	148504-51-2		C <sub>23</sub> H <sub>22</sub> N <sub>6</sub> O
Risarestat	Antidiabetic	79714-31-1		C <sub>16</sub> H <sub>21</sub> NO <sub>4</sub> S
Risedronic Acid	Bone Resorption Inhibitor	105462-24-6		C <sub>7</sub> H <sub>11</sub> NO <sub>7</sub> P <sub>2</sub>
Risocaine	Anesthetic	94-12-2		C <sub>10</sub> H <sub>13</sub> NO <sub>2</sub>
Risotilide	Antiarrhythmic	120688-08-6		C <sub>15</sub> H <sub>27</sub> N <sub>3</sub> O <sub>4</sub> S <sub>2</sub>
Rispenzepine	Bronchodilator	96449-05-7		C <sub>19</sub> H <sub>20</sub> N <sub>4</sub> O <sub>2</sub>
Risperidone	Antipsychotic	106266-06-2	Y	C <sub>23</sub> H <sub>27</sub> FN <sub>4</sub> O <sub>2</sub>
Ristianol Phosphate	Immunomodulator	78092-65-6		C <sub>8</sub> H <sub>11</sub> NOS
Ritanserin	Anxiolytic	87051-43-2		C <sub>27</sub> H <sub>25</sub> F <sub>2</sub> N <sub>3</sub> OS
Ritiometan	Unclassified	34914-39-1		C <sub>7</sub> H <sub>10</sub> O <sub>6</sub> S <sub>3</sub>
Ritipenem	Antibiotic	84845-57-8		C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> O <sub>6</sub> S



Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Ritobegron	Antidiabetic	255734-04-4		C <sub>21</sub> H <sub>27</sub> NO <sub>5</sub>
Ritodrine	Tocolytic	26652-09-5		C <sub>17</sub> H <sub>21</sub> NO <sub>3</sub>
Ritolukast	Bronchodilator	111974-60-8		C <sub>17</sub> H <sub>13</sub> F <sub>3</sub> N <sub>2</sub> O <sub>3</sub> S
Ritonavir	Antiviral	155213-67-5	Y	C <sub>37</sub> H <sub>48</sub> N <sub>6</sub> O <sub>5</sub> S <sub>2</sub>
Ritropirronium Bromide	Neuromuscular Blocking Agent	58493-54-2		C <sub>19</sub> H <sub>28</sub> BrNO <sub>3</sub>
Ritrosulfan	Antineoplastic	4148-16-7		C <sub>10</sub> H <sub>24</sub> N <sub>2</sub> O <sub>8</sub> S <sub>2</sub>
Rivanieline	Nootropic	15585-43-0		C <sub>10</sub> H <sub>14</sub> N <sub>2</sub>
Rivaroxaban	Anticoagulant	366789-02-8	Y	C <sub>19</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>5</sub> S
Rivastigmine	Nootropic	123441-03-2	Y	C <sub>14</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>
Rivenprost	Anticoagulant	256382-08-8		C <sub>24</sub> H <sub>34</sub> O <sub>6</sub> S
Rivoglitazone	Antidiabetic	185428-18-6		C <sub>20</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub> S
Rizatriptan Benzoate	Antimigraine	144034-80-0	Y	C <sub>15</sub> H <sub>19</sub> N <sub>5</sub>
Rizatriptan Benzoate	Antimigraine	65-85-0	Y	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>
Robenacoxib	Antiinflammatory	220991-32-2		C <sub>16</sub> H <sub>13</sub> F <sub>4</sub> NO <sub>2</sub>
Robenidine	Antibiotic	25875-51-8		C <sub>15</sub> H <sub>13</sub> Cl <sub>2</sub> N <sub>5</sub>
Rocastine	Antihistaminic	91833-49-7		C <sub>13</sub> H <sub>19</sub> N <sub>3</sub> OS
Roceprofant	Antithrombotic	132579-32-9		C <sub>26</sub> H <sub>23</sub> ClN <sub>6</sub> O <sub>5</sub> S <sub>2</sub>
Rociclovir	Antiviral	108436-80-2		C <sub>15</sub> H <sub>25</sub> N <sub>5</sub> O <sub>3</sub>
Rociverine	Antispasmodic	53716-44-2		C <sub>20</sub> H <sub>37</sub> NO <sub>3</sub>
Rocuronium	Neuromuscular Blocking Agent	143558-00-3		C <sub>32</sub> H <sub>53</sub> N <sub>2</sub> O <sub>4</sub>
Rodocaine	Anesthetic	38821-80-6		C <sub>18</sub> H <sub>25</sub> ClN <sub>2</sub> O
Rodorbucicin	Antineoplastic	96497-67-5		C <sub>48</sub> H <sub>64</sub> N <sub>2</sub> O <sub>17</sub>
Rofecoxib	Antiinflammatory	162011-90-7		C <sub>17</sub> H <sub>14</sub> O <sub>4</sub> S
Rofelodine	Muscle Relaxant	76696-97-4		C <sub>13</sub> H <sub>14</sub> N <sub>2</sub> O
Rofleponide	Steroid	144459-70-1		C <sub>25</sub> H <sub>34</sub> F <sub>2</sub> O <sub>6</sub>
Roflumilast	Bronchodilator	162401-32-3	Y	C <sub>17</sub> H <sub>14</sub> Cl <sub>2</sub> F <sub>2</sub> N <sub>2</sub> O <sub>3</sub>
Roflurane	Anesthetic	679-90-3		C <sub>3</sub> H <sub>4</sub> BrF <sub>3</sub> O
Rogletimide	Antineoplastic	92788-10-8		C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Rokitamycin	Antibiotic	74014-51-0		C <sub>42</sub> H <sub>69</sub> NO <sub>15</sub>
Rolafagrel	Antithrombotic	89781-55-5		C <sub>14</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>
Roletamide	Sedative	10078-46-3		C <sub>16</sub> H <sub>19</sub> NO <sub>4</sub>
Rolgamidine	Antidiarrheal	66608-04-6		C <sub>9</sub> H <sub>16</sub> N <sub>4</sub> O
Rolicyclidine	Cholinergic	2201-39-0		C <sub>16</sub> H <sub>23</sub> N
Rolicyprine	Antidepressant	2829-19-8		C <sub>14</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>
Rolipram	Antidepressant	61413-54-5		C <sub>16</sub> H <sub>21</sub> NO <sub>3</sub>
Rolitetracycline	Antibiotic	751-97-3		C <sub>27</sub> H <sub>33</sub> N <sub>3</sub> O <sub>8</sub>
Rolodine	Muscle Relaxant	1866-43-9		C <sub>14</sub> H <sub>14</sub> N <sub>4</sub>
Rolziracetam	Nootropic	18356-28-0		C <sub>7</sub> H <sub>9</sub> NO <sub>2</sub>
Romazarit	Antiinflammatory	109543-76-2	Y	C <sub>15</sub> H <sub>16</sub> ClNO <sub>4</sub>
Romergoline	Antiparkinsonian	107052-56-2		C <sub>20</sub> H <sub>22</sub> N <sub>4</sub> O <sub>2</sub>
Romifenone	Antiarrhythmic	38373-83-0		C <sub>13</sub> H <sub>17</sub> NO <sub>3</sub>
Romifidine	Sedative	65896-16-4		C <sub>9</sub> H <sub>9</sub> BrFN <sub>3</sub>
Romurtide	Immunomodulator	78113-36-7		C <sub>43</sub> H <sub>78</sub> N <sub>6</sub> O <sub>13</sub>
Ronactolol	Antiarrhythmic	90895-85-5		C <sub>20</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub>
Ronidazole	Antiprotozoal	7681-76-7		C <sub>6</sub> H <sub>8</sub> N <sub>4</sub> O <sub>4</sub>
Ronifibrate	Antihyperlipidemic	42597-57-9	Y	C <sub>19</sub> H <sub>20</sub> ClNO <sub>5</sub>
Ronipamil	Vasodilator	85247-77-4		C <sub>32</sub> H <sub>48</sub> N <sub>2</sub>
Ropinirole	Antiparkinsonian	91374-21-9	Y	C <sub>16</sub> H <sub>24</sub> N <sub>2</sub> O
Ropitoin	Antiarrhythmic	56079-81-3		C <sub>30</sub> H <sub>33</sub> N <sub>3</sub> O <sub>3</sub>
Ropivacaine	Anesthetic	84057-95-4		C <sub>17</sub> H <sub>26</sub> N <sub>2</sub> O
Ropizine	Anticonvulsant	3601-19-2		C <sub>24</sub> H <sub>26</sub> N <sub>4</sub>
Roquinimex	Immunomodulator	84088-42-6		C <sub>18</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>
Rosaprostol	Ant ulcerative	56695-65-9		C <sub>18</sub> H <sub>34</sub> O <sub>3</sub>
Rosaramicin	Antibacterial	35834-26-5		C <sub>31</sub> H <sub>51</sub> NO <sub>9</sub>
Rosiglitazone	Antidiabetic	122320-73-4	Y	C <sub>18</sub> H <sub>19</sub> N <sub>3</sub> O <sub>5</sub> S
Rosoxacin	Antibacterial	40034-42-2		C <sub>17</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>
Rostafuroxin	Antihypertensive	156722-18-8	Y	C <sub>23</sub> H <sub>34</sub> O <sub>4</sub>
Rostaporfin	Ophthalmic	284041-10-7		C <sub>37</sub> H <sub>42</sub> Cl <sub>2</sub> N <sub>4</sub> O <sub>2</sub> Sn
Rosterolone	Androgen	79243-67-7		C <sub>23</sub> H <sub>38</sub> O <sub>2</sub>
Rosuvastatin	Antihyperlipidemic	287714-41-4	Y	C <sub>22</sub> H <sub>28</sub> FN <sub>3</sub> O <sub>6</sub> S
Rotamicillin	Antibiotic	55530-41-1		C <sub>28</sub> H <sub>31</sub> N <sub>5</sub> O <sub>5</sub> S

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Rotenone	Antibacterial	83-79-4		C <sub>23</sub> H <sub>22</sub> O <sub>6</sub>
Rotigaptide	Antiarrhythmic	355151-12-1		C <sub>28</sub> H <sub>39</sub> N <sub>7</sub> O <sub>9</sub>
Rotigotine	Antiparkinsonian	99755-59-6		C <sub>19</sub> H <sub>25</sub> NOS
Rotoxamine	Antihistaminic	5560-77-0		C <sub>16</sub> H <sub>19</sub> ClN <sub>2</sub> O
Rotraxate	Antiuclerative	92071-51-7		C <sub>17</sub> H <sub>23</sub> NO <sub>3</sub>
Roxadimate	Dermatologic	58882-17-0		C <sub>15</sub> H <sub>23</sub> NO <sub>4</sub>
Roxarsone	Antibacterial	121-19-7		C <sub>6</sub> H <sub>6</sub> AsNO <sub>6</sub>
Roxatidine Acetate	Antiuclerative	78628-28-1		C <sub>19</sub> H <sub>28</sub> N <sub>2</sub> O <sub>4</sub>
Roxibolone	Steroid	60023-92-9		C <sub>21</sub> H <sub>28</sub> O <sub>5</sub>
Roxifiban Acetate	Antithrombotic	170902-47-3		C <sub>21</sub> H <sub>29</sub> N <sub>5</sub> O <sub>6</sub>
Roxindole	Antidepressant	112192-04-8		C <sub>23</sub> H <sub>26</sub> N <sub>2</sub> O
Roxithromycin	Antibiotic	80214-83-1	Y	C <sub>41</sub> H <sub>76</sub> N <sub>2</sub> O <sub>15</sub>
Roxolonium Metilsulfate	Antihypertensive	53862-80-9		C <sub>38</sub> H <sub>63</sub> NO <sub>8</sub> S
Roxoperone	Antipsychotic	2804-00-4		C <sub>19</sub> H <sub>23</sub> FN <sub>2</sub> O <sub>3</sub>
Rubitecan	Antineoplastic	91421-42-0		C <sub>20</sub> H <sub>15</sub> N <sub>3</sub> O <sub>6</sub>
Ruboxistaurin	Antineoplastic	169939-94-0		C <sub>28</sub> H <sub>28</sub> N <sub>4</sub> O <sub>3</sub>
Rufinamide	Anticonvulsant	106308-44-5	Y	C <sub>10</sub> H <sub>8</sub> F <sub>2</sub> N <sub>4</sub> O
Rufloxacin	Antibiotic	101363-10-4	Y	C <sub>17</sub> H <sub>18</sub> FN <sub>3</sub> O <sub>3</sub> S
Rupatadine	Antihistaminic	158876-82-5	Y	C <sub>26</sub> H <sub>26</sub> ClN <sub>3</sub>
Rupintrivir	Antiviral	223537-30-2		C <sub>31</sub> H <sub>39</sub> FN <sub>4</sub> O <sub>7</sub>
Rutamycin	Antifungal	1404-59-7		C <sub>44</sub> H <sub>72</sub> O <sub>11</sub>
Rutin	Capillary Protectant	153-18-4		C <sub>27</sub> H <sub>30</sub> O <sub>16</sub>
Ruvazone	Analgesic	20228-27-7		C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub>
Ruzadolane	Unclassified	115762-17-9		C <sub>18</sub> H <sub>19</sub> F <sub>2</sub> N <sub>5</sub> S
Sabarubicin	Antineoplastic	211100-13-9		C <sub>32</sub> H <sub>37</sub> NO <sub>13</sub>
Sabcomeline	Nootropic	159912-53-5		C <sub>10</sub> H <sub>15</sub> N <sub>3</sub> O
Sabeluzole	Anticonvulsant	104383-17-7		C <sub>22</sub> H <sub>26</sub> FN <sub>3</sub> O <sub>2</sub> S
Sabiporide	Cardiotonic	261505-80-0		C <sub>18</sub> H <sub>19</sub> F <sub>3</sub> N <sub>6</sub> O <sub>2</sub>
Safinamide	Diuretic	133865-89-1	Y	C <sub>17</sub> H <sub>19</sub> FN <sub>2</sub> O <sub>2</sub>
Safingol	Antineoplastic	15639-50-6		C <sub>18</sub> H <sub>39</sub> NO <sub>2</sub>
Safironil	Dermatologic	134377-69-8		C <sub>15</sub> H <sub>23</sub> N <sub>3</sub> O <sub>4</sub>
Safrazine	Antipsychotic	33419-68-0		C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>
Sagandipine	Antihypertensive	126294-30-2		C <sub>27</sub> H <sub>31</sub> FN <sub>2</sub> O <sub>5</sub>
Salacetamide	Analgesic	487-48-9		C <sub>9</sub> H <sub>9</sub> NO <sub>3</sub>
Salafibrate	Antihyperlipidemic	64496-66-8		C <sub>32</sub> H <sub>32</sub> Cl <sub>2</sub> O <sub>10</sub>
Salantel	Anthelmintic	36093-47-7		C <sub>20</sub> H <sub>11</sub> Cl <sub>2</sub> I <sub>2</sub> NO <sub>3</sub>
Salazodine	Antihypertensive	22933-72-8		C <sub>18</sub> H <sub>15</sub> N <sub>5</sub> O <sub>6</sub> S
Salazosulfadimidine	Antibiotic	2315-08-4		C <sub>19</sub> H <sub>17</sub> N <sub>5</sub> O <sub>5</sub> S
Salazosulfamide	Antibiotic	139-56-0		C <sub>13</sub> H <sub>11</sub> N <sub>3</sub> O <sub>5</sub> S
Salazosulfthiazole	Antibiotic	515-58-2		C <sub>16</sub> H <sub>12</sub> N <sub>4</sub> O <sub>5</sub> S <sub>2</sub>
Salcaproic Acid	Unclassified	183990-46-7		C <sub>15</sub> H <sub>21</sub> NO <sub>4</sub>
Salclobuzic Acid	Unclassified	387825-03-8		C <sub>11</sub> H <sub>12</sub> ClNO <sub>4</sub>
Salcolex	Analgesic	2016-36-6		C <sub>7</sub> H <sub>5</sub> O <sub>3</sub> .C <sub>5</sub> H <sub>14</sub> NO
Salethamide Maleate	Analgesic	46803-81-0		C <sub>13</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>
Salfluverine	Antispasmodic	587-49-5		C <sub>14</sub> H <sub>10</sub> F <sub>3</sub> NO <sub>2</sub>
Salicin	Analgesic	138-52-3		C <sub>13</sub> H <sub>18</sub> O <sub>7</sub>
Salicyl Alcohol	Anesthetic	90-01-7		C <sub>7</sub> H <sub>8</sub> O <sub>2</sub>
Salicylamide	Analgesic	65-45-2		C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub>
Salicylanilide	Antifungal	87-17-2		C <sub>13</sub> H <sub>11</sub> NO <sub>2</sub>
Salicylic Acid	Dermatologic	69-72-7	Y	C <sub>7</sub> H <sub>6</sub> O <sub>3</sub>
Salicylic Anhydride Diacetate	Antiinflammatory	1466-82-6		C <sub>18</sub> H <sub>14</sub> O <sub>7</sub>
Salicylic Acid	Antiinflammatory	487-54-7		C <sub>9</sub> H <sub>9</sub> NO <sub>4</sub>
Salinazid	Antibiotic	495-84-1		C <sub>13</sub> H <sub>11</sub> N <sub>3</sub> O <sub>2</sub>
Salinomycin	Antibiotic	53003-10-4		C <sub>42</sub> H <sub>70</sub> O <sub>11</sub>
Salmefamol	Bronchodilator	18910-65-1		C <sub>19</sub> H <sub>25</sub> NO <sub>4</sub>
Salmeterol	Bronchodilator	89365-50-4		C <sub>25</sub> H <sub>37</sub> NO <sub>4</sub>
Salmeterol Xinafoate	Bronchodilator	86-48-6		C <sub>11</sub> H <sub>8</sub> O <sub>3</sub>
Salmisteine	Mucolytic	89767-59-9		C <sub>14</sub> H <sub>15</sub> NO <sub>6</sub> S
Salnacedin	Antiinflammatory	87573-01-1		C <sub>12</sub> H <sub>13</sub> NO <sub>5</sub> S
Salprotoside	Cardiotonic	33779-37-2		C <sub>25</sub> H <sub>30</sub> O <sub>10</sub>
Salsalate	Analgesic	552-94-3	Y	C <sub>14</sub> H <sub>10</sub> O <sub>5</sub>
Salverine	Analgesic	6376-26-7		C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub>
Sameridine	Anesthetic	143257-97-0		C <sub>21</sub> H <sub>34</sub> N <sub>2</sub> O

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Samixogrel	Antithrombotic	133276-80-9		C <sub>25</sub> H <sub>25</sub> ClN <sub>2</sub> O <sub>4</sub> S
Sampatrilat	Antihypertensive	129981-36-8		C <sub>26</sub> H <sub>40</sub> N <sub>4</sub> O <sub>5</sub> S
Sampirtine	Analgesic	115911-28-9		C <sub>12</sub> H <sub>12</sub> FN <sub>3</sub>
Sancycline	Antibacterial	808-26-4		C <sub>21</sub> H <sub>22</sub> N <sub>2</sub> O <sub>7</sub>
Sanfetrinem Cilexetil	Antibacterial	141646-08-4		C <sub>23</sub> H <sub>33</sub> NO <sub>8</sub>
Sanfetrinem Sodium	Antibacterial	156769-21-0		C <sub>14</sub> H <sub>19</sub> NO <sub>5</sub>
Santonin	Anthelmintic	481-06-1		C <sub>15</sub> H <sub>18</sub> O <sub>3</sub>
Saperconazole	Antifungal	110588-57-3		C <sub>35</sub> H <sub>38</sub> F <sub>2</sub> N <sub>8</sub> O <sub>4</sub>
Saprisartan Potassium	Antihypertensive	146623-69-0		C <sub>25</sub> H <sub>22</sub> BrF <sub>3</sub> N <sub>4</sub> O <sub>4</sub> S
Saquinavir	Antiviral	127779-20-8	Y	C <sub>38</sub> H <sub>50</sub> N <sub>6</sub> O <sub>5</sub>
Sarafloxacin	Antibiotic	98105-99-8	Y	C <sub>20</sub> H <sub>17</sub> F <sub>2</sub> N <sub>3</sub> O <sub>3</sub>
Sarakalim	Antihypertensive	148430-28-8		C <sub>20</sub> H <sub>19</sub> F <sub>3</sub> N <sub>2</sub> O <sub>4</sub>
Saralasin	Antihypertensive	34273-10-4		C <sub>42</sub> H <sub>65</sub> N <sub>13</sub> O <sub>10</sub>
Sarcolysin	Antineoplastic	531-76-0		C <sub>13</sub> H <sub>18</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Sardomozide	Antipsychotic	149400-88-4		C <sub>11</sub> H <sub>14</sub> N <sub>6</sub>
Saredutant	Bronchodilator	142001-63-6		C <sub>31</sub> H <sub>35</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>2</sub>
Saripidem	Sedative	103844-86-6		C <sub>19</sub> H <sub>20</sub> ClN <sub>3</sub> O
Sarizotan	Antiparkinsonian	351862-32-3		C <sub>22</sub> H <sub>21</sub> FN <sub>2</sub> O
Sarmazenil	Anxiolytic	78771-13-8		C <sub>15</sub> H <sub>14</sub> ClN <sub>3</sub> O <sub>3</sub>
Sarmoxicillin	Antibacterial	67337-44-4		C <sub>21</sub> H <sub>27</sub> N <sub>3</sub> O <sub>5</sub> S
Sarpicillin	Antibacterial	40966-79-8		C <sub>21</sub> H <sub>27</sub> N <sub>3</sub> O <sub>5</sub> S
Sarpogrelate	Antithrombotic	125926-17-2		C <sub>24</sub> H <sub>31</sub> NO <sub>6</sub>
Satavaptan	Hepatoprotectant	185913-78-4		C <sub>33</sub> H <sub>45</sub> N <sub>3</sub> O <sub>8</sub> S
Saterinone	Cardiotonic	102669-89-6		C <sub>27</sub> H <sub>30</sub> N <sub>4</sub> O <sub>4</sub>
Satigrel	Antithrombotic	111753-73-2		C <sub>20</sub> H <sub>19</sub> NO <sub>4</sub>
Satranidazole	Antiamoebic	56302-13-7		C <sub>8</sub> H <sub>11</sub> N <sub>5</sub> O <sub>5</sub> S
Saviprazole	Antiulcerative	121617-11-6		C <sub>15</sub> H <sub>10</sub> F <sub>7</sub> N <sub>3</sub> O <sub>2</sub> S <sub>2</sub>
Savoxepin	Antidepressant	79262-46-7		C <sub>25</sub> H <sub>26</sub> N <sub>2</sub> O
Saxagliptin	Antidiabetic	361442-04-8		C <sub>18</sub> H <sub>25</sub> N <sub>3</sub> O <sub>2</sub>
Scopinast	Antihistamine	145574-90-9		C <sub>31</sub> H <sub>31</sub> F <sub>2</sub> NO <sub>5</sub>
Scopolamine	Antispasmodic	51-34-3		C <sub>17</sub> H <sub>21</sub> NO <sub>4</sub>
Secalciferol	Steroid	55721-11-4		C <sub>27</sub> H <sub>44</sub> O <sub>3</sub>
Seclazone	Antiinflammatory	29050-11-1		C <sub>10</sub> H <sub>8</sub> ClNO <sub>3</sub>
Secnidazole	Antiamoebic	3366-95-8	Y	C <sub>7</sub> H <sub>11</sub> N <sub>3</sub> O <sub>3</sub>
Secobarbital	Sedative	76-73-3	Y	C <sub>12</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>
Secoverine	Antispasmodic	57558-44-8		C <sub>22</sub> H <sub>35</sub> NO <sub>2</sub>
Sedecamycin	Antibacterial	23477-98-7		C <sub>27</sub> H <sub>35</sub> NO <sub>8</sub>
Seganserlin	Antidepressant	87729-89-3		C <sub>29</sub> H <sub>27</sub> F <sub>2</sub> N <sub>3</sub> O
Segesterone	Progestogen	7690-08-6		C <sub>21</sub> H <sub>28</sub> O <sub>3</sub>
Seglitide	Antidiabetic	81377-02-8		C <sub>44</sub> H <sub>56</sub> N <sub>8</sub> O <sub>7</sub>
Selamectin	Anthelmintic	220119-17-5		C <sub>43</sub> H <sub>63</sub> NO <sub>11</sub>
Selegiline	Antiparkinsonian	14611-51-9	Y	C <sub>13</sub> H <sub>17</sub> N
Seletracetam	Anticonvulsant	357336-74-4		C <sub>10</sub> H <sub>14</sub> F <sub>2</sub> N <sub>2</sub> O
Selfotel	Antipsychotic	110347-85-8		C <sub>7</sub> H <sub>14</sub> NO <sub>5</sub> P
Seliciclib	Antineoplastic	186692-46-6	Y	C <sub>19</sub> H <sub>26</sub> N <sub>6</sub> O
Selodenson	Antiarrhythmic	110299-05-3		C <sub>17</sub> H <sub>24</sub> N <sub>6</sub> O <sub>4</sub>
Selprazine	Antipsychotic	103997-59-7		C <sub>24</sub> H <sub>31</sub> N <sub>3</sub> O <sub>3</sub>
Semapimod	Antiinflammatory	352513-83-8	Y	C <sub>34</sub> H <sub>52</sub> N <sub>18</sub> O <sub>2</sub>
Sematilide	Antiarrhythmic	101526-83-4		C <sub>14</sub> H <sub>23</sub> N <sub>3</sub> O <sub>3</sub> S
Semaxanib	Antineoplastic	194413-58-6		C <sub>15</sub> H <sub>14</sub> N <sub>2</sub> O
Semduramicin	Antibiotic	113378-31-7		C <sub>45</sub> H <sub>76</sub> O <sub>16</sub>
Semorphone	Analgesic	88939-40-6		C <sub>19</sub> H <sub>23</sub> NO <sub>5</sub>
Semotiadil	Antianginal	116476-13-2		C <sub>29</sub> H <sub>32</sub> N <sub>2</sub> O <sub>6</sub> S
Semustine	Antineoplastic	13909-09-6		C <sub>10</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>2</sub>
Senazodan	Cardiotonic	98326-32-0		C <sub>15</sub> H <sub>14</sub> N <sub>4</sub> O
Seocalcitol	Steroid	134404-52-7		C <sub>30</sub> H <sub>46</sub> O <sub>3</sub>
Seperidol	Antipsychotic	10457-91-7		C <sub>22</sub> H <sub>22</sub> ClF <sub>4</sub> NO <sub>2</sub>
Sepimostat	Anticoagulant	103926-64-3		C <sub>21</sub> H <sub>19</sub> N <sub>5</sub> O <sub>2</sub>
Seprilose	Antirheumatic	133692-55-4		C <sub>16</sub> H <sub>30</sub> O <sub>6</sub>
Seproxtetine	Antidepressant	126924-38-7		C <sub>16</sub> H <sub>16</sub> F <sub>3</sub> NO
Sequifenadine	Antihistaminic	57734-69-7		C <sub>22</sub> H <sub>27</sub> NO
Seratrovast	Antiinflammatory	112665-43-7	Y	C <sub>22</sub> H <sub>26</sub> O <sub>4</sub>
Serazapine	Anxiolytic	115313-22-9		C <sub>22</sub> H <sub>23</sub> N <sub>3</sub> O <sub>2</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Serfibrate	Antihyperlipidemic	54657-98-6		C <sub>16</sub> H <sub>20</sub> ClNO <sub>5</sub> S
Sergolexole Maleate	Antimigraine	108674-86-8		C <sub>26</sub> H <sub>36</sub> N <sub>2</sub> O <sub>3</sub>
Sermetacin	Antiinflammatory	57645-05-3		C <sub>22</sub> H <sub>21</sub> ClN <sub>2</sub> O <sub>6</sub>
Sertaconazole	Antifungal	99592-32-2		C <sub>20</sub> H <sub>15</sub> Cl <sub>3</sub> N <sub>2</sub> O <sub>5</sub> S
Sertindole	Antipsychotic	106516-24-9	Y	C <sub>24</sub> H <sub>26</sub> ClFN <sub>4</sub> O
Sertraline	Antidepressant	79617-96-2	Y	C <sub>17</sub> H <sub>17</sub> Cl <sub>2</sub> N
Setastine	Antihistaminic	64294-95-7	Y	C <sub>22</sub> H <sub>28</sub> ClNO
Setazindol	Antidepressant	28570-99-2		C <sub>15</sub> H <sub>16</sub> ClNO
Setipafant	Antithrombotic	132418-35-0		C <sub>26</sub> H <sub>23</sub> ClN <sub>6</sub> O <sub>2</sub> S
Setiptiline	Antidepressant	57262-94-9		C <sub>19</sub> H <sub>19</sub> N
Setoperone	Antipsychotic	86487-64-1		C <sub>21</sub> H <sub>24</sub> FN <sub>3</sub> O <sub>2</sub> S
Sevotroplum Mesilate	Bronchodilator	88199-75-1		C <sub>24</sub> H <sub>29</sub> NO <sub>5</sub> S <sub>2</sub>
Sevoflurane	Anesthetic	28523-86-6		C <sub>4</sub> H <sub>3</sub> F <sub>7</sub> O
Sevopramide	Antidepressant	57227-17-5		C <sub>29</sub> H <sub>43</sub> N <sub>3</sub> O <sub>3</sub>
Sezolamide	Antiglaucoma	123308-22-5		C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub> S <sub>3</sub>
Sibenaedet	Respiratory Stimulant	154189-40-9		C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> O <sub>5</sub> S <sub>2</sub>
Sibopirdine	Nootropic	122955-18-4		C <sub>23</sub> H <sub>18</sub> N <sub>4</sub>
Sibrafiban	Antithrombotic	172927-65-0		C <sub>20</sub> H <sub>28</sub> N <sub>4</sub> O <sub>6</sub>
Sibutramine	Antiobesity	106650-56-0		C <sub>17</sub> H <sub>26</sub> ClN
Siccanin	Antifungal	22733-60-4		C <sub>22</sub> H <sub>30</sub> O <sub>3</sub>
Sifaprazine	Sedative	131635-06-8		C <sub>18</sub> H <sub>22</sub> N <sub>2</sub>
Siguazodan	Cardiotonic	115344-47-3		C <sub>14</sub> H <sub>16</sub> N <sub>6</sub> O
Silandrone	Androgen	5055-42-5		C <sub>22</sub> H <sub>36</sub> O <sub>2</sub> Si
Sildenafil	Erectile Dysfunction	139755-83-2	Y	C <sub>22</sub> H <sub>30</sub> N <sub>6</sub> O <sub>4</sub> S
Silibinin	Hepatic Protectant	22888-70-6		C <sub>25</sub> H <sub>22</sub> O <sub>10</sub>
Silicristin	Hepatic Protectant	33889-69-9		C <sub>25</sub> H <sub>22</sub> O <sub>10</sub>
Silidianin	Hepatic Protectant	29782-68-1		C <sub>25</sub> H <sub>22</sub> O <sub>10</sub>
Silodosin	Urologic	160970-54-7	Y	C <sub>25</sub> H <sub>32</sub> F <sub>3</sub> N <sub>3</sub> O <sub>4</sub>
Silperisone	Muscle Relaxant	140944-31-6		C <sub>15</sub> H <sub>24</sub> FNSi
Siltenzepine	Anticonvulsant	98374-54-0		C <sub>19</sub> H <sub>20</sub> ClN <sub>3</sub> O <sub>4</sub>
Silver Sulfadiazine	Antibacterial	22199-08-2		C <sub>10</sub> H <sub>9</sub> AgN <sub>4</sub> O <sub>2</sub> S
Simendan	Cardiotonic	131741-08-7		C <sub>14</sub> H <sub>12</sub> N <sub>6</sub> O
Simetride	Analgesic	154-82-5		C <sub>28</sub> H <sub>38</sub> N <sub>2</sub> O <sub>6</sub>
Simfibrate	Antihyperlipidemic	14929-11-4		C <sub>23</sub> H <sub>26</sub> Cl <sub>2</sub> O <sub>6</sub>
Simotaxel	Antineoplastic	791635-59-1		C <sub>46</sub> H <sub>57</sub> NO <sub>15</sub> S
Simtrazene	Antineoplastic	5579-27-1		C <sub>14</sub> H <sub>16</sub> N <sub>4</sub>
Simvastatin	Antihyperlipidemic	79902-63-9	Y	C <sub>25</sub> H <sub>38</sub> O <sub>5</sub>
Sinefungin	Antifungal	58944-73-3		C <sub>15</sub> H <sub>23</sub> N <sub>7</sub> O <sub>5</sub>
Sinitrodil	Antihypertensive	143248-63-9		C <sub>10</sub> H <sub>10</sub> N <sub>2</sub> O <sub>5</sub>
Sintropium Bromide	Antispasmodic	79467-19-9		C <sub>19</sub> H <sub>36</sub> BrNO <sub>2</sub>
Sipatrigine	Anticonvulsant	130800-90-7		C <sub>15</sub> H <sub>16</sub> Cl <sub>3</sub> N <sub>5</sub>
Sipoglitazar	Antidiabetic	342026-92-0		C <sub>25</sub> H <sub>25</sub> N <sub>3</sub> O <sub>4</sub> S
Siramesine	Antipsychotic	147817-50-3		C <sub>30</sub> H <sub>31</sub> FN <sub>2</sub> O
Siratiazem	Antihypertensive	138778-28-6		C <sub>24</sub> H <sub>30</sub> N <sub>2</sub> O <sub>4</sub> S
Sirolimus	Immunosuppressant	53123-88-9	Y	C <sub>51</sub> H <sub>79</sub> NO <sub>13</sub>
Sisomicin	Antibacterial	32385-11-8		C <sub>19</sub> H <sub>37</sub> N <sub>5</sub> O <sub>7</sub>
Sitafloxacin	Antibacterial	127254-12-0	Y	C <sub>19</sub> H <sub>18</sub> ClF <sub>2</sub> N <sub>3</sub> O <sub>3</sub>
Sitalidone	Diuretic	119636-74-7		C <sub>23</sub> H <sub>29</sub> ClN <sub>2</sub> O <sub>5</sub> S
Sitamaquine	Antimalarial	57695-04-2		C <sub>21</sub> H <sub>33</sub> N <sub>3</sub> O
Sitaxentan	Antihypertensive	184036-34-8		C <sub>18</sub> H <sub>15</sub> ClN <sub>2</sub> O <sub>6</sub> S <sub>2</sub>
Sitofibrate	Antihyperlipidemic	55902-94-8		C <sub>39</sub> H <sub>59</sub> ClO <sub>3</sub>
Sitogluside	Unclassified	474-58-8		C <sub>35</sub> H <sub>60</sub> O <sub>6</sub>
Sitosterol	Steroid	83-46-5		C <sub>29</sub> H <sub>50</sub> O
Sivelestat	Respiratory Stimulant	127373-66-4		C <sub>20</sub> H <sub>22</sub> N <sub>2</sub> O <sub>7</sub> S
Soblidotin	Antineoplastic	149606-27-9		C <sub>39</sub> H <sub>67</sub> N <sub>5</sub> O <sub>6</sub>
Sobuzoxane	Antineoplastic	98631-95-9		C <sub>22</sub> H <sub>34</sub> N <sub>4</sub> O <sub>10</sub>
Cacodylate	Anthelminthic	15132-04-4		C <sub>2</sub> H <sub>6</sub> AsO <sub>2</sub>
Dehydroacetate	Choleretic	45990-85-0		C <sub>8</sub> H <sub>7</sub> O <sub>4</sub>
Dibunate	Antitussive	14992-58-6		C <sub>18</sub> H <sub>24</sub> O <sub>3</sub> S
Dichloroacetic Acid	Nootropic	79-43-6		C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub> O <sub>2</sub>
Sodium Ethasulfate	Respiratory Stimulant	72214-01-8		C <sub>8</sub> H <sub>18</sub> O <sub>4</sub> S
Sodium Gentisate	Analgesic	490-79-9		C <sub>7</sub> H <sub>6</sub> O <sub>4</sub>
Gluconate	Plasma Volume Expander	608-59-3		C <sub>6</sub> H <sub>11</sub> O <sub>7</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Glucosulfone	Antibiotic	551-89-3		C <sub>24</sub> H <sub>36</sub> N <sub>2</sub> O <sub>18</sub> S <sub>3</sub>
Gualenate	Antiinflammatory	16915-32-5		C <sub>15</sub> H <sub>18</sub> O <sub>3</sub> S
Hydroxybenzylphosphinate	Unclassified	52705-43-8		C <sub>7</sub> H <sub>9</sub> O <sub>3</sub> P
Monofluorophosphate	Dermatologic	13537-32-1		FH <sub>2</sub> O <sub>3</sub> P
Oxybate	Anesthetic	591-81-1		C <sub>4</sub> H <sub>8</sub> O <sub>3</sub>
Phenylacetate	Antidote	7631-42-7		C <sub>8</sub> H <sub>7</sub> O <sub>2</sub>
Picofosfate	Unclassified	36175-06-1		C <sub>18</sub> H <sub>17</sub> NO <sub>8</sub> P <sub>2</sub>
Picosulfate	Laxative	10040-34-3	Y	C <sub>18</sub> H <sub>15</sub> N <sub>2</sub> O <sub>8</sub> S <sub>2</sub>
Stibocaptate	Antiprotozoal	1986-66-9		C <sub>12</sub> H <sub>12</sub> O <sub>12</sub> S <sub>6</sub> Sb <sub>2</sub>
Stibogluconate	Antiprotozoal	100817-46-7		C <sub>12</sub> H <sub>20</sub> O <sub>17</sub> Sb <sub>2</sub>
Succinate	Respiratory Stimulant	56-14-4	Y	C <sub>4</sub> H <sub>4</sub> O <sub>4</sub>
Sofalcone	Ant ulcerative	64506-49-6		C <sub>27</sub> H <sub>30</sub> O <sub>6</sub>
Solabegron	Antidiabetic	252920-94-8		C <sub>23</sub> H <sub>23</sub> ClN <sub>2</sub> O <sub>3</sub>
Solasulfone	Antibiotic	118-84-3		C <sub>30</sub> H <sub>32</sub> N <sub>2</sub> O <sub>14</sub> S <sub>5</sub>
Solifenacin	Antispasmodic	242478-37-1	Y	C <sub>23</sub> H <sub>26</sub> N <sub>2</sub> O <sub>2</sub>
Solimastat	Antineoplastic	226072-63-5		C <sub>20</sub> H <sub>32</sub> N <sub>4</sub> O <sub>5</sub>
Solpecainol	Antiarrhythmic	155321-96-3		C <sub>18</sub> H <sub>23</sub> NO <sub>3</sub>
Solypertine Tartrate	Antihypertensive	4448-96-8		C <sub>22</sub> H <sub>25</sub> N <sub>3</sub> O <sub>3</sub>
Somantadine	Antiviral	79594-24-4		C <sub>14</sub> H <sub>25</sub> N
Soneclozan	Antibacterial	3380-30-1		C <sub>12</sub> H <sub>8</sub> Cl <sub>2</sub> O <sub>2</sub>
Sonepiprazole	Antipsychotic	170858-33-0		C <sub>21</sub> H <sub>27</sub> N <sub>3</sub> O <sub>3</sub> S
Sopitazine	Antihistaminic	23492-69-5		C <sub>20</sub> H <sub>23</sub> N <sub>3</sub> OS
Sopromidine	Antihistaminic	79313-75-0		C <sub>14</sub> H <sub>23</sub> N <sub>7</sub> S
Soquinolol	Antihypertensive	61563-18-6		C <sub>17</sub> H <sub>26</sub> N <sub>2</sub> O <sub>3</sub>
Sorafenib	Antineoplastic	284461-73-0	Y	C <sub>21</sub> H <sub>16</sub> ClF <sub>3</sub> N <sub>4</sub> O <sub>3</sub>
Soraprazan	Ant ulcerative	261944-46-1		C <sub>21</sub> H <sub>25</sub> N <sub>3</sub> O <sub>3</sub>
Sorbinate	Antihyperlipidemic	6184-06-1		C <sub>42</sub> H <sub>32</sub> N <sub>6</sub> O <sub>12</sub>
Sorbiniol	Antidiabetic	68367-52-2		C <sub>11</sub> H <sub>9</sub> FN <sub>2</sub> O <sub>3</sub>
Soretolide	Anticonvulsant	130403-08-6		C <sub>13</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Sorivudine	Antiviral	77181-69-2		C <sub>11</sub> H <sub>13</sub> BrN <sub>2</sub> O <sub>6</sub>
Sornidipine	Vasodilator	95105-77-4		C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>9</sub>
Sotalol	Antianginal	3930-20-9	Y	C <sub>12</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> S
Soterinol	Bronchodilator	13642-52-9		C <sub>12</sub> H <sub>20</sub> N <sub>2</sub> O <sub>4</sub> S
Sotirimod	Dermatologic	227318-75-4		C <sub>14</sub> H <sub>17</sub> N <sub>5</sub>
Spaglumic Acid	Antihistaminic	4910-46-7		C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> O <sub>8</sub>
Sparfloxacin	Antibiotic	110871-86-8	Y	C <sub>19</sub> H <sub>22</sub> F <sub>2</sub> N <sub>4</sub> O <sub>3</sub>
Sparfosate Sodium	Antineoplastic	51321-79-0		C <sub>6</sub> H <sub>10</sub> NO <sub>8</sub> P
Sparsomycin	Antineoplastic	1404-64-4		C <sub>13</sub> H <sub>19</sub> N <sub>3</sub> O <sub>5</sub> S <sub>2</sub>
Sparteine	Cardiotonic	90-39-1		C <sub>15</sub> H <sub>26</sub> N <sub>2</sub>
Spectinomycin	Antibiotic	1695-77-8		C <sub>14</sub> H <sub>24</sub> N <sub>2</sub> O <sub>7</sub>
Spiclamine	Antidepressant	90243-97-3		C <sub>20</sub> H <sub>25</sub> ClN <sub>2</sub> O
Spiclomazine	Antipsychotic	24527-27-3		C <sub>22</sub> H <sub>24</sub> ClN <sub>3</sub> OS <sub>2</sub>
Spiiperone	Antipsychotic	749-02-0		C <sub>23</sub> H <sub>26</sub> FN <sub>3</sub> O <sub>2</sub>
Spiradoline Mesylate	Analgesic	87151-85-7		C <sub>22</sub> H <sub>30</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Spiramide	Nootropic	510-74-7		C <sub>22</sub> H <sub>26</sub> FN <sub>3</sub> O <sub>2</sub>
Spirapril	Antihypertensive	83647-97-6	Y	C <sub>22</sub> H <sub>30</sub> N <sub>2</sub> O <sub>5</sub> S <sub>2</sub>
Spiraprilat	Antihypertensive	83602-05-5		C <sub>20</sub> H <sub>26</sub> N <sub>2</sub> O <sub>5</sub> S <sub>2</sub>
Spirendolol	Antihypertensive	81840-58-6		C <sub>21</sub> H <sub>31</sub> NO <sub>3</sub>
Spirgetine	Unclassified	144-45-6		C <sub>10</sub> H <sub>20</sub> N <sub>4</sub>
Spirilene	Antipsychotic	357-66-4		C <sub>24</sub> H <sub>28</sub> FN <sub>3</sub> O
Spiriprostil	Prostaglandin	122946-42-3		C <sub>20</sub> H <sub>34</sub> N <sub>2</sub> O <sub>4</sub>
Spirobarbital Sodium	Sedative	72035-36-0		C <sub>12</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub> S
Spirofyline	Bronchodilator	98204-48-9		C <sub>24</sub> H <sub>28</sub> N <sub>6</sub> O <sub>5</sub>
Spirogermanium	Antineoplastic	41992-23-8		C <sub>17</sub> H <sub>36</sub> GeN <sub>2</sub>
Spiroglumide	Ant ulcerative	137795-35-8		C <sub>21</sub> H <sub>26</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>4</sub>
Spiromustine	Antineoplastic	56605-16-4		C <sub>14</sub> H <sub>23</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>2</sub>
Spirocholactone	Diuretic	1952-01-7	Y	C <sub>24</sub> H <sub>32</sub> O <sub>4</sub> S
Spirorenone	Steroid	74220-07-8		C <sub>24</sub> H <sub>28</sub> O <sub>3</sub>
Spiroxasone	Diuretic	6673-97-8		C <sub>24</sub> H <sub>34</sub> O <sub>3</sub> S
Spiroaxtrine	Vasodilator	1054-88-2		C <sub>22</sub> H <sub>25</sub> N <sub>3</sub> O <sub>3</sub>
Spiropepin	Antidepressant	47254-05-7		C <sub>19</sub> H <sub>21</sub> NO <sub>3</sub>
Spizofurone	Ant ulcerative	72492-12-7		C <sub>12</sub> H <sub>10</sub> O <sub>3</sub>
Squalamine Lactate	Antineoplastic	148717-90-2		C <sub>34</sub> H <sub>65</sub> N <sub>3</sub> O <sub>5</sub> S

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Stacofylline	Bronchodilator	98833-92-2		C <sub>20</sub> H <sub>33</sub> N <sub>7</sub> O <sub>3</sub>
Stallimycin	Antibacterial	636-47-5		C <sub>22</sub> H <sub>27</sub> N <sub>9</sub> O <sub>4</sub>
Stanolone	Androgen	521-18-6		C <sub>19</sub> H <sub>30</sub> O <sub>2</sub>
Stanozolol	Steroid	10418-03-8		C <sub>21</sub> H <sub>32</sub> N <sub>2</sub> O
Stavudine	Antiviral	3056-17-5	Y	C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub>
Stearylsulfamide	Diuretic	498-78-2		C <sub>24</sub> H <sub>42</sub> N <sub>2</sub> O <sub>3</sub> S
Steffimycin	Antibacterial	11033-34-4		C <sub>28</sub> H <sub>30</sub> O <sub>13</sub>
Stenbolone Acetate	Steroid	1242-56-4		C <sub>22</sub> H <sub>32</sub> O <sub>3</sub>
Stepronin	Mucolytic	72324-18-6		C <sub>10</sub> H <sub>11</sub> NO <sub>4</sub> S <sub>2</sub>
Stercuronium Iodide	Muscle Relaxant	30033-10-4		C <sub>26</sub> H <sub>43</sub> N <sub>2</sub> I
Stevaladil	Unclassified	6535-03-1		C <sub>27</sub> H <sub>45</sub> NO <sub>4</sub>
Stilbamidine Isethionate	Antiprotozoal	122-06-5		C <sub>16</sub> H <sub>16</sub> N <sub>4</sub>
Stilbazium Iodide	Anthelminthic	3784-99-4		C <sub>31</sub> H <sub>36</sub> IN <sub>3</sub>
Stilonium Iodide	Antispasmodic	77257-42-2		C <sub>22</sub> H <sub>30</sub> INO
Stirimazole	Antifungal	30529-16-9		C <sub>14</sub> H <sub>11</sub> N <sub>3</sub> O <sub>4</sub>
Stiripentol	Anticonvulsant	49763-96-4	Y	C <sub>14</sub> H <sub>18</sub> O <sub>3</sub>
Stirocainide	Antiarrhythmic	78372-27-7		C <sub>22</sub> H <sub>34</sub> N <sub>2</sub> O
Streptomycin Sulfate	Antibiotic	57-92-1		C <sub>21</sub> H <sub>39</sub> N <sub>7</sub> O <sub>12</sub>
Streptonicozid	Antibacterial	4480-58-4		C <sub>27</sub> H <sub>44</sub> N <sub>10</sub> O <sub>12</sub>
Streptonigrin	Antineoplastic	3930-19-6		C <sub>25</sub> H <sub>22</sub> N <sub>4</sub> O <sub>8</sub>
Streptozocin	Antineoplastic	18883-66-4		C <sub>8</sub> H <sub>15</sub> N <sub>3</sub> O <sub>7</sub>
Strinoline	Antiarrhythmic	39862-58-3		C <sub>10</sub> H <sub>6</sub> N <sub>4</sub>
Strychnine	Nootropic	57-24-9		C <sub>21</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>
Subathizone	Antibacterial	121-55-1		C <sub>10</sub> H <sub>13</sub> N <sub>3</sub> O <sub>2</sub> S <sub>2</sub>
Subendazole	Anthelminthic	54340-66-8		C <sub>10</sub> H <sub>5</sub> Cl <sub>3</sub> N <sub>4</sub> S <sub>3</sub>
Succimer	Antidote	304-55-2		C <sub>4</sub> H <sub>6</sub> O <sub>4</sub> S <sub>2</sub>
Succinchlorimide	Anticonvulsant	128-09-6		C <sub>4</sub> H <sub>4</sub> ClNO <sub>2</sub>
Succinylcholine	Neuromuscular Blocking Agent	306-40-1		C <sub>14</sub> H <sub>30</sub> N <sub>2</sub> O <sub>42+</sub>
Succinylsulfathiazole	Antibiotic	116-43-8		C <sub>13</sub> H <sub>13</sub> N <sub>3</sub> O <sub>5</sub> S <sub>2</sub>
Succisulfone	Antibiotic	5934-14-5		C <sub>16</sub> H <sub>16</sub> N <sub>2</sub> O <sub>5</sub> S
Suclofenide	Anticonvulsant	30279-49-3		C <sub>16</sub> H <sub>13</sub> ClN <sub>2</sub> O <sub>4</sub> S
Sucralose	Antilulcerative	56038-13-2		C <sub>12</sub> H <sub>19</sub> Cl <sub>3</sub> O <sub>8</sub>
Sucralox	Unclassified	57-50-1		C <sub>12</sub> H <sub>22</sub> O <sub>11</sub>
Sucrosolate Potassium	Antilulcerative	57680-56-5		C <sub>12</sub> H <sub>22</sub> O <sub>35</sub> S <sub>8</sub>
Sudexanox	Antihistaminic	58761-87-8		C <sub>21</sub> H <sub>23</sub> NO <sub>5</sub> S
Sudoxicam	Antiinflammatory	34042-85-8		C <sub>13</sub> H <sub>11</sub> N <sub>3</sub> O <sub>4</sub> S <sub>2</sub>
Sufentanil	Analgesic	56030-54-7		C <sub>22</sub> H <sub>30</sub> N <sub>2</sub> O <sub>2</sub> S
Sufosfamide	Antineoplastic	37753-10-9		C <sub>8</sub> H <sub>18</sub> ClN <sub>2</sub> O <sub>5</sub> PS
Sufotidine	Antilulcerative	80343-63-1		C <sub>20</sub> H <sub>31</sub> N <sub>5</sub> O <sub>3</sub> S
Sufugolix	Pituitary	308831-61-0		C <sub>36</sub> H <sub>31</sub> F <sub>2</sub> N <sub>5</sub> O <sub>4</sub> S
Sulamserod	Antiarrhythmic	219757-90-1		C <sub>19</sub> H <sub>28</sub> ClN <sub>3</sub> O <sub>5</sub> S
Sulazepam	Anxiolytic	2898-13-7		C <sub>16</sub> H <sub>13</sub> ClN <sub>2</sub> O <sub>3</sub> S
Sulazuril	Antibiotic	108258-89-5		C <sub>17</sub> H <sub>15</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>5</sub> S
Sulbactam Pivoxil	Antibacterial	69388-79-0		C <sub>14</sub> H <sub>21</sub> NO <sub>7</sub> S
Sulbactam	Antibiotic	68373-14-8		C <sub>8</sub> H <sub>11</sub> NO <sub>5</sub> S
Sulbenicillin	Antibiotic	41744-40-5		C <sub>16</sub> H <sub>18</sub> N <sub>2</sub> O <sub>7</sub> S <sub>2</sub>
Sulbenox	Steroid	58095-31-1		C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> S
Sulbentine	Antifungal	350-12-9		C <sub>17</sub> H <sub>18</sub> N <sub>2</sub> S <sub>2</sub>
Sulclamide	Antitussive	2455-92-7		C <sub>7</sub> H <sub>7</sub> ClN <sub>2</sub> O <sub>3</sub> S
Sulconazole	Antifungal	61318-90-9		C <sub>18</sub> H <sub>15</sub> Cl <sub>3</sub> N <sub>2</sub> S
Sulfabenz	Antibacterial	127-77-5		C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> S
Sulfabenzamide	Antibacterial	127-71-9		C <sub>13</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub> S
Sulfabromomethazine Sodium	Antibiotic	116-45-0		C <sub>12</sub> H <sub>13</sub> BrN <sub>4</sub> O <sub>2</sub> S
Sulfacarbamide	Antibiotic	547-44-4		C <sub>7</sub> H <sub>9</sub> N <sub>3</sub> O <sub>3</sub> S
Sulfacecole	Unclassified	21662-79-3		C <sub>14</sub> H <sub>17</sub> N <sub>3</sub> O <sub>5</sub> S
Sulfacetamide	Antibiotic	144-80-9		C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> S
Sulfachlorpyridazine	Antibiotic	80-32-0		C <sub>10</sub> H <sub>9</sub> ClN <sub>4</sub> O <sub>2</sub> S
Sulfachrysoidine	Antibiotic	485-41-6		C <sub>13</sub> H <sub>13</sub> N <sub>5</sub> O <sub>4</sub> S
Sulfacloamide	Antibacterial	4015-18-3		C <sub>12</sub> H <sub>13</sub> ClN <sub>4</sub> O <sub>2</sub> S
Sulfaclozazole	Unclassified	54063-55-7		C <sub>16</sub> H <sub>15</sub> ClN <sub>4</sub> O <sub>2</sub> S
Sulfaclozine	Antibiotic	102-65-8		C <sub>10</sub> H <sub>9</sub> ClN <sub>4</sub> O <sub>2</sub> S
Sulfacytine	Antibacterial	17784-12-2		C <sub>12</sub> H <sub>14</sub> N <sub>4</sub> O <sub>3</sub> S

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Sulfadiazine	Antibiotic	68-35-9		C <sub>10</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub> S
Sulfadiazine	Antibiotic	115-68-4		C <sub>11</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub> S
Sulfadimethoxine	Antibiotic	122-11-2		C <sub>12</sub> H <sub>14</sub> N <sub>4</sub> O <sub>4</sub> S
Sulfadoxine	Antibiotic	2447-57-6		C <sub>12</sub> H <sub>14</sub> N <sub>4</sub> O <sub>4</sub> S
Sulfaethidole	Antibiotic	94-19-9		C <sub>10</sub> H <sub>12</sub> N <sub>4</sub> O <sub>2</sub> S <sub>2</sub>
Sulfaguanidine	Antibiotic	57-67-0		C <sub>7</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub> S
Sulfaguanole	Antibiotic	27031-08-9		C <sub>12</sub> H <sub>15</sub> N <sub>5</sub> O <sub>3</sub> S
Sulfalene	Antibacterial	152-47-6		C <sub>11</sub> H <sub>12</sub> N <sub>4</sub> O <sub>3</sub> S
Sulfaloxic Acid	Antibiotic	14376-16-0		C <sub>16</sub> H <sub>15</sub> N <sub>3</sub> O <sub>7</sub> S
Sulfamazone	Antiinflammatory	65761-24-2		C <sub>23</sub> H <sub>24</sub> N <sub>6</sub> O <sub>7</sub> S <sub>2</sub>
Sulfamerazine	Antibiotic	127-79-7		C <sub>11</sub> H <sub>12</sub> N <sub>4</sub> O <sub>2</sub> S
Sulfameter	Antibiotic	651-06-9		C <sub>11</sub> H <sub>12</sub> N <sub>4</sub> O <sub>3</sub> S
Sulfamethazine	Antibiotic	57-68-1		C <sub>12</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub> S
Sulfamethizole	Antibiotic	144-82-1		C <sub>9</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub> S <sub>2</sub>
Sulfamethoxazole	Antibiotic	723-46-6		C <sub>10</sub> H <sub>11</sub> N <sub>3</sub> O <sub>3</sub> S
Sulfamethoxy-pyridazine	Antibiotic	80-35-3		C <sub>11</sub> H <sub>12</sub> N <sub>4</sub> O <sub>3</sub> S
Sulfamethoxy-pyridazine Acetyl	Antibiotic	3568-43-2		C <sub>13</sub> H <sub>14</sub> N <sub>4</sub> O <sub>4</sub> S
Sulfametomidine	Antibiotic	3772-76-7		C <sub>12</sub> H <sub>14</sub> N <sub>4</sub> O <sub>3</sub> S
Sulfametrole	Antibiotic	32909-92-5		C <sub>9</sub> H <sub>10</sub> N <sub>4</sub> O <sub>3</sub> S <sub>2</sub>
Sulfamonomethoxine	Antibiotic	1220-83-3		C <sub>11</sub> H <sub>12</sub> N <sub>4</sub> O <sub>3</sub> S
Sulfamoxole	Antibacterial	729-99-7		C <sub>11</sub> H <sub>13</sub> N <sub>3</sub> O <sub>3</sub> S
Sulfanilamide	Antibiotic	63-74-1		C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> S
Sulfanilate Zinc	Antibiotic	121-57-3		C <sub>6</sub> H <sub>7</sub> NO <sub>3</sub> S
Sulfantran	Antibacterial	122-16-7		C <sub>14</sub> H <sub>13</sub> N <sub>3</sub> O <sub>3</sub> S
Sulfaperin	Antibiotic	599-88-2		C <sub>11</sub> H <sub>12</sub> N <sub>4</sub> O <sub>2</sub> S
Sulfaphenazole	Antibiotic	526-08-9		C <sub>15</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub> S
Sulfaproxyline	Antibiotic	116-42-7		C <sub>16</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub> S
Sulfapyrazine	Antibiotic	116-44-9		C <sub>10</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub> S
Sulfapyridine	Antibiotic	144-83-2		C <sub>11</sub> H <sub>11</sub> N <sub>3</sub> O <sub>2</sub> S
Sulfaquinolaxine	Antiprotozoal	59-40-5		C <sub>14</sub> H <sub>12</sub> N <sub>4</sub> O <sub>2</sub> S
Sulfarsphenamine	Antibacterial	534-93-0		C <sub>14</sub> H <sub>16</sub> As <sub>2</sub> N <sub>2</sub> O <sub>8</sub> S <sub>2</sub>
Sulfasalazine	Antiinflammatory	599-79-1	Y	C <sub>18</sub> H <sub>14</sub> N <sub>4</sub> O <sub>5</sub> S
Sulfasomizole	Antibacterial	632-00-8		C <sub>10</sub> H <sub>11</sub> N <sub>3</sub> O <sub>2</sub> S <sub>2</sub>
Sulfasuccinamide	Antibiotic	3563-14-2		C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> O <sub>5</sub> S
Sulfasymazine	Antibiotic	1984-94-7		C <sub>13</sub> H <sub>17</sub> N <sub>5</sub> O <sub>2</sub> S
Sulfathiazole	Antibiotic	72-14-0		C <sub>9</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub> S <sub>2</sub>
Sulfathiourea	Antibiotic	515-49-1		C <sub>7</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub> S <sub>2</sub>
Sulfatroxazole	Antibacterial	23256-23-7		C <sub>11</sub> H <sub>13</sub> N <sub>3</sub> O <sub>3</sub> S
Sulfatrozole	Antiprotozoal	13369-07-8		C <sub>10</sub> H <sub>12</sub> N <sub>4</sub> O <sub>3</sub> S <sub>2</sub>
Sulfazamet	Antibacterial	852-19-7		C <sub>16</sub> H <sub>16</sub> N <sub>4</sub> O <sub>2</sub> S
Sulfinalol	Antihypertensive	66264-77-5		C <sub>20</sub> H <sub>27</sub> NO <sub>4</sub> S
Sulfinpyrazone	Antiurolithic	57-96-5	Y	C <sub>23</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> S
Sulfiram	Ectoparasiticide	95-05-6		C <sub>10</sub> H <sub>20</sub> N <sub>2</sub> S <sub>3</sub>
Sulfisomidine	Antibiotic	515-64-0		C <sub>12</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub> S
Sulfisoxazole	Antibiotic	127-69-5	Y	C <sub>11</sub> H <sub>13</sub> N <sub>3</sub> O <sub>3</sub> S
Sulfisoxazole Acetyl	Antibacterial	80-74-0		C <sub>13</sub> H <sub>15</sub> N <sub>3</sub> O <sub>4</sub> S
Sulfonethylmethane	Sedative	76-20-0		C <sub>8</sub> H <sub>18</sub> O <sub>4</sub> S <sub>2</sub>
Sulfonmethane	Sedative	115-24-2		C <sub>7</sub> H <sub>16</sub> O <sub>4</sub> S <sub>2</sub>
Sulfonterol	Bronchodilator	42461-79-0		C <sub>14</sub> H <sub>23</sub> NO <sub>4</sub> S
Sulforidazine	Antipsychotic	14759-06-9		C <sub>21</sub> H <sub>26</sub> N <sub>2</sub> O <sub>2</sub> S <sub>2</sub>
Sulfosalicylic Acid	Antiinflammatory	97-05-2		C <sub>7</sub> H <sub>6</sub> O <sub>6</sub> S
Sulfoxone	Antibiotic	144-76-3		C <sub>14</sub> H <sub>16</sub> N <sub>2</sub> O <sub>6</sub> S <sub>3</sub>
Sulicrinat	Diuretic	90207-12-8		C <sub>15</sub> H <sub>10</sub> Cl <sub>3</sub> NO <sub>6</sub> S
Sulindac	Antineoplastic	38194-50-2	Y	C <sub>20</sub> H <sub>17</sub> FO <sub>3</sub> S
Sulisatin	Laxative	54935-03-4		C <sub>21</sub> H <sub>17</sub> NO <sub>9</sub> S <sub>2</sub>
Sulisobenzone	Dermatologic	4065-45-6		C <sub>14</sub> H <sub>12</sub> O <sub>6</sub> S
Sulmarin	Hemostatic	29334-07-4		C <sub>10</sub> H <sub>8</sub> O <sub>10</sub> S <sub>2</sub>
Sulmazole	Cardiotonic	73384-60-8		C <sub>14</sub> H <sub>13</sub> N <sub>3</sub> O <sub>2</sub> S
Sulmepride	Gastroprokinetic	57479-88-6		C <sub>14</sub> H <sub>21</sub> N <sub>3</sub> O <sub>4</sub> S
Sulnidazole	Antiprotozoal	51022-76-5		C <sub>9</sub> H <sub>14</sub> N <sub>4</sub> O <sub>3</sub> S
Sulocarbilate	Ophthalmic	121-64-2		C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O <sub>5</sub> S
Suloctidil	Vasodilator	54767-75-8		C <sub>20</sub> H <sub>35</sub> NOS
Sulofenur	Antineoplastic	110311-27-8		C <sub>16</sub> H <sub>15</sub> ClN <sub>2</sub> O <sub>3</sub> S

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Sulopenem	Antibacterial	120788-07-0		C <sub>12</sub> H <sub>15</sub> NO <sub>5</sub> S <sub>3</sub>
Sulosemide	Diuretic	82666-62-4		C <sub>17</sub> H <sub>16</sub> N <sub>2</sub> O <sub>7</sub> S <sub>2</sub>
Sulotroban	Anticoagulant	72131-33-0		C <sub>16</sub> H <sub>17</sub> NO <sub>5</sub> S
Suloxifen Oxalate	Bronchodilator	25827-12-7		C <sub>18</sub> H <sub>24</sub> N <sub>2</sub> O <sub>5</sub> S
Sulpiride	Antipsychotic	15676-16-1	Y	C <sub>15</sub> H <sub>23</sub> N <sub>3</sub> O <sub>4</sub> S
Sulprosal	Unclassified	58703-77-8		C <sub>10</sub> H <sub>12</sub> O <sub>6</sub> S
Sulprostone	Prostaglandin	60325-46-4		C <sub>23</sub> H <sub>31</sub> NO <sub>7</sub> S
Sultamicillin	Antibacterial	76497-13-7		C <sub>25</sub> H <sub>30</sub> N <sub>4</sub> O <sub>9</sub> S <sub>2</sub>
Sulthiame	Anticonvulsant	61-56-3		C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub> S <sub>2</sub>
Sultopride	Antipsychotic	53583-79-2	Y	C <sub>17</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub> S
Sultosilic Acid	Antihyperlipidemic	57775-26-5		C <sub>13</sub> H <sub>12</sub> O <sub>7</sub> S <sub>2</sub>
Sultroponium	Antispasmodic	15130-91-3		C <sub>20</sub> H <sub>29</sub> NO <sub>6</sub> S
Sulukast	Bronchodilator	98116-53-1		C <sub>25</sub> H <sub>36</sub> N <sub>4</sub> O <sub>5</sub> S
Sulverapride	Antiemetic	73747-20-3		C <sub>16</sub> H <sub>25</sub> N <sub>3</sub> O <sub>5</sub> S
Sumacetamol	Analgesic	69217-67-0		C <sub>15</sub> H <sub>20</sub> N <sub>2</sub> O <sub>4</sub> S
Sumanriole	Antiparkinsonian	179386-43-7		C <sub>11</sub> H <sub>13</sub> N <sub>3</sub> O
Sumarotene	Dermatologic	105687-93-2		C <sub>24</sub> H <sub>30</sub> O <sub>2</sub> S
Sumatriptan	Antimigraine	103628-46-2		C <sub>14</sub> H <sub>21</sub> N <sub>3</sub> O <sub>2</sub> S
Sumetizide	Antidiabetic	32059-27-1		C <sub>12</sub> H <sub>13</sub> ClN <sub>4</sub> O <sub>6</sub> S <sub>2</sub>
Sunagrel	Anticoagulant	85418-85-5		C <sub>25</sub> H <sub>32</sub> N <sub>2</sub> O <sub>2</sub> S
Suncillin Sodium	Antibacterial	22164-94-9		C <sub>16</sub> H <sub>19</sub> N <sub>3</sub> O <sub>7</sub> S <sub>2</sub>
Sunepitron	Antidepressant	131831-03-3		C <sub>17</sub> H <sub>24</sub> ClN <sub>5</sub> O <sub>2</sub>
Sunitinib	Antineoplastic	557795-19-4	Y	C <sub>22</sub> H <sub>27</sub> FN <sub>4</sub> O <sub>2</sub>
Supidimide	Sedative	49785-74-2		C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub> S
Suplatast Tosilate	Antihistaminic	94055-76-2	Y	C <sub>23</sub> H <sub>33</sub> NO <sub>7</sub> S <sub>2</sub>
Suproclone	Sedative	76535-71-2		C <sub>22</sub> H <sub>22</sub> ClN <sub>5</sub> O <sub>4</sub> S <sub>2</sub>
Suprofen	Antiinflammatory	40828-46-4		C <sub>14</sub> H <sub>12</sub> O <sub>3</sub> S
Suricainide Maleate	Antiarrhythmic	85053-46-9		C <sub>18</sub> H <sub>31</sub> N <sub>3</sub> O <sub>3</sub> S
Suriclone	Anxiolytic	53813-83-5		C <sub>20</sub> H <sub>20</sub> ClN <sub>5</sub> O <sub>3</sub> S <sub>2</sub>
Surinabant	Antibiotic	288104-79-0		C <sub>23</sub> H <sub>23</sub> Br <sub>2</sub> Cl <sub>2</sub> N <sub>4</sub> O
Suritazole	Antidepressant	110623-33-1		C <sub>10</sub> H <sub>10</sub> FN <sub>3</sub> S
Suronacrine Maleate	Neuromuscular Blocking Agent	104675-35-6		C <sub>20</sub> H <sub>20</sub> N <sub>2</sub> O
Susalimod	Immunomodulator	149556-49-0		C <sub>21</sub> H <sub>16</sub> N <sub>2</sub> O <sub>5</sub> S
Suxamethonium Bromide	Muscle Relaxant	55-94-7		C <sub>14</sub> H <sub>30</sub> Br <sub>2</sub> N <sub>2</sub> O <sub>4</sub>
Suxemerid Sulfate	Antitussive	47662-15-7		C <sub>24</sub> H <sub>44</sub> N <sub>2</sub> O <sub>4</sub>
Suxethonium Chloride	Neuromuscular Blocking Agent	54063-57-9		C <sub>16</sub> H <sub>34</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>4</sub>
Suxibuzone	Antiinflammatory	27470-51-5		C <sub>24</sub> H <sub>26</sub> N <sub>2</sub> O <sub>6</sub>
Symclosene	Antibacterial	87-90-1		C <sub>3</sub> Cl <sub>3</sub> N <sub>3</sub> O <sub>3</sub>
Symetine	Antiamoebic	15599-45-8		C <sub>30</sub> H <sub>48</sub> N <sub>2</sub> O <sub>2</sub>
Syrosingopine	Antihypertensive	84-36-6		C <sub>35</sub> H <sub>42</sub> N <sub>2</sub> O <sub>11</sub>
Tabilautide	Immunomodulator	78088-46-7		C <sub>27</sub> H <sub>49</sub> N <sub>5</sub> O <sub>8</sub>
Tabimorelin	Cardiotonic	193079-69-5		C <sub>32</sub> H <sub>40</sub> N <sub>4</sub> O <sub>3</sub>
Tacalcitol	Dermatologic	57333-96-7		C <sub>27</sub> H <sub>44</sub> O <sub>3</sub>
Tacapenem	Antibiotic	193811-33-5		C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O <sub>5</sub> S
Tacedinaline	Antineoplastic	112522-64-2		C <sub>15</sub> H <sub>15</sub> N <sub>3</sub> O <sub>2</sub>
Taclamine	Anxiolytic	34061-33-1		C <sub>21</sub> H <sub>23</sub> N
Tacrine	Nootropic	321-64-2	Y	C <sub>13</sub> H <sub>14</sub> N <sub>2</sub>
Tacrolimus	Immunosuppressant	104987-11-3	Y	C <sub>44</sub> H <sub>69</sub> NO <sub>12</sub>
Tadalafil	Erectile Dysfunction	171596-29-5	Y	C <sub>22</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub>
Tafenoquine	Antimalarial	106635-80-7		C <sub>24</sub> H <sub>28</sub> F <sub>3</sub> N <sub>3</sub> O <sub>3</sub>
Tafluprost	Prostaglandin	209860-87-7		C <sub>25</sub> H <sub>34</sub> F <sub>2</sub> O <sub>5</sub>
Taglutimide	Sedative	14166-26-8		C <sub>14</sub> H <sub>16</sub> N <sub>2</sub> O <sub>4</sub>
Tagorizine	Antihistaminic	118420-47-6		C <sub>30</sub> H <sub>36</sub> N <sub>4</sub> O
Talabostat	Hematinic	149682-77-9		C <sub>9</sub> H <sub>19</sub> BN <sub>2</sub> O <sub>3</sub>
Talaglumetad	Antineoplastic	441765-98-6		C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> O <sub>5</sub>
Talampanel	Antiseizure	161832-65-1		C <sub>19</sub> H <sub>19</sub> N <sub>3</sub> O <sub>3</sub>
Talampicillin	Antibacterial	47747-56-8		C <sub>24</sub> H <sub>23</sub> N <sub>3</sub> O <sub>6</sub> S
Talaporfin Sodium	Antineoplastic	110230-98-3		C <sub>38</sub> H <sub>41</sub> N <sub>5</sub> O <sub>9</sub>
Talastine	Antihistaminic	16188-61-7		C <sub>19</sub> H <sub>21</sub> N <sub>3</sub> O
Talbutal	Sedative	115-44-6		C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>
Taleranol	Pituitary	42422-68-4		C <sub>18</sub> H <sub>26</sub> O <sub>5</sub>



Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Talibegron	Antiobesity	146376-58-1		C <sub>18</sub> H <sub>21</sub> NO <sub>4</sub>
Talinolol	Antihypertensive	57460-41-0	Y	C <sub>20</sub> H <sub>33</sub> N <sub>3</sub> O <sub>3</sub>
Talipexole	Antiparkinsonian	101626-70-4	Y	C <sub>10</sub> H <sub>15</sub> N <sub>3</sub> S
Tallimustine	Antineoplastic	115308-98-0		C <sub>32</sub> H <sub>38</sub> Cl <sub>2</sub> N <sub>10</sub> O <sub>4</sub>
Talmetacin	Analgesic	67489-39-8		C <sub>27</sub> H <sub>20</sub> ClNO <sub>6</sub>
Talmetoprim	Antibiotic	66093-35-4		C <sub>22</sub> H <sub>20</sub> N <sub>4</sub> O <sub>5</sub>
Talnetant	Antispasmodic	174636-32-9		C <sub>25</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>
Talniflumate	Antiinflammatory	66898-62-2	Y	C <sub>21</sub> H <sub>13</sub> F <sub>3</sub> N <sub>2</sub> O <sub>4</sub>
Talopram	Antidepressant	7182-51-6		C <sub>20</sub> H <sub>25</sub> NO
Talosalate	Analgesic	66898-60-0		C <sub>17</sub> H <sub>12</sub> O <sub>6</sub>
Talotrexin Ammonium	Antineoplastic	113857-87-7		C <sub>27</sub> H <sub>27</sub> N <sub>9</sub> O <sub>6</sub>
Taloximine	Bronchodilator	17243-68-4		C <sub>12</sub> H <sub>16</sub> N <sub>4</sub> O <sub>2</sub>
Talsaclidine Fumarate	Nootropic	147025-53-4		C <sub>10</sub> H <sub>15</sub> NO
Talsupram	Antidepressant	21489-20-3	Y	C <sub>20</sub> H <sub>25</sub> NS
Taltirelin	Pituitary	103300-74-9	Y	C <sub>17</sub> H <sub>23</sub> N <sub>7</sub> O <sub>5</sub>
Taltobulin	Antineoplastic	228266-40-8		C <sub>27</sub> H <sub>43</sub> N <sub>3</sub> O <sub>4</sub>
Taltrimide	Anticonvulsant	81428-04-8		C <sub>13</sub> H <sub>16</sub> N <sub>2</sub> O <sub>4</sub> S
Talviraline	Antiviral	163451-80-7		C <sub>15</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> S <sub>2</sub>
Tameridone	Sedative	102144-78-5		C <sub>22</sub> H <sub>26</sub> N <sub>6</sub> O <sub>2</sub>
Tameticillin	Antibacterial	56211-43-9		C <sub>23</sub> H <sub>33</sub> N <sub>3</sub> O <sub>6</sub> S
Tametriline	Antidepressant	52795-02-5		C <sub>17</sub> H <sub>19</sub> N
Tamibarotene	Immunomodulator	94497-51-5	Y	C <sub>22</sub> H <sub>25</sub> NO <sub>3</sub>
Tamitinol	Nootropic	59429-50-4		C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> OS
Tamolarizine	Vasodilator	93035-32-6		C <sub>27</sub> H <sub>32</sub> N <sub>2</sub> O <sub>3</sub>
Tamoxifen	Antineoplastic	10540-29-1	Y	C <sub>26</sub> H <sub>29</sub> NO
Tampramine Fumarate	Antidepressant	83166-17-0		C <sub>23</sub> H <sub>24</sub> N <sub>4</sub>
Tamsulosin	Antineoplastic	106133-20-4	Y	C <sub>20</sub> H <sub>28</sub> N <sub>2</sub> O <sub>5</sub> S
Tanaproget	Contraceptive	304853-42-7		C <sub>16</sub> H <sub>15</sub> N <sub>3</sub> OS
Tandamine	Antidepressant	42408-80-0		C <sub>18</sub> H <sub>26</sub> N <sub>2</sub> S
Tandospirone Citrate	Anxiolytic	87760-53-0	Y	C <sub>21</sub> H <sub>29</sub> N <sub>5</sub> O <sub>2</sub>
Tandutinib	Antineoplastic	387867-13-2		C <sub>31</sub> H <sub>42</sub> N <sub>6</sub> O <sub>4</sub>
Taniplon	Sedative	106073-01-2		C <sub>14</sub> H <sub>15</sub> N <sub>5</sub> O <sub>2</sub>
Tanogitran	Unclassified	637328-69-9		C <sub>25</sub> H <sub>31</sub> N <sub>7</sub> O <sub>3</sub>
Tanomastat	Antirheumatic	179545-77-8		C <sub>23</sub> H <sub>19</sub> ClO <sub>3</sub> S
Tapentadol	Analgesic	175591-23-8	Y	C <sub>14</sub> H <sub>23</sub> NO
Taprizosin	Antihypertensive	210538-44-6		C <sub>25</sub> H <sub>26</sub> N <sub>6</sub> O <sub>4</sub> S
Taprostene	Antithrombotic	108945-35-3		C <sub>24</sub> H <sub>30</sub> O <sub>5</sub>
Tarazepide	Antispasmodic	141374-81-4		C <sub>28</sub> H <sub>24</sub> N <sub>4</sub> O <sub>2</sub>
Tariquidar	Antineoplastic	206873-63-4		C <sub>38</sub> H <sub>38</sub> N <sub>4</sub> O <sub>6</sub>
Tartaric Acid	Antibacterial	87-69-4		C <sub>4</sub> H <sub>6</sub> O <sub>6</sub>
Tasidotin	Antineoplastic	192658-64-3		C <sub>32</sub> H <sub>58</sub> N <sub>6</sub> O <sub>5</sub>
Tasosartan	Antihypertensive	145733-36-4		C <sub>23</sub> H <sub>21</sub> N <sub>7</sub> O
Tasquinimod	Nootropic	254964-60-8	Y	C <sub>20</sub> H <sub>17</sub> F <sub>3</sub> N <sub>2</sub> O <sub>4</sub>
Tasuldine	Mucolytic	88579-39-9		C <sub>10</sub> H <sub>9</sub> N <sub>3</sub> S
Taurocholic Acid	Choleretic	81-24-3		C <sub>26</sub> H <sub>45</sub> NO <sub>7</sub> S
Taurolidine	Antibacterial	19388-87-5		C <sub>7</sub> H <sub>16</sub> N <sub>4</sub> O <sub>4</sub> S <sub>2</sub>
Tauromustine	Antineoplastic	85977-49-7		C <sub>7</sub> H <sub>15</sub> ClN <sub>4</sub> O <sub>4</sub> S
Tauroselcholic Acid	Gastroprokinetic	75018-71-2		C <sub>26</sub> H <sub>45</sub> NO <sub>7</sub> SSe
Taurosteine	Mucolytic	124066-33-7		C <sub>7</sub> H <sub>9</sub> NO <sub>4</sub> S <sub>2</sub>
Taurultam	Antineoplastic	38668-01-8		C <sub>3</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> S
Tazadolene Succinate	Analgesic	87936-75-2		C <sub>16</sub> H <sub>21</sub> N
Tazanolast	Antihistaminic	82989-25-1		C <sub>13</sub> H <sub>15</sub> N <sub>5</sub> O <sub>3</sub>
Tazarotene	Dermatologic	118292-40-3		C <sub>21</sub> H <sub>21</sub> NO <sub>2</sub> S
Tazasubrate	Antihyperlipidemic	79071-15-1		C <sub>18</sub> H <sub>17</sub> NO <sub>3</sub> S <sub>2</sub>
Tazeprofen	Antiinflammatory	76816-33-6		C <sub>16</sub> H <sub>13</sub> NO <sub>2</sub> S
Tazifylline	Antihistaminic	79712-55-3		C <sub>23</sub> H <sub>32</sub> N <sub>6</sub> O <sub>3</sub> S
Taziprinone	Cardiotonic	79253-92-2		C <sub>22</sub> H <sub>31</sub> N <sub>3</sub> O <sub>3</sub>
Tazobactam	Antibiotic	89786-04-9		C <sub>10</sub> H <sub>12</sub> N <sub>4</sub> O <sub>5</sub> S
Tazofelone	Immunomodulator	107902-67-0		C <sub>18</sub> H <sub>27</sub> NO <sub>2</sub> S
Tazolol	Cardiotonic	39832-48-9		C <sub>9</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub> S
Tazomeline Citrate	Nootropic	131987-54-7		C <sub>14</sub> H <sub>23</sub> N <sub>3</sub> S <sub>2</sub>
Tebanicline Tosylate	Analgesic	198283-73-7		C <sub>9</sub> H <sub>11</sub> ClN <sub>2</sub> O
Tebatizole	Antiurolytic	54147-28-3		C <sub>12</sub> H <sub>21</sub> N <sub>3</sub> S

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Tebipenem Pivoxil	Antibiotic	161715-24-8	Y	C <sub>22</sub> H <sub>31</sub> N <sub>3</sub> O <sub>6</sub> S <sub>2</sub>
Tebufelone	Analgesic	112018-00-5		C <sub>20</sub> H <sub>28</sub> O <sub>2</sub>
Tebuquine	Antimalarial	74129-03-6		C <sub>26</sub> H <sub>25</sub> Cl <sub>2</sub> N <sub>3</sub> O
Tecadenoson	Antiarrhythmic	204512-90-3		C <sub>14</sub> H <sub>19</sub> N <sub>5</sub> O
Tecalcet	Pituitary	148717-54-8		C <sub>18</sub> H <sub>22</sub> ClNO
Tecastemizole	Antihistaminic	75970-99-9		C <sub>19</sub> H <sub>21</sub> FN <sub>4</sub>
Teclotiazide	Diuretic	4267-05-4		C <sub>8</sub> H <sub>7</sub> Cl <sub>4</sub> N <sub>3</sub> O <sub>4</sub> S <sub>2</sub>
Teclozan	Antiamoebic	5560-78-1		C <sub>20</sub> H <sub>28</sub> Cl <sub>4</sub> N <sub>2</sub> O <sub>4</sub>
Tedisamil	Antiarrhythmic	90961-53-8		C <sub>19</sub> H <sub>32</sub> N <sub>2</sub>
Tefazoline	Adrenergic	1082-56-0		C <sub>14</sub> H <sub>18</sub> N <sub>2</sub>
Tefenperate	Unclassified	77342-26-8		C <sub>29</sub> H <sub>37</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>4</sub>
Tefludazine	Antipsychotic	80273-79-6		C <sub>22</sub> H <sub>24</sub> F <sub>4</sub> N <sub>2</sub> O
Teflurane	Anesthetic	124-72-1		C <sub>2</sub> HBrF <sub>4</sub>
Teflutixol	Antipsychotic	55837-23-5		C <sub>23</sub> H <sub>26</sub> F <sub>4</sub> N <sub>2</sub> OS
Tegafur	Antineoplastic	17902-23-7	Y	C <sub>8</sub> H <sub>9</sub> FN <sub>2</sub> O <sub>3</sub>
Tegaserod	Gastroprokinetic	145158-71-0	Y	C <sub>16</sub> H <sub>23</sub> N <sub>5</sub> O
Teglicar	Unclassified	250694-07-6		C <sub>22</sub> H <sub>45</sub> N <sub>3</sub> O <sub>3</sub>
Telbivudine	Antiviral	3424-98-4	Y	C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>5</sub>
Telenzepine	Antiulcerative	80880-90-6		C <sub>19</sub> H <sub>22</sub> N <sub>4</sub> O <sub>2</sub> S
Telinavir	Antiviral	143224-34-4		C <sub>33</sub> H <sub>44</sub> N <sub>6</sub> O <sub>5</sub>
Telithromycin	Antibiotic	191114-48-4	Y	C <sub>43</sub> H <sub>65</sub> N <sub>5</sub> O <sub>10</sub>
Telmesteine	Mucolytic	122946-43-4		C <sub>7</sub> H <sub>11</sub> NO <sub>4</sub> S
Telmisartan	Antihypertensive	144701-48-4	Y	C <sub>33</sub> H <sub>30</sub> N <sub>4</sub> O <sub>2</sub>
Teloxantrone	Antineoplastic	91441-48-4		C <sub>21</sub> H <sub>25</sub> N <sub>5</sub> O <sub>4</sub>
Teludipine	Antihypertensive	108687-08-7		C <sub>28</sub> H <sub>38</sub> N <sub>2</sub> O <sub>6</sub>
Temafloxacin	Antibacterial	108319-06-8		C <sub>21</sub> H <sub>18</sub> F <sub>3</sub> N <sub>3</sub> O <sub>3</sub>
Temarotene	Immunomodulator	75078-91-0		C <sub>23</sub> H <sub>28</sub>
Temazepam	Sedative	846-50-4	Y	C <sub>16</sub> H <sub>13</sub> ClN <sub>2</sub> O <sub>2</sub>
Temefos	Ectoparasiticide	3383-96-8	Y	C <sub>16</sub> H <sub>20</sub> O <sub>6</sub> P <sub>2</sub> S <sub>3</sub>
Temelastine	Antihistaminic	86181-42-2		C <sub>21</sub> H <sub>24</sub> BrN <sub>5</sub> O
Temiverine	Antispasmodic	173324-94-2		C <sub>24</sub> H <sub>35</sub> NO <sub>3</sub>
Temocapril	Antihypertensive	111902-57-9	Y	C <sub>23</sub> H <sub>28</sub> N <sub>2</sub> O <sub>5</sub> S <sub>2</sub>
Temocaprilat	Antihypertensive	110221-53-9		C <sub>21</sub> H <sub>24</sub> N <sub>2</sub> O <sub>5</sub> S <sub>2</sub>
Temocillin	Antibacterial	66148-78-5		C <sub>16</sub> H <sub>18</sub> N <sub>2</sub> O <sub>7</sub> S <sub>2</sub>
Temodox	Steroid	34499-96-2		C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>5</sub>
Temporfin	Antineoplastic	122341-38-2		C <sub>44</sub> H <sub>32</sub> N <sub>4</sub> O <sub>4</sub>
Temozolomide	Antineoplastic	85622-93-1	Y	C <sub>6</sub> H <sub>6</sub> N <sub>6</sub> O <sub>2</sub>
Tenamfetamine	Nootropic	4764-17-4		C <sub>10</sub> H <sub>13</sub> NO <sub>2</sub>
Tenatoprazole	Antihypertensive	113712-98-4		C <sub>16</sub> H <sub>18</sub> N <sub>4</sub> O <sub>3</sub> S
Tenidap	Antiinflammatory	120210-48-2		C <sub>14</sub> H <sub>9</sub> ClN <sub>2</sub> O <sub>3</sub> S
Tenilapine	Antipsychotic	82650-83-7		C <sub>17</sub> H <sub>16</sub> N <sub>4</sub> S <sub>2</sub>
Teniloxazine	Antidepressant	62473-79-4		C <sub>16</sub> H <sub>19</sub> NO <sub>2</sub> S
Tenilsetam	Nootropic	86696-86-8		C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> OS
Teniposide	Antineoplastic	29767-20-2	Y	C <sub>32</sub> H <sub>32</sub> O <sub>13</sub> S
Tenivastatin Calcium	Antihyperlipidemic	121009-77-6		C <sub>25</sub> H <sub>40</sub> O <sub>6</sub>
Tenocyclidine	Antiparkinsonian	21500-98-1		C <sub>15</sub> H <sub>23</sub> NS
Tenofovir	Antiviral	147127-20-6	Y	C <sub>9</sub> H <sub>14</sub> N <sub>5</sub> O <sub>4</sub> P
Tenofovir Disoproxil Fumarate	Antiviral	201341-05-1	Y	C <sub>19</sub> H <sub>30</sub> N <sub>5</sub> O <sub>10</sub> P
Tenonitrozole	Antiprotozoal	3810-35-3		C <sub>8</sub> H <sub>5</sub> N <sub>3</sub> O <sub>3</sub> S <sub>2</sub>
Tenosal	Unclassified	95232-68-1		C <sub>12</sub> H <sub>8</sub> O <sub>4</sub> S
Tenosiprol	Antiinflammatory	129336-81-8		C <sub>10</sub> H <sub>11</sub> NO <sub>4</sub> S
Tenoxicam	Antiinflammatory	59804-37-4	Y	C <sub>13</sub> H <sub>11</sub> N <sub>3</sub> O <sub>4</sub> S <sub>2</sub>
Tenylidone	Diuretic	893-01-6		C <sub>16</sub> H <sub>14</sub> OS <sub>2</sub>
Teopranitol	Vasodilator	81792-35-0		C <sub>16</sub> H <sub>22</sub> N <sub>6</sub> O <sub>7</sub>
Teoprolol	Antihypertensive	65184-10-3		C <sub>23</sub> H <sub>30</sub> N <sub>6</sub> O <sub>4</sub>
Tepirindole	Nootropic	72808-81-2		C <sub>16</sub> H <sub>19</sub> ClN <sub>2</sub>
Tepoxalin	Dermatologic	103475-41-8		C <sub>20</sub> H <sub>20</sub> ClN <sub>3</sub> O <sub>3</sub>
Teprenone	Antiulcerative	6809-52-5	Y	C <sub>23</sub> H <sub>38</sub> O
Terazosin	Antihypertensive	63590-64-7	Y	C <sub>19</sub> H <sub>25</sub> N <sub>5</sub> O <sub>4</sub>
Terbequinil	Antipsychotic	113079-82-6		C <sub>15</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>
Terbinafine	Antifungal	91161-71-6	Y	C <sub>21</sub> H <sub>25</sub> N
Terbogrel	Antithrombotic	149979-74-8		C <sub>23</sub> H <sub>27</sub> N <sub>5</sub> O <sub>2</sub>
Terbucromil	Antihistaminic	37456-21-6		C <sub>18</sub> H <sub>22</sub> O <sub>4</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Terbufibrol	Antihyperlipidemic	56488-59-6		C <sub>20</sub> H <sub>24</sub> O <sub>5</sub>
Terbuficin	Unclassified	15534-92-6		C <sub>30</sub> H <sub>44</sub> O <sub>4</sub>
Terbuprol	Choleretic	13021-53-9		C <sub>8</sub> H <sub>18</sub> O <sub>3</sub>
Terbutaline	Bronchodilator	23031-25-6	Y	C <sub>12</sub> H <sub>19</sub> NO <sub>3</sub>
Terciprazine	Antipsychotic	56693-15-3		C <sub>22</sub> H <sub>29</sub> F <sub>3</sub> N <sub>2</sub> O <sub>2</sub>
Terconazole	Antifungal	67915-31-5		C <sub>26</sub> H <sub>31</sub> Cl <sub>2</sub> N <sub>5</sub> O <sub>3</sub>
Terdecamycin	Antibacterial	113167-61-6		C <sub>31</sub> H <sub>43</sub> N <sub>3</sub> O <sub>8</sub>
Terestigmine	Muscle Relaxant	147650-57-5		C <sub>21</sub> H <sub>33</sub> N <sub>3</sub> O <sub>3</sub>
Terfenadine	Antihistaminic	50679-08-8		C <sub>32</sub> H <sub>41</sub> NO <sub>2</sub>
Terflavoxate	Muscle Relaxant	86433-40-1		C <sub>26</sub> H <sub>29</sub> NO <sub>4</sub>
Terfluranol	Steroid	64396-09-4		C <sub>17</sub> H <sub>17</sub> F <sub>3</sub> O <sub>2</sub>
Terguride	Antiparkinsonian	37686-84-3	Y	C <sub>20</sub> H <sub>28</sub> N <sub>4</sub> O
Teriflunomide	Antirheumatic	163451-81-8	Y	C <sub>12</sub> H <sub>9</sub> F <sub>3</sub> N <sub>2</sub> O <sub>2</sub>
Terikalant	Antiarrhythmic	132338-79-5		C <sub>24</sub> H <sub>31</sub> NO <sub>3</sub>
Terizidone	Antibacterial	25683-71-0		C <sub>14</sub> H <sub>14</sub> N <sub>4</sub> O <sub>4</sub>
Terlakiren	Antihypertensive	119625-78-4		C <sub>31</sub> H <sub>48</sub> N <sub>4</sub> O <sub>7</sub> S
Ternidazole	Antiprotozoal	1077-93-6		C <sub>7</sub> H <sub>11</sub> N <sub>3</sub> O <sub>3</sub>
Terodiline	Vasodilator	15793-40-5		C <sub>20</sub> H <sub>27</sub> N
Terofenamate	Antiinflammatory	29098-15-5		C <sub>17</sub> H <sub>17</sub> Cl <sub>2</sub> NO <sub>3</sub>
Teroxalene	Unclassified	14728-33-7		C <sub>28</sub> H <sub>41</sub> ClN <sub>2</sub> O
Teroxirone	Antineoplastic	59653-73-5		C <sub>12</sub> H <sub>15</sub> N <sub>3</sub> O <sub>6</sub>
Terpin	Expectorant	80-53-5		C <sub>10</sub> H <sub>20</sub> O <sub>2</sub>
Tertatolol	Antihypertensive	83688-84-0	Y	C <sub>16</sub> H <sub>25</sub> NO <sub>2</sub> S
Terutroban	Antithrombotic	165538-40-9	Y	C <sub>20</sub> H <sub>22</sub> ClNO <sub>4</sub> S
Tesaglitazar	Antidiabetic	251565-85-2		C <sub>20</sub> H <sub>24</sub> O <sub>7</sub> S
Tesetaxel	Antineoplastic	333754-36-2		C <sub>46</sub> H <sub>60</sub> FN <sub>3</sub> O <sub>13</sub>
Tesicam	Antiinflammatory	21925-88-2		C <sub>16</sub> H <sub>11</sub> ClN <sub>2</sub> O <sub>3</sub>
Tesimide	Antiinflammatory	35423-09-7		C <sub>16</sub> H <sub>15</sub> NO <sub>2</sub>
Tesmilifene	Antihistaminic	98774-23-3		C <sub>19</sub> H <sub>25</sub> NO
Tesofensine	Antiparkinsonian	195875-84-4		C <sub>17</sub> H <sub>23</sub> Cl <sub>2</sub> NO
Testolactone	Antineoplastic	968-93-4		C <sub>19</sub> H <sub>24</sub> O <sub>3</sub>
Testosterone	Androgen	58-22-0		C <sub>19</sub> H <sub>28</sub> O <sub>2</sub>
Tetomilast	Bronchodilator	145739-56-6		C <sub>19</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub> S
Tetrabarbital	Sedative	76-23-3		C <sub>12</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub>
Tetrabenzazine	Antipsychotic	58-46-8	Y	C <sub>19</sub> H <sub>27</sub> NO <sub>3</sub>
Tetracaine	Anesthetic	94-24-6		C <sub>15</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub>
Tetrachloroethylene	Anthelminthic	127-18-4		C <sub>2</sub> Cl <sub>4</sub>
Tetracycline	Antibiotic	60-54-8		C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>8</sub>
Tetradonium Bromide	Antiarrhythmic	1119-97-7		C <sub>17</sub> H <sub>38</sub> BrN
Tetragestrin	Antispasmodic	1947-37-1		C <sub>29</sub> H <sub>36</sub> N <sub>6</sub> O <sub>6</sub> S
Tetrahydrozoline	Decongestant	84-22-0		C <sub>13</sub> H <sub>16</sub> N <sub>2</sub>
Tetramisole	Anthelminthic	5036-02-2		C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> S
Tetrantoin	Anticonvulsant	52094-70-9		C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>
Tetraxetan	Antidote	60239-18-1		C <sub>16</sub> H <sub>28</sub> N <sub>4</sub> O <sub>8</sub>
Tetrazepam	Muscle Relaxant	10379-14-3		C <sub>16</sub> H <sub>17</sub> ClN <sub>2</sub> O
Tetrazolast Meglumine	Antihistaminic	95104-27-1		C <sub>10</sub> H <sub>6</sub> N <sub>8</sub>
Tetripofen	Analgesic	28168-10-7		C <sub>15</sub> H <sub>18</sub> O <sub>2</sub>
Tetronasin 5930	Antibiotic	75139-06-9		C <sub>35</sub> H <sub>54</sub> O <sub>8</sub>
Tetroquinone	Dermatologic	319-89-1		C <sub>6</sub> H <sub>4</sub> O <sub>6</sub>
Tetroxoprim	Antibacterial	53808-87-0		C <sub>16</sub> H <sub>22</sub> N <sub>4</sub> O <sub>4</sub>
Tetrydamine	Analgesic	17289-49-5		C <sub>9</sub> H <sub>15</sub> N <sub>3</sub>
Texacromil	Antihistaminic	77005-28-8		C <sub>14</sub> H <sub>14</sub> O <sub>6</sub> S
Tezacitabine	Antineoplastic	130306-02-4		C <sub>10</sub> H <sub>12</sub> FN <sub>3</sub> O <sub>4</sub>
Tezosentan	Anesthetic	180384-57-0		C <sub>27</sub> H <sub>27</sub> N <sub>9</sub> O <sub>6</sub> S
Thalidomide	Immunomodulator	50-35-1	Y	C <sub>13</sub> H <sub>10</sub> N <sub>2</sub> O <sub>4</sub>
Thebacon	Analgesic	466-90-0		C <sub>20</sub> H <sub>23</sub> NO <sub>4</sub>
Thenalidine	Antihistaminic	86-12-4		C <sub>17</sub> H <sub>22</sub> N <sub>2</sub> S
Thenium Closylate	Anthelminthic	4304-40-9		C <sub>21</sub> H <sub>24</sub> ClNO <sub>4</sub> S <sub>2</sub>
Thenylidamine	Antihistaminic	91-79-2		C <sub>14</sub> H <sub>19</sub> N <sub>3</sub> S
Theobromine	Diuretic	83-67-0		C <sub>7</sub> H <sub>8</sub> N <sub>4</sub> O <sub>2</sub>
Theodrenaline	Bronchodilator	13460-98-5		C <sub>17</sub> H <sub>21</sub> N <sub>5</sub> O <sub>5</sub>
Theofibrate	Antihyperlipidemic	54504-70-0		C <sub>19</sub> H <sub>21</sub> ClN <sub>4</sub> O <sub>5</sub>
Theophylline	Bronchodilator	58-55-9	Y	C <sub>7</sub> H <sub>8</sub> N <sub>4</sub> O <sub>2</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Thiabendazole	Anthelmintic	148-79-8		C <sub>10</sub> H <sub>7</sub> N <sub>3</sub> S
Thiacetarsamide	Anthelmintic	531-72-6		C <sub>11</sub> H <sub>12</sub> AsNO <sub>5</sub> S <sub>2</sub>
Thialbarbital	Anesthetic	467-36-7		C <sub>13</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub> S
Thiambutosine	Antibiotic	500-89-0		C <sub>19</sub> H <sub>25</sub> N <sub>3</sub> OS
Thiamiprine	Antineoplastic	5581-52-2		C <sub>9</sub> H <sub>8</sub> N <sub>8</sub> O <sub>2</sub> S
Thiamphenicol	Antibiotic	15318-45-3		C <sub>12</sub> H <sub>15</sub> Cl <sub>2</sub> NO <sub>5</sub> S
Thiamylal	Anesthetic	77-27-0		C <sub>12</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub> S
Thiazesim	Antidepressant	5845-26-1		C <sub>19</sub> H <sub>22</sub> N <sub>2</sub> OS
Thiazinamium Chloride	Antihistaminic	4320-13-2		C <sub>18</sub> H <sub>23</sub> ClN <sub>2</sub> S
Thiazinamium Metilsulfate	Antihistaminic	58-34-4		C <sub>19</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub> S <sub>2</sub>
Thiazolsulfone	Antibiotic	473-30-3		C <sub>9</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub> S <sub>2</sub>
Thiethylperazine	Antiemetic	1420-55-9		C <sub>22</sub> H <sub>29</sub> N <sub>3</sub> S
Thiocarbanidin	Antibiotic	92-97-7		C <sub>22</sub> H <sub>23</sub> N <sub>3</sub> O <sub>2</sub> S
Thiocarbarsone	Antiamebic	120-02-5		C <sub>11</sub> H <sub>13</sub> AsN <sub>2</sub> O <sub>5</sub> S <sub>2</sub>
Thiocolchicoside	Muscle Relaxant	602-41-5	Y	C <sub>27</sub> H <sub>33</sub> NO <sub>10</sub> S
Thioctic Acid	Hepatic Protectant	1077-28-7		C <sub>8</sub> H <sub>14</sub> O <sub>2</sub> S <sub>2</sub>
Thioctic Acid Amide	Unclassified	940-69-2		C <sub>8</sub> H <sub>15</sub> NOS <sub>2</sub>
Thiodiglycol	Antineoplastic	111-48-8		C <sub>4</sub> H <sub>10</sub> O <sub>2</sub> S
Thiofuradene	Antibacterial	2240-21-3		C <sub>8</sub> H <sub>8</sub> N <sub>4</sub> O <sub>3</sub> S
Thioguanine	Antineoplastic	154-42-7	Y	C <sub>5</sub> H <sub>5</sub> N <sub>5</sub> S
Thiohexamide	Antidiabetic	3692-44-2		C <sub>14</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> S <sub>2</sub>
Thioinosine	Immunosuppressant	574-25-4		C <sub>10</sub> H <sub>12</sub> N <sub>4</sub> O <sub>4</sub> S
Thiopental	Anesthetic	76-75-5		C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub> S
Thiopropazate	Antipsychotic	84-06-0		C <sub>23</sub> H <sub>28</sub> ClN <sub>3</sub> O <sub>2</sub> S
Thiopropazine	Antipsychotic	316-81-4		C <sub>22</sub> H <sub>30</sub> N <sub>4</sub> O <sub>2</sub> S <sub>2</sub>
Thioridazine	Antipsychotic	50-52-2	Y	C <sub>21</sub> H <sub>26</sub> N <sub>2</sub> S <sub>2</sub>
Thiotepa	Antineoplastic	52-24-4		C <sub>6</sub> H <sub>12</sub> N <sub>3</sub> PS
Thiotetrabarbital	Sedative	467-38-9		C <sub>12</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub> S
Thiothixene	Antipsychotic	3313-26-6	Y	C <sub>23</sub> H <sub>29</sub> N <sub>3</sub> O <sub>2</sub> S <sub>2</sub>
Thiouracil	Thyroid	141-90-2		C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> OS
Thiourea	Antineoplastic	62-56-6		CH <sub>4</sub> N <sub>2</sub> S
Thiphenamil	Muscle Relaxant	82-99-5		C <sub>20</sub> H <sub>25</sub> NOS
Thipencillin Potassium	Antibacterial	26552-51-2		C <sub>16</sub> H <sub>17</sub> KN <sub>2</sub> O <sub>4</sub> S <sub>2</sub>
Thonzylamine	Antihistaminic	91-85-0		C <sub>16</sub> H <sub>22</sub> N <sub>4</sub> O
Thozalinone	Antidepressant	655-05-0		C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>
Thurfyl Nicotinate	Antiinflammatory	70-19-9		C <sub>11</sub> H <sub>13</sub> NO <sub>3</sub>
Thymocartin	Immunomodulator	85466-18-8		C <sub>21</sub> H <sub>40</sub> N <sub>8</sub> O <sub>7</sub>
Thymoctonan	Antiviral	107489-37-2		C <sub>43</sub> H <sub>67</sub> N <sub>9</sub> O <sub>13</sub>
Thymol	Antibacterial	89-83-8		C <sub>10</sub> H <sub>14</sub> O
Thymopentin	Immunosuppressant	69558-55-0		C <sub>30</sub> H <sub>49</sub> N <sub>9</sub> O <sub>9</sub>
Thymotriganin	Immunomodulator	85465-82-3		C <sub>16</sub> H <sub>31</sub> N <sub>7</sub> O <sub>6</sub>
Thyromedan	Thyroid	15301-96-9		C <sub>21</sub> H <sub>24</sub> I <sub>3</sub> NO <sub>4</sub>
Thyropropic Acid	Antihyperlipidemic	51-26-3		C <sub>15</sub> H <sub>11</sub> I <sub>3</sub> O <sub>4</sub>
Thyroxine	Thyroid	51-48-9		C <sub>15</sub> H <sub>11</sub> I <sub>4</sub> NO <sub>4</sub>
Tiacrilast	Antihistaminic	78299-53-3		C <sub>12</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> S
Tiadenol	Antihyperlipidemic	6964-20-1		C <sub>14</sub> H <sub>30</sub> O <sub>2</sub> S <sub>2</sub>
Tiafibrate	Antihyperlipidemic	55837-28-0		C <sub>34</sub> H <sub>48</sub> Cl <sub>2</sub> O <sub>6</sub> S <sub>2</sub>
Tiagabine	Anticonvulsant	115103-54-3	Y	C <sub>20</sub> H <sub>25</sub> NO <sub>2</sub> S <sub>2</sub>
Tiamenidine	Antihypertensive	31428-61-2		C <sub>8</sub> H <sub>10</sub> ClN <sub>3</sub> S
Tiametonium Iodide	Cholinergic	10433-71-3		C <sub>12</sub> H <sub>30</sub> I <sub>2</sub> N <sub>2</sub> S
Tiamulin Fumarate	Antibacterial	55297-95-5		C <sub>28</sub> H <sub>47</sub> NO <sub>4</sub> S
Tianafac	Antiinflammatory	51527-19-6		C <sub>11</sub> H <sub>9</sub> ClO <sub>2</sub> S
Tianeptine	Antidepressant	72797-41-2	Y	C <sub>21</sub> H <sub>25</sub> ClN <sub>2</sub> O <sub>4</sub> S
Tiapamil	Antiarrhythmic	57010-31-8		C <sub>26</sub> H <sub>37</sub> NO <sub>8</sub> S <sub>2</sub>
Tiapirinol	Antibacterial	14785-50-3		C <sub>12</sub> H <sub>16</sub> N <sub>2</sub> O <sub>4</sub> S
Tiapride	Antispasmodic	51012-32-9	Y	C <sub>15</sub> H <sub>24</sub> N <sub>2</sub> O <sub>4</sub> S
Tiaprofenic Acid	Antiinflammatory	33005-95-7	Y	C <sub>14</sub> H <sub>12</sub> O <sub>3</sub> S
Tiaprost	Prostaglandin	71116-82-0		C <sub>20</sub> H <sub>28</sub> O <sub>6</sub> S
Tiamamide	Antiinflammatory	32527-55-2		C <sub>15</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>3</sub> S
Tiazofurin	Antineoplastic	60084-10-8		C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O <sub>5</sub> S
Tiazuril	Antibacterial	35319-70-1		C <sub>17</sub> H <sub>14</sub> ClN <sub>3</sub> O <sub>2</sub> S
Tibalosin	Antihypertensive	63996-84-9		C <sub>21</sub> H <sub>27</sub> NOS
Tibeglisene	Unclassified	134993-74-1		C <sub>18</sub> H <sub>15</sub> ClO <sub>4</sub> S

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Tibenelast Sodium	Bronchodilator	97852-72-7		C <sub>13</sub> H <sub>14</sub> O <sub>4</sub> S
Tibenzate	Unclassified	13402-51-2		C <sub>14</sub> H <sub>12</sub> OS
Tibezonium Iodide	Antibacterial	54663-47-7	Y	C <sub>28</sub> H <sub>32</sub> IN <sub>3</sub> S <sub>2</sub>
Tibolone	Steroid	5630-53-5	Y	C <sub>21</sub> H <sub>28</sub> O <sub>2</sub>
Tibric Acid	Antihyperlipidemic	7087-94-8		C <sub>14</sub> H <sub>18</sub> ClNO <sub>4</sub> S
Ticabesone Propionate	Glucocorticoid	73205-13-7		C <sub>25</sub> H <sub>32</sub> F <sub>2</sub> O <sub>5</sub> S
Ticalopride	Antiemetic	202590-69-0		C <sub>14</sub> H <sub>20</sub> CIN <sub>3</sub> O <sub>3</sub>
Ticarbodine	Anthelminthic	31932-09-9		C <sub>15</sub> H <sub>19</sub> F <sub>3</sub> N <sub>2</sub> S
Ticarcillin Cresyl Sodium	Antibacterial	59070-07-4		C <sub>22</sub> H <sub>22</sub> N <sub>2</sub> O <sub>6</sub> S <sub>2</sub>
Ticarcillin	Antibacterial	34787-01-4		C <sub>15</sub> H <sub>16</sub> N <sub>2</sub> O <sub>6</sub> S <sub>2</sub>
Ticlatone	Antibacterial	70-10-0		C <sub>7</sub> H <sub>4</sub> CINOS
Ticlopidine	Antithrombotic	55142-85-3	Y	C <sub>14</sub> H <sub>14</sub> CINS
Ticolubant	Dermatologic	154413-61-3		C <sub>23</sub> H <sub>19</sub> Cl <sub>2</sub> NO <sub>5</sub> S
Ticrynafen	Diuretic	40180-04-9		C <sub>13</sub> H <sub>8</sub> Cl <sub>2</sub> O <sub>4</sub> S
Tidembersat	Antimigraine	175013-73-7		C <sub>20</sub> H <sub>19</sub> F <sub>2</sub> NO <sub>4</sub>
Tidiacic	Unclassified	30097-06-4		C <sub>5</sub> H <sub>7</sub> NO <sub>4</sub> S
Tiemonium Iodide	Antispasmodic	144-12-7		C <sub>18</sub> H <sub>24</sub> INO <sub>2</sub> S
Tienocarbine	Antipsychotic	75458-65-0		C <sub>15</sub> H <sub>16</sub> N <sub>2</sub> S
Tienopramine	Antidepressant	37967-98-9		C <sub>17</sub> H <sub>20</sub> N <sub>2</sub> S
Tienoxolol	Diuretic	90055-97-3		C <sub>21</sub> H <sub>28</sub> N <sub>2</sub> O <sub>5</sub> S
Tifacogin	Anticoagulant	148883-56-1		C <sub>12</sub> H <sub>13</sub> NS
Tifemoxone	Antidepressant	39754-64-8		C <sub>11</sub> H <sub>13</sub> NO <sub>2</sub> S
Tifenazoxide	Antihypertensive	279215-43-9		C <sub>9</sub> H <sub>10</sub> CIN <sub>3</sub> O <sub>2</sub> S <sub>2</sub>
Tiflamizole	Antiinflammatory	62894-89-7		C <sub>17</sub> H <sub>10</sub> F <sub>6</sub> N <sub>2</sub> O <sub>2</sub> S
Tiflorex	Anorexic	53993-67-2		C <sub>12</sub> H <sub>16</sub> F <sub>3</sub> NS
Tifluadom	Analgesic	83386-35-0		C <sub>22</sub> H <sub>20</sub> FN <sub>3</sub> OS
Tiflucarbine	Antidepressant	89875-86-5		C <sub>16</sub> H <sub>17</sub> FN <sub>2</sub> S
Tiformin	Antidiabetic	4210-97-3		C <sub>5</sub> H <sub>12</sub> N <sub>4</sub> O
Tifurac Sodium	Analgesic	97483-17-5		C <sub>18</sub> H <sub>14</sub> O <sub>4</sub> S
Tigecycline	Antibiotic	220620-09-7		C <sub>29</sub> H <sub>39</sub> N <sub>5</sub> O <sub>8</sub>
Tigemonam Dicholine	Antibacterial	102916-21-2		C <sub>22</sub> H <sub>41</sub> N <sub>7</sub> O <sub>11</sub> S <sub>2</sub>
Tigestol	Progestogen	896-71-9		C <sub>20</sub> H <sub>28</sub> O
Tigluidine	Antispasmodic	495-83-0		C <sub>13</sub> H <sub>21</sub> NO <sub>2</sub>
Tilarginine	Antineoplastic	17035-90-4		C <sub>7</sub> H <sub>16</sub> N <sub>4</sub> O <sub>2</sub>
Tilbroquinol	Antibiotic	7175-09-9		C <sub>10</sub> H <sub>8</sub> BrNO
Tiletamine	Anesthetic	14176-49-9		C <sub>12</sub> H <sub>17</sub> NOS
Tilidine	Analgesic	51931-66-9	Y	C <sub>17</sub> H <sub>23</sub> NO <sub>2</sub>
Tiliquinol	Antibiotic	5541-67-3		C <sub>10</sub> H <sub>9</sub> NO
Tilisolol	Antiarrhythmic	85136-71-6	Y	C <sub>17</sub> H <sub>24</sub> N <sub>2</sub> O <sub>3</sub>
Tilmacoxib	Antirheumatic	180200-68-4		C <sub>16</sub> H <sub>19</sub> FN <sub>2</sub> O <sub>3</sub> S
Tilmicosin	Antibacterial	108050-54-0		C <sub>46</sub> H <sub>80</sub> N <sub>2</sub> O <sub>13</sub>
Tilnoprofen Arbamel	Antiinflammatory	118635-52-2		C <sub>20</sub> H <sub>22</sub> N <sub>2</sub> O <sub>4</sub>
Tilomisole	Immunomodulator	58433-11-7		C <sub>17</sub> H <sub>11</sub> CIN <sub>2</sub> O <sub>2</sub> S
Tilorone	Antiviral	27591-97-5		C <sub>25</sub> H <sub>34</sub> N <sub>2</sub> O <sub>3</sub>
Tilozepine	Analgesic	42239-60-1		C <sub>17</sub> H <sub>18</sub> CIN <sub>3</sub> S
Tilsuprost	Prostaglandin	80225-28-1		C <sub>20</sub> H <sub>33</sub> NO <sub>4</sub> S
Tiludronate	Bone Resorption Inhibitor	89987-06-4		C <sub>7</sub> H <sub>9</sub> ClO <sub>6</sub> P <sub>2</sub> S
Timcodar	Antineoplastic	179033-51-3		C <sub>43</sub> H <sub>45</sub> CIN <sub>4</sub> O <sub>6</sub>
Timefurone	Antihyperlipidemic	76301-19-4		C <sub>15</sub> H <sub>14</sub> O <sub>5</sub> S
Timegadin	Antiinflammatory	71079-19-1		C <sub>20</sub> H <sub>23</sub> N <sub>5</sub> S
Timelotem	Antipsychotic	96306-34-2		C <sub>17</sub> H <sub>18</sub> FN <sub>3</sub> S
Timepidium Bromide	Mydriatic	35035-05-3		C <sub>17</sub> H <sub>22</sub> BrNOS <sub>2</sub>
Timiperone	Antipsychotic	57648-21-2		C <sub>22</sub> H <sub>24</sub> FN <sub>3</sub> OS
Timirdine	Antipsychotic	100417-09-2		C <sub>9</sub> H <sub>10</sub> CIN <sub>3</sub> S
Timobesone Acetate	Steroid	79578-14-6		C <sub>24</sub> H <sub>31</sub> FO <sub>5</sub> S
Timofibrate	Antihyperlipidemic	64179-54-0		C <sub>14</sub> H <sub>16</sub> ClNO <sub>4</sub> S
Timolol	Antihypertensive	26839-75-8	Y	C <sub>13</sub> H <sub>24</sub> N <sub>4</sub> O <sub>3</sub> S
Timonacic	Hepatic Protectant	444-27-9	Y	C <sub>4</sub> H <sub>7</sub> NO <sub>2</sub> S
Timoprazole	Antilucerative	57237-97-5		C <sub>13</sub> H <sub>11</sub> N <sub>3</sub> OS
Tinabitol	Antihypertensive	50708-95-7		C <sub>23</sub> H <sub>34</sub> O <sub>2</sub> S
Tinazoline	Antihypertensive	62882-99-9		C <sub>11</sub> H <sub>11</sub> N <sub>3</sub> S
Tinidazole	Antiprotozoal	19387-91-8	Y	C <sub>8</sub> H <sub>13</sub> N <sub>3</sub> O <sub>4</sub> S
Tinisulpride	Gastroprokinetic	69387-87-7		C <sub>20</sub> H <sub>29</sub> N <sub>3</sub> O <sub>4</sub> S

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Tinofedrine	Vasodilator	36702-83-7		C <sub>20</sub> H <sub>21</sub> NOS <sub>2</sub>
Tinoridine	Analgesic	24237-54-5		C <sub>17</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub> S
Tiocarlide	Antibacterial	910-86-1		C <sub>23</sub> H <sub>32</sub> N <sub>2</sub> O <sub>2</sub> S
Tiocloमारol	Anticoagulant	22619-35-8		C <sub>22</sub> H <sub>16</sub> Cl <sub>2</sub> O <sub>4</sub> S
Tioconazole	Antifungal	65899-73-2		C <sub>16</sub> H <sub>13</sub> Cl <sub>3</sub> N <sub>2</sub> OS
Tioctilate	Hepatic Protectant	10489-23-3		C <sub>15</sub> H <sub>22</sub> OS
Tiodazosin	Antihypertensive	66969-81-1		C <sub>18</sub> H <sub>21</sub> N <sub>7</sub> O <sub>4</sub> S
Tiodonium Chloride	Antibacterial	38070-41-6		C <sub>10</sub> H <sub>7</sub> Cl <sub>2</sub> IS
Tiomergine	Antipsychotic	57935-49-6		C <sub>21</sub> H <sub>21</sub> N <sub>3</sub> S
Tiomesterone	Androgen	2205-73-4		C <sub>24</sub> H <sub>34</sub> O <sub>4</sub> S <sub>2</sub>
Tioperidone	Antipsychotic	52618-67-4		C <sub>25</sub> H <sub>32</sub> N <sub>4</sub> O <sub>2</sub> S
Tiopinac	Antiinflammatory	61220-69-7		C <sub>16</sub> H <sub>12</sub> O <sub>3</sub> S
Tiopronin	Antidote	1953-02-2		C <sub>5</sub> H <sub>9</sub> NO <sub>3</sub> S
Tiopropamine	Antihistaminic	39516-21-7		C <sub>24</sub> H <sub>27</sub> NS
Tiospirone	Antipsychotic	87691-91-6		C <sub>24</sub> H <sub>32</sub> N <sub>4</sub> O <sub>2</sub> S
Tiotidine	Antihistaminic	69014-14-8		C <sub>10</sub> H <sub>16</sub> N <sub>8</sub> S <sub>2</sub>
Tiotropium	Bronchodilator	186691-13-4		C <sub>19</sub> H <sub>22</sub> NO <sub>4</sub> S <sub>2</sub>
Tioxacin	Antibiotic	34976-39-1		C <sub>14</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub> S
Tioxamast	Antihistaminic	74531-88-7		C <sub>14</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub> S
Tioxaprofen	Antiinflammatory	40198-53-6		C <sub>18</sub> H <sub>13</sub> Cl <sub>2</sub> NO <sub>3</sub> S
Tioxidazole	Anthelminthic	61570-90-9		C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub> S
Tioxolone	Dermatologic	4991-65-5		C <sub>7</sub> H <sub>4</sub> O <sub>3</sub> S
Tipentosin	Antihypertensive	95588-08-2		C <sub>21</sub> H <sub>25</sub> NO <sub>3</sub> S
Tipepidine	Antitussive	5169-78-8		C <sub>15</sub> H <sub>17</sub> NS <sub>2</sub>
Tipetropium Bromide	Antispasmodic	54376-91-9		C <sub>25</sub> H <sub>32</sub> BrNSOS
Tipifarnib	Antineoplastic	192185-72-1	Y	C <sub>27</sub> H <sub>22</sub> Cl <sub>2</sub> N <sub>4</sub> O
Tipindole	Antidepressant	7489-66-9		C <sub>16</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub> S
Tiplasinin	Anticoagulant	393105-53-8		C <sub>24</sub> H <sub>16</sub> F <sub>3</sub> NO <sub>4</sub>
Tipranavir	Antiviral	174484-41-4	Y	C <sub>31</sub> H <sub>33</sub> F <sub>3</sub> N <sub>2</sub> O <sub>5</sub> S
Tipredane	Steroid	85197-77-9		C <sub>22</sub> H <sub>31</sub> FO <sub>2</sub> S <sub>2</sub>
Tiprenolol	Antihypertensive	26481-51-6		C <sub>13</sub> H <sub>21</sub> NO <sub>2</sub> S
Tiprinast Meglumine	Antihistaminic	83153-39-3		C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub> S
Tipropidil	Vasodilator	70895-45-3		C <sub>20</sub> H <sub>35</sub> NO <sub>2</sub> S
Tiprostanide	Prostaglandin	67040-53-3		C <sub>33</sub> H <sub>45</sub> NO <sub>6</sub> S
Tiprotimod	Immunomodulator	105523-37-3		C <sub>10</sub> H <sub>13</sub> NO <sub>4</sub> S <sub>2</sub>
Tiqueside	Antihyperlipidemic	99759-19-0		C <sub>39</sub> H <sub>64</sub> O <sub>13</sub>
Tiquinamide	Mydriatic	53400-67-2		C <sub>11</sub> H <sub>14</sub> N <sub>2</sub> S
Tiquizium Bromide	Antispasmodic	71731-58-3		C <sub>19</sub> H <sub>24</sub> BrNS <sub>2</sub>
Tiracizine	Antidepressant	83275-56-3		C <sub>21</sub> H <sub>25</sub> N <sub>3</sub> O <sub>3</sub>
Tirapazamine	Antineoplastic	27314-97-2		C <sub>7</sub> H <sub>6</sub> N <sub>4</sub> O <sub>2</sub>
Tiratricol	Thyroid	51-24-1		C <sub>14</sub> H <sub>9</sub> I <sub>3</sub> O <sub>4</sub>
Tirilazad	Capillary Protectant	110101-66-1		C <sub>38</sub> H <sub>52</sub> N <sub>6</sub> O <sub>2</sub>
Tirofiban	Antithrombotic	144494-65-5		C <sub>22</sub> H <sub>36</sub> N <sub>2</sub> O <sub>5</sub> S
Tiropamide	Antispasmodic	55837-29-1		C <sub>28</sub> H <sub>41</sub> N <sub>3</sub> O <sub>3</sub>
Tisocromide	Antipsychotic	35423-51-9		C <sub>19</sub> H <sub>30</sub> N <sub>2</sub> O <sub>6</sub> S
Tisopurine	Antineoplastic	5334-23-6		C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> S
Tisoquone	Antineoplastic	40692-37-3		C <sub>17</sub> H <sub>17</sub> NS
Tivanidazole	Antiprotozoal	80680-05-3		C <sub>11</sub> H <sub>13</sub> N <sub>5</sub> O <sub>2</sub> S
Tiviciclovir	Antiviral	103024-93-7		C <sub>9</sub> H <sub>13</sub> N <sub>5</sub> O <sub>3</sub>
Tivirapine	Antiviral	137332-54-8		C <sub>16</sub> H <sub>20</sub> CIN <sub>3</sub> S
Tixadil	Unclassified	2949-95-3		C <sub>24</sub> H <sub>25</sub> NS
Tixanox	Antihistaminic	40691-50-7		C <sub>15</sub> H <sub>10</sub> O <sub>5</sub> S
Tixocortol Pivalate	Antiinflammatory	55560-96-8		C <sub>26</sub> H <sub>38</sub> O <sub>5</sub> S
Tizabrin	Unclassified	83573-53-9		C <sub>8</sub> H <sub>15</sub> NO <sub>3</sub> S
Tizanidine	Antispasmodic	51322-75-9	Y	C <sub>9</sub> H <sub>8</sub> CIN <sub>5</sub> S
Tizolemide	Diuretic	56488-58-5		C <sub>11</sub> H <sub>14</sub> CIN <sub>3</sub> O <sub>3</sub> S <sub>2</sub>
Tizoprolol Acid	Antihyperlipidemic	30709-69-4		C <sub>7</sub> H <sub>9</sub> NO <sub>2</sub> S
Tnp-470	Antineoplastic	129298-91-5		C <sub>19</sub> H <sub>28</sub> CINO <sub>6</sub>
Tobicillin	Antibiotic	151287-22-8		C <sub>27</sub> H <sub>30</sub> N <sub>2</sub> O <sub>6</sub> S
Toborinone	Cardiotonic	143343-83-3		C <sub>21</sub> H <sub>24</sub> N <sub>2</sub> O <sub>5</sub>
Tobramycin	Antibiotic	32986-56-4		C <sub>18</sub> H <sub>37</sub> N <sub>5</sub> O <sub>9</sub>
Tobuterol	Bronchodilator	75626-99-2		C <sub>28</sub> H <sub>31</sub> NO <sub>5</sub>
Tocainide	Antiarrhythmic	41708-72-9		C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> O

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Tocamphyl	Choleretic	465-27-0		C <sub>19</sub> H <sub>26</sub> O <sub>4</sub>
Tocladesine	Antineoplastic	41941-56-4		C <sub>10</sub> H <sub>11</sub> ClN <sub>5</sub> O <sub>6</sub> P
Tocofenoxate	Antidepressant	61343-44-0		C <sub>37</sub> H <sub>55</sub> ClO <sub>4</sub>
Tocofibrate	Antihyperlipidemic	50465-39-9		C <sub>39</sub> H <sub>59</sub> ClO <sub>4</sub>
Todralazine	Antihypertensive	14679-73-3		C <sub>11</sub> H <sub>12</sub> N <sub>4</sub> O <sub>2</sub>
Tofenacin	Antidepressant	15301-93-6		C <sub>17</sub> H <sub>21</sub> NO
Tofetridine	Analgesic	40173-75-9		C <sub>15</sub> H <sub>21</sub> NO
Tofimilast	Bronchodilator	185954-27-2		C <sub>18</sub> H <sub>21</sub> N <sub>5</sub> S
Tofisoline	Unclassified	29726-99-6		C <sub>22</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub>
Tofisopam	Anxiolytic	22345-47-7		C <sub>22</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub>
Tolafentrine	Erectile Dysfunction	139308-65-9		C <sub>28</sub> H <sub>31</sub> N <sub>3</sub> O <sub>4</sub> S
Tolamolol	Vasodilator	38103-61-6		C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> O <sub>4</sub>
Tolazamide	Antidiabetic	1156-19-0		C <sub>14</sub> H <sub>21</sub> N <sub>3</sub> O <sub>3</sub> S
Tolazoline	Vasodilator	59-98-3		C <sub>10</sub> H <sub>12</sub> N <sub>2</sub>
Tolboxane	Antianginal	2430-46-8		C <sub>14</sub> H <sub>21</sub> BO <sub>2</sub>
Tolbutamide	Antidiabetic	64-77-7		C <sub>12</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub> S
Tolcapone	Antiparkinsonian	134308-13-7	Y	C <sub>14</sub> H <sub>11</sub> NO <sub>5</sub>
Tolciclate	Antifungal	50838-36-3		C <sub>20</sub> H <sub>21</sub> NOS
Toldimfos	Antineoplastic	57808-64-7		C <sub>9</sub> H <sub>14</sub> NO <sub>2</sub> P
Tolfamide	Antibiotic	70788-29-3		C <sub>8</sub> H <sub>12</sub> N <sub>3</sub> O <sub>2</sub> P
Tolfenamic Acid	Antiinflammatory	13710-19-5		C <sub>14</sub> H <sub>12</sub> ClNO <sub>2</sub>
Tolgabide	Anticonvulsant	86914-11-6		C <sub>18</sub> H <sub>18</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Tolimidone	Antiulcerative	41964-07-2		C <sub>11</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>
Tolindate	Antifungal	27877-51-6		C <sub>18</sub> H <sub>19</sub> NOS
Toliodium Chloride	Antibacterial	19028-28-5		C <sub>14</sub> H <sub>14</sub> ClI
Toliprolol	Antianginal	2933-94-0		C <sub>13</sub> H <sub>21</sub> NO <sub>2</sub>
Tolmesoxide	Antihypertensive	38452-29-8		C <sub>10</sub> H <sub>14</sub> O <sub>3</sub> S
Tolmetin	Antiinflammatory	26171-23-3		C <sub>15</sub> H <sub>15</sub> NO <sub>3</sub>
Tolnaftate	Antifungal	2398-96-1		C <sub>19</sub> H <sub>17</sub> NOS
Tolnapersine	Antihypertensive	70312-00-4		C <sub>21</sub> H <sub>26</sub> N <sub>2</sub> O
Tolnidamine	Antihistaminic	50454-68-7		C <sub>16</sub> H <sub>13</sub> ClN <sub>2</sub> O <sub>2</sub>
Tolconium Metilsulfate	Antifungal	552-92-1		C <sub>23</sub> H <sub>43</sub> NO <sub>4</sub> S
Tolonidine	Antihypertensive	4201-22-3		C <sub>10</sub> H <sub>12</sub> ClN <sub>3</sub>
Toloxatone	Antidepressant	29218-27-7		C <sub>11</sub> H <sub>13</sub> NO <sub>3</sub>
Tolpadol	Analgesic	77502-27-3		C <sub>28</sub> H <sub>26</sub> N <sub>4</sub> O <sub>2</sub>
Tolpentamide	Antispasmodic	1027-87-8		C <sub>13</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub> S
Tolperisone	Muscle Relaxant	728-88-1	Y	C <sub>16</sub> H <sub>23</sub> NO
Tolpiprazole	Antipsychotic	20326-13-0		C <sub>17</sub> H <sub>24</sub> N <sub>4</sub>
Tolpronine	Analgesic	97-57-4		C <sub>15</sub> H <sub>21</sub> NO <sub>2</sub>
Tolpropamine	Antihistaminic	5632-44-0		C <sub>18</sub> H <sub>23</sub> N
Tolpyrramide	Antidiabetic	5588-38-5		C <sub>12</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub> S
Tolquinzole	Unclassified	6187-50-4		C <sub>16</sub> H <sub>23</sub> NO
Tolrestat	Antidiabetic	82964-04-3		C <sub>16</sub> H <sub>14</sub> F <sub>3</sub> NO <sub>3</sub> S
Tolterodine	Misc- Urologic	124937-51-5	Y	C <sub>22</sub> H <sub>31</sub> NO
Toltrazuril	Antibacterial	69004-03-1		C <sub>18</sub> H <sub>14</sub> F <sub>3</sub> N <sub>3</sub> O <sub>4</sub> S
Tolufazepam	Anxiolytic	86273-92-9		C <sub>24</sub> H <sub>20</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>3</sub> S
Tolvaptan	Cardiotonic	150683-30-0	Y	C <sub>26</sub> H <sub>25</sub> ClN <sub>2</sub> O <sub>3</sub>
Tolycaine	Anesthetic	3686-58-6		C <sub>15</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub>
Tomeglovir	Antiviral	233254-24-5		C <sub>23</sub> H <sub>27</sub> N <sub>3</sub> O <sub>4</sub> S
Tomelukast	Bronchodilator	88107-10-2		C <sub>16</sub> H <sub>22</sub> N <sub>4</sub> O <sub>3</sub>
Tomoglumide	Gastroprokinetic	97964-54-0		C <sub>24</sub> H <sub>38</sub> N <sub>2</sub> O <sub>4</sub>
Tomoxiprole	Antiinflammatory	76145-76-1		C <sub>21</sub> H <sub>20</sub> N <sub>2</sub> O
Tonabersat	Antimigraine	175013-84-0		C <sub>20</sub> H <sub>19</sub> ClFNO <sub>4</sub>
Tonazocine Mesylate	Analgesic	71461-18-2		C <sub>23</sub> H <sub>35</sub> NO <sub>2</sub>
Topicaïne	Analgesic	76-91-5		C <sub>26</sub> H <sub>37</sub> NO <sub>4</sub>
Topilutamide	Sedative	260980-89-0		C <sub>13</sub> H <sub>11</sub> F <sub>6</sub> N <sub>3</sub> O <sub>5</sub>
Topiramate	Anticonvulsant	97240-79-4	Y	C <sub>12</sub> H <sub>21</sub> NO <sub>8</sub> S
Topixantrone	Antineoplastic	156090-18-5		C <sub>21</sub> H <sub>26</sub> N <sub>6</sub> O <sub>2</sub>
Topotecan	Antineoplastic	123948-87-8	Y	C <sub>23</sub> H <sub>23</sub> N <sub>3</sub> O <sub>5</sub>
Toprilidone	Analgesic	54063-58-0		C <sub>19</sub> H <sub>25</sub> N <sub>3</sub> O
Topterone	Steroid	60607-35-4		C <sub>22</sub> H <sub>34</sub> O <sub>2</sub>
Toquizine	Mydriatic	7125-71-5		C <sub>23</sub> H <sub>29</sub> N <sub>5</sub> O
Torbafylline	Bronchodilator	105102-21-4		C <sub>16</sub> H <sub>26</sub> N <sub>4</sub> O <sub>4</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Torcetrapib	Antihyperlipidemic	262352-17-0		C <sub>26</sub> H <sub>25</sub> F <sub>9</sub> N <sub>2</sub> O <sub>4</sub>
Torcitabine	Antiviral	40093-94-5		C <sub>9</sub> H <sub>13</sub> N <sub>3</sub> O <sub>4</sub>
Toremifene	Antineoplastic	89778-26-7	Y	C <sub>26</sub> H <sub>28</sub> ClNO
Toripristone	Progestogen	91935-26-1		C <sub>31</sub> H <sub>39</sub> NO <sub>2</sub>
Torsemide	Diuretic	56211-40-6		C <sub>16</sub> H <sub>20</sub> N <sub>4</sub> O <sub>5</sub> S
Tosagestin	Contraceptive	110072-15-6		C <sub>21</sub> H <sub>24</sub> O <sub>2</sub>
Tosifen	Antianginal	32295-18-4		C <sub>17</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> S
Tosufloxacin	Antibiotic	100490-36-6	Y	C <sub>19</sub> H <sub>15</sub> F <sub>3</sub> N <sub>4</sub> O <sub>3</sub>
Tosulur	Unclassified	87051-13-6		C <sub>11</sub> H <sub>15</sub> NO <sub>5</sub> S
Trabectedin	Antineoplastic	114899-77-3		C <sub>39</sub> H <sub>43</sub> N <sub>3</sub> O <sub>11</sub> S
Traboxopine	Antipsychotic	103624-59-5		C <sub>19</sub> H <sub>23</sub> ClN <sub>2</sub> O <sub>2</sub>
Tracazolate	Sedative	41094-88-6		C <sub>16</sub> H <sub>24</sub> N <sub>4</sub> O <sub>2</sub>
Tradecamide	Unclassified	132787-19-0		C <sub>15</sub> H <sub>31</sub> NO <sub>2</sub>
Tralonide	Glucocorticoid	21365-49-1		C <sub>24</sub> H <sub>28</sub> Cl <sub>2</sub> F <sub>2</sub> O <sub>4</sub>
Tramadol	Analgesic	27203-92-5	Y	C <sub>16</sub> H <sub>25</sub> NO <sub>2</sub>
Tramazoline	Decongestant	1082-57-1		C <sub>13</sub> H <sub>17</sub> N <sub>3</sub>
Tramiprosate	Nootropic	3687-18-1		C <sub>3</sub> H <sub>9</sub> NO <sub>3</sub> S
Trandolapril	Antihypertensive	87679-37-6		C <sub>24</sub> H <sub>34</sub> N <sub>2</sub> O <sub>5</sub>
Trandolaprilat	Antihypertensive	87679-71-8		C <sub>22</sub> H <sub>30</sub> N <sub>2</sub> O <sub>5</sub>
Tranexamic Acid	Hemostatic	1197-18-8		C <sub>8</sub> H <sub>15</sub> NO <sub>2</sub>
Tranilast	Antihistaminic	53902-12-8		C <sub>18</sub> H <sub>17</sub> NO <sub>5</sub>
Transcainide	Antiarrhythmic	88296-62-2		C <sub>22</sub> H <sub>35</sub> N <sub>3</sub> O <sub>2</sub>
Trantelium Bromide	Antispasmodic	4047-34-1		C <sub>23</sub> H <sub>26</sub> NO <sub>3</sub> .Br
Tranylcypromine	Antidepressant	155-09-9		C <sub>9</sub> H <sub>11</sub> N
Trapenacaine	Anesthetic	104485-01-0		C <sub>22</sub> H <sub>34</sub> N <sub>2</sub> O <sub>3</sub>
Trapidil	Vasodilator	15421-84-8		C <sub>10</sub> H <sub>15</sub> N <sub>5</sub>
Travoprost	Antiglaucoma	157283-68-6		C <sub>26</sub> H <sub>35</sub> F <sub>3</sub> O <sub>6</sub>
Traxanox	Antihistaminic	58712-69-9		C <sub>13</sub> H <sub>6</sub> ClN <sub>5</sub> O <sub>2</sub>
Traxoprodil Mesylate	Nootropic	134234-12-1		C <sub>20</sub> H <sub>25</sub> NO <sub>3</sub>
Trazitiline	Antidepressant	26070-23-5		C <sub>21</sub> H <sub>24</sub> N <sub>2</sub>
Trazium Esilate	Antidepressant	97110-59-3		C <sub>19</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>4</sub> S
Trazodone	Antidepressant	19794-93-5	Y	C <sub>19</sub> H <sub>22</sub> ClN <sub>5</sub> O
Trazolopride	Antiemetic	86365-92-6		C <sub>20</sub> H <sub>23</sub> N <sub>5</sub> O <sub>2</sub>
Trebenzomine	Antidepressant	23915-73-3		C <sub>12</sub> H <sub>17</sub> NO
Trecadrine	Antidiabetic	108767-50-6		C <sub>27</sub> H <sub>29</sub> NO
Trecetilide	Antiarrhythmic	180918-68-7		C <sub>21</sub> H <sub>37</sub> FN <sub>2</sub> O <sub>3</sub> S
Trefentanil	Analgesic	120656-74-8		C <sub>25</sub> H <sub>31</sub> FN <sub>6</sub> O <sub>2</sub>
Trelnarizine	Antihistaminic	123205-52-7		C <sub>28</sub> H <sub>30</sub> F <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Treloxinate	Antihyperlipidemic	30910-27-1		C <sub>16</sub> H <sub>12</sub> Cl <sub>2</sub> O <sub>4</sub>
Trenbolone Acetate	Steroid	10161-34-9		C <sub>20</sub> H <sub>24</sub> O <sub>3</sub>
Trengestone	Progestogen	5192-84-7		C <sub>21</sub> H <sub>25</sub> ClO <sub>2</sub>
Trenizine	Antihistaminic	89224-07-7		C <sub>31</sub> H <sub>40</sub> N <sub>2</sub> O
Treosulfan	Antineoplastic	299-75-2	Y	C <sub>6</sub> H <sub>14</sub> O <sub>8</sub> S <sub>2</sub>
Trepibutone	Choleretic	41826-92-0		C <sub>16</sub> H <sub>22</sub> O <sub>6</sub>
Trepipam Maleate	Sedative	56030-50-3		C <sub>19</sub> H <sub>23</sub> NO <sub>2</sub>
Trepirium Iodide	Antihypertensive	1018-34-4		C <sub>12</sub> H <sub>26</sub> I <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Treprostinil	Antihypertensive	81846-19-7	Y	C <sub>23</sub> H <sub>34</sub> O <sub>5</sub>
Treptilamine	Antispasmodic	58313-74-9		C <sub>20</sub> H <sub>27</sub> NO
Trequinsin	Antihypertensive	79855-88-2		C <sub>24</sub> H <sub>27</sub> N <sub>3</sub> O <sub>3</sub>
Tresperimus	Immunosuppressant	160677-67-8		C <sub>17</sub> H <sub>37</sub> N <sub>7</sub> O <sub>3</sub>
Trestolone Acetate	Androgen	6157-87-5		C <sub>21</sub> H <sub>30</sub> O <sub>3</sub>
Tretazicar	Antineoplastic	21919-05-1		C <sub>9</sub> H <sub>8</sub> N <sub>4</sub> O <sub>5</sub>
Trethinium Tosilate	Unclassified	1748-43-2		C <sub>19</sub> H <sub>25</sub> NO <sub>3</sub> S
Tretinoin	Antineoplastic	302-79-4	Y	C <sub>20</sub> H <sub>28</sub> O <sub>2</sub>
Tretinoin Tocoferil	Dermatologic	40516-48-1		C <sub>49</sub> H <sub>76</sub> O <sub>3</sub>
Tretoquinol	Bronchodilator	30418-38-3		C <sub>19</sub> H <sub>23</sub> NO <sub>5</sub>
Triacetin	Antifungal	102-76-1		C <sub>9</sub> H <sub>14</sub> O <sub>6</sub>
Triafungin	Antifungal	55242-77-8		C <sub>13</sub> H <sub>10</sub> N <sub>4</sub>
Triamcinolone	Glucocorticoid	124-94-7		C <sub>21</sub> H <sub>27</sub> FO <sub>6</sub>
Triamcinolone Acetonide	Glucocorticoid	76-25-5		C <sub>24</sub> H <sub>31</sub> FO <sub>6</sub>
Triamcinolone Benetonide	Glucocorticoid	31002-79-6		C <sub>35</sub> H <sub>42</sub> FN <sub>8</sub> O <sub>8</sub>
Triamcinolone Diacetate	Glucocorticoid	67-78-7		C <sub>25</sub> H <sub>31</sub> FO <sub>8</sub>
Triamcinolone Furetonide	Glucocorticoid	4989-94-0		C <sub>33</sub> H <sub>35</sub> FO <sub>8</sub>



Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Triamcinolone Hexacetonide	Antiinflammatory	5611-51-8		C <sub>30</sub> H <sub>41</sub> FO <sub>7</sub>
Triampyzine Sulfate	Mydriatic	6503-95-3		C <sub>9</sub> H <sub>15</sub> N <sub>3</sub>
Triamterene	Diuretic	396-01-0		C <sub>12</sub> H <sub>11</sub> N <sub>7</sub>
Triaziquone	Antineoplastic	68-76-8		C <sub>12</sub> H <sub>13</sub> N <sub>3</sub> O <sub>2</sub>
Triazolam	Sedative	28911-01-5	Y	C <sub>17</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>4</sub>
Tribendilol	Antihypertensive	96258-13-8		C <sub>18</sub> H <sub>22</sub> N <sub>4</sub> O <sub>4</sub>
Tribenoside	Dermatologic	10310-32-4		C <sub>29</sub> H <sub>34</sub> O <sub>6</sub>
Tribromoethanol	Anesthetic	75-80-9		C <sub>2</sub> H <sub>3</sub> Br <sub>3</sub> O
Tribromsalan	Antibacterial	87-10-5		C <sub>13</sub> H <sub>8</sub> Br <sub>3</sub> NO <sub>2</sub>
Tribuzone	Antiinflammatory	13221-27-7		C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>3</sub>
Tricetamide	Sedative	363-20-2		C <sub>16</sub> H <sub>24</sub> N <sub>2</sub> O <sub>5</sub>
Trichlormethiazide	Diuretic	133-67-5		C <sub>8</sub> H <sub>8</sub> Cl <sub>3</sub> N <sub>3</sub> O <sub>4</sub> S <sub>2</sub>
Trichlormethine	Antineoplastic	555-77-1		C <sub>6</sub> H <sub>12</sub> Cl <sub>3</sub> N
2,2,2-Trichloroethanol	Sedative	115-20-8		C <sub>2</sub> H <sub>3</sub> Cl <sub>3</sub> O
Trichloroethylene	Anesthetic	79-01-6		C <sub>2</sub> HCl <sub>3</sub>
Triciribine	Antineoplastic	35943-35-2		C <sub>13</sub> H <sub>16</sub> N <sub>6</sub> O <sub>4</sub>
Triclabendazole	Anthelmintic	68786-66-3		C <sub>14</sub> H <sub>9</sub> Cl <sub>3</sub> N <sub>2</sub> O <sub>5</sub>
Triclacetamol	Analgesic	6340-87-0		C <sub>8</sub> H <sub>6</sub> Cl <sub>3</sub> NO <sub>2</sub>
Triclazate	Anorexic	7009-76-9		C <sub>20</sub> H <sub>23</sub> NO <sub>3</sub>
Triclodazol	Antiprotozoal	56-28-0		C <sub>17</sub> H <sub>15</sub> Cl <sub>3</sub> N <sub>2</sub> O <sub>2</sub>
Triclofenol Piperazine	Anthelmintic	95-95-4		C <sub>6</sub> H <sub>3</sub> Cl <sub>3</sub> O
Triclofos	Sedative	306-52-5		C <sub>2</sub> H <sub>4</sub> Cl <sub>3</sub> O <sub>4</sub> P
Triclofylline	Bronchodilator	17243-70-8		C <sub>11</sub> H <sub>13</sub> Cl <sub>3</sub> N <sub>4</sub> O <sub>4</sub>
Triclonide	Antiinflammatory	26849-57-0		C <sub>24</sub> H <sub>28</sub> Cl <sub>3</sub> FO <sub>4</sub>
Tricyclamol Chloride	Antiparkinsonian	3818-88-0		C <sub>20</sub> H <sub>32</sub> ClNO
Tridihexethyl	Antispasmodic	60-49-1		C <sub>21</sub> H <sub>36</sub> NO+
Tridihexethyl Iodide	Mydriatic	125-99-5		C <sub>21</sub> H <sub>36</sub> INO
Tridolgosir	Antineoplastic	72741-87-8		C <sub>8</sub> H <sub>15</sub> NO <sub>3</sub>
Trientine	Antidote	112-24-3		C <sub>6</sub> H <sub>18</sub> N <sub>4</sub>
Triethylamine	Antiinflammatory	121-44-8		C <sub>6</sub> H <sub>15</sub> N
Triethylene Glycol	Antineoplastic	112-27-6		C <sub>6</sub> H <sub>14</sub> O <sub>4</sub>
Triethylene Glycol Diacetate	Antineoplastic	111-21-7		C <sub>10</sub> H <sub>18</sub> O <sub>6</sub>
Triethylenemelamine	Antineoplastic	51-18-3		C <sub>9</sub> H <sub>12</sub> N <sub>6</sub>
Trifenagrel	Antithrombotic	84203-09-8		C <sub>25</sub> H <sub>25</sub> N <sub>3</sub> O
Trifezolac	Antiinflammatory	32710-91-1		C <sub>23</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>
Triflocin	Diuretic	13422-16-7		C <sub>13</sub> H <sub>9</sub> F <sub>3</sub> N <sub>2</sub> O <sub>2</sub>
Triflubazam	Anxiolytic	22365-40-8		C <sub>17</sub> H <sub>13</sub> F <sub>3</sub> N <sub>2</sub> O <sub>2</sub>
Triflumidate	Antiinflammatory	24243-89-8		C <sub>17</sub> H <sub>14</sub> F <sub>3</sub> NO <sub>5</sub> S
Trifluomeprazine	Analgesic	2622-37-9		C <sub>19</sub> H <sub>21</sub> F <sub>3</sub> N <sub>2</sub> S
Trifluoperazine	Antipsychotic	117-89-5		C <sub>21</sub> H <sub>24</sub> F <sub>3</sub> N <sub>3</sub> S
Trifluoperidol	Antipsychotic	749-13-3		C <sub>22</sub> H <sub>23</sub> F <sub>4</sub> NO <sub>2</sub>
Triflupromazine	Antipsychotic	146-54-3		C <sub>18</sub> H <sub>19</sub> F <sub>3</sub> N <sub>2</sub> S
Trifluridine	Antiviral	70-00-8		C <sub>10</sub> H <sub>11</sub> F <sub>3</sub> N <sub>2</sub> O <sub>5</sub>
Triflusal	Antithrombotic	322-79-2		C <sub>10</sub> H <sub>7</sub> F <sub>3</sub> O <sub>4</sub>
Trigevolol	Antihypertensive	76812-98-1		C <sub>21</sub> H <sub>28</sub> N <sub>2</sub> O <sub>7</sub>
Trihexyphenidyl	Antiparkinsonian	144-11-6		C <sub>20</sub> H <sub>31</sub> NO
Triletide	Anticoagulant	62087-96-1		C <sub>27</sub> H <sub>31</sub> N <sub>5</sub> O <sub>5</sub>
Trilostane	Pituitary	13647-35-3		C <sub>20</sub> H <sub>27</sub> NO <sub>3</sub>
Trimazosin	Antihypertensive	35795-16-5		C <sub>20</sub> H <sub>29</sub> N <sub>5</sub> O <sub>6</sub>
Trimebutine	Antispasmodic	39133-31-8		C <sub>22</sub> H <sub>29</sub> NO <sub>5</sub>
Trimecaine	Anesthetic	616-68-2		C <sub>15</sub> H <sub>24</sub> N <sub>2</sub> O
Trimedoxime Bromide	Antidote	56-97-3		C <sub>15</sub> H <sub>18</sub> Br <sub>2</sub> N <sub>4</sub> O <sub>2</sub>
Trimegestone	Progestogen	74513-62-5		C <sub>22</sub> H <sub>30</sub> O <sub>3</sub>
Trimeperidine	Analgesic	64-39-1		C <sub>17</sub> H <sub>25</sub> NO <sub>2</sub>
Trimetazidine	Antianginal	5011-34-7		C <sub>14</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub>
Trimethadione	Anticonvulsant	127-48-0		C <sub>6</sub> H <sub>9</sub> NO <sub>3</sub>
Trimethamide	Nootropic	5789-72-0		C <sub>17</sub> H <sub>21</sub> N <sub>3</sub> O <sub>4</sub>
Trimethaphan Camsylate	Antihypertensive	68-91-7		C <sub>22</sub> H <sub>25</sub> N <sub>2</sub> OS.C <sub>10</sub> H <sub>15</sub> O <sub>4</sub> S
Trimethidinium Methosulfate	Antihypertensive	14149-43-0		C <sub>19</sub> H <sub>42</sub> N <sub>2</sub> O <sub>8</sub> S <sub>2</sub>
Trimethobenzamide	Antiemetic	138-56-7		C <sub>21</sub> H <sub>28</sub> N <sub>2</sub> O <sub>5</sub>
Trimethoprim	Antibacterial	738-70-5	Y	C <sub>14</sub> H <sub>18</sub> N <sub>4</sub> O <sub>3</sub>
Trimethylcetylammmonium Pentachlorophenate	Antibacterial	87-76-3		C <sub>19</sub> H <sub>42</sub> N.C <sub>6</sub> Cl <sub>5</sub> O

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Trimetozine	Anxiolytic	635-41-6		C <sub>14</sub> H <sub>19</sub> NO <sub>5</sub>
Trimetrexate	Antineoplastic	52128-35-5		C <sub>19</sub> H <sub>23</sub> N <sub>5</sub> O <sub>3</sub>
Trimetrexate Glucuronate	Antineoplastic	6556-12-3		C <sub>6</sub> H <sub>10</sub> O <sub>7</sub>
Trimexiline	Unclassified	64015-58-3		C <sub>17</sub> H <sub>29</sub> N
Trimipramine	Antidepressant	739-71-9		C <sub>20</sub> H <sub>26</sub> N <sub>2</sub>
Trimoprostil	Antilucerative	69900-72-7		C <sub>23</sub> H <sub>38</sub> O <sub>4</sub>
Trimoxamine	Antihypertensive	15686-23-4		C <sub>15</sub> H <sub>23</sub> NO <sub>3</sub>
Trioxifene Mesylate	Estrogen	68307-81-3		C <sub>30</sub> H <sub>31</sub> NO <sub>3</sub>
Trioxsalen	Dermatologic	3902-71-4		C <sub>14</sub> H <sub>12</sub> O <sub>3</sub>
Tripamide	Diuretic	73803-48-2		C <sub>16</sub> H <sub>20</sub> ClN <sub>3</sub> O <sub>3</sub> S
Triparanol	Antihyperlipidemic	78-41-1		C <sub>27</sub> H <sub>32</sub> ClNO <sub>2</sub>
Tripelennamine	Antihistaminic	91-81-6		C <sub>16</sub> H <sub>21</sub> N <sub>3</sub>
Tripolidine	Antihistaminic	486-12-4		C <sub>19</sub> H <sub>22</sub> N <sub>2</sub>
Tritiozine	Antilucerative	35619-65-9		C <sub>14</sub> H <sub>19</sub> NO <sub>4</sub> S
Tritoqualine	Antihistaminic	14504-73-5		C <sub>26</sub> H <sub>32</sub> N <sub>2</sub> O <sub>8</sub>
Trixolane	Unclassified	47420-28-0		C <sub>18</sub> H <sub>27</sub> NO <sub>6</sub>
Trizoxime	Antibiotic	35710-57-7		C <sub>16</sub> H <sub>15</sub> N <sub>5</sub> O <sub>2</sub>
Trocimine	Antipsychotic	14368-24-2		C <sub>17</sub> H <sub>25</sub> NO <sub>4</sub>
Trodusquemine	Antiobesity	186139-09-3		C <sub>37</sub> H <sub>72</sub> N <sub>4</sub> O <sub>5</sub> S
Trofosfamide	Antineoplastic	22089-22-1		C <sub>9</sub> H <sub>18</sub> Cl <sub>3</sub> N <sub>3</sub> O <sub>2</sub> P
Troglitazone	Antidiabetic	97322-87-7		C <sub>24</sub> H <sub>27</sub> NO <sub>5</sub> S
Trolamine	Analgesic	102-71-6		C <sub>6</sub> H <sub>15</sub> NO <sub>3</sub>
Troleandomycin	Antibiotic	2751-09-9		C <sub>41</sub> H <sub>67</sub> NO <sub>15</sub>
Trolnitrate Phosphate	Antianginal	7077-34-1		C <sub>6</sub> H <sub>12</sub> N <sub>4</sub> O <sub>9</sub>
Tromantadine	Antiviral	53783-83-8		C <sub>16</sub> H <sub>28</sub> N <sub>2</sub> O <sub>2</sub>
Tromethamine	Oxytocic	77-86-1		C <sub>4</sub> H <sub>11</sub> NO <sub>3</sub>
Tropabazate	Unclassified	64294-94-6		C <sub>15</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub>
Tropanserine	Antidepressant	85181-40-4		C <sub>17</sub> H <sub>23</sub> NO <sub>2</sub>
Tropapride	Antipsychotic	76352-13-1		C <sub>23</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub>
Tropatepine	Antipsychotic	27574-24-9		C <sub>22</sub> H <sub>23</sub> NS
Tropenziline Bromide	Antispasmodic	143-92-0		C <sub>24</sub> H <sub>30</sub> BrNO <sub>4</sub>
Tropicamide	Mydriatic	1508-75-4		C <sub>17</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>
Tropigline	Unclassified	533-08-4		C <sub>13</sub> H <sub>21</sub> NO <sub>2</sub>
Tropirine	Antihistamine	19410-02-7		C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O
Tropisetron	Antiemetic	89565-68-4	Y	C <sub>17</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>
Tropodifene	Antihypertensive	15790-02-0		C <sub>25</sub> H <sub>29</sub> NO <sub>4</sub>
Troquidazole	Antiprotozoal	108001-60-1		C <sub>14</sub> H <sub>15</sub> N <sub>5</sub> O <sub>3</sub>
Trospectomycin	Antibiotic	88669-04-9		C <sub>17</sub> H <sub>30</sub> N <sub>2</sub> O <sub>7</sub>
Trospium	Antispasmodic	47608-32-2		C <sub>25</sub> H <sub>30</sub> ClNO <sub>3</sub>
Trovafloxacin	Antibacterial	147059-72-1	Y	C <sub>20</sub> H <sub>15</sub> F <sub>3</sub> N <sub>4</sub> O <sub>3</sub>
Trovirdine	Antiviral	149488-17-5		C <sub>13</sub> H <sub>13</sub> BrN <sub>4</sub> S
Troxacitabine	Antineoplastic	145918-75-8		C <sub>8</sub> H <sub>11</sub> N <sub>3</sub> O <sub>4</sub>
Troxerutin	Capillary Protectant	7085-55-4		C <sub>33</sub> H <sub>42</sub> O <sub>19</sub>
Troxipide	Antilucerative	30751-05-4		C <sub>15</sub> H <sub>22</sub> N <sub>2</sub> O <sub>4</sub>
Troxypyrrolium Tosilate	Mydriatic	3612-98-4		C <sub>25</sub> H <sub>35</sub> NO <sub>8</sub> S
Truxicuriem Iodide	Muscle Relaxant	4304-01-2		C <sub>34</sub> H <sub>52</sub> I <sub>2</sub> N <sub>2</sub> O <sub>4</sub>
Truxipicuriem Iodide	Muscle Relaxant	35515-77-6		C <sub>38</sub> H <sub>56</sub> I <sub>2</sub> N <sub>2</sub> O <sub>4</sub>
Tryparsamide	Antiprotozoal	618-25-7		C <sub>8</sub> H <sub>11</sub> AsN <sub>2</sub> O <sub>4</sub>
Tuaminoheptane	Decongestant	123-82-0		C <sub>7</sub> H <sub>17</sub> N
Tubocurarine	Neuromuscular Blocking Agent	57-95-4		C <sub>37</sub> H <sub>41</sub> N <sub>2</sub> O <sub>6</sub>
Tubulozole	Antineoplastic	84697-22-3		C <sub>23</sub> H <sub>23</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>4</sub> S
Tucarezol	Immunomodulator	84290-27-7		C <sub>13</sub> H <sub>12</sub> O <sub>5</sub>
Tuclazepam	Anxiolytic	51037-88-8		C <sub>17</sub> H <sub>16</sub> Cl <sub>2</sub> N <sub>2</sub> O
Tulathromycin	Antibacterial	217500-96-4		C <sub>41</sub> H <sub>79</sub> N <sub>3</sub> O <sub>12</sub>
Tulobuterol	Bronchodilator	41570-61-0		C <sub>12</sub> H <sub>18</sub> ClNO
Tulopafant	Anticoagulant	116289-53-3		C <sub>25</sub> H <sub>19</sub> N <sub>3</sub> O <sub>2</sub> S
Turosteride	Antineoplastic	137099-09-3		C <sub>27</sub> H <sub>45</sub> N <sub>3</sub> O <sub>3</sub>
Tuvatidine	Antilucerative	91257-14-6		C <sub>10</sub> H <sub>17</sub> N <sub>9</sub> O <sub>2</sub> S <sub>3</sub>
Tybamate	Anxiolytic	4268-36-4		C <sub>13</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub>
Tylosin	Antibiotic	1401-69-0		C <sub>46</sub> H <sub>77</sub> NO <sub>17</sub>
Tymazoline	Decongestant	24243-97-8		C <sub>14</sub> H <sub>20</sub> N <sub>2</sub> O
Ubenimex	Immunomodulator	58970-76-6		C <sub>16</sub> H <sub>24</sub> N <sub>2</sub> O <sub>4</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Ubidecarenone	Antihypertensive	303-98-0		C <sub>59</sub> H <sub>90</sub> O <sub>4</sub>
Ubisindine	Unclassified	26070-78-0		C <sub>20</sub> H <sub>24</sub> N <sub>2</sub> O
Udenafil	Erectile Dysfunction	268203-93-6	Y	C <sub>25</sub> H <sub>36</sub> N <sub>6</sub> O <sub>4</sub> S
Ufenamate	Antiinflammatory	67330-25-0		C <sub>18</sub> H <sub>18</sub> F <sub>3</sub> NO <sub>2</sub>
Ufiprazole	Anxiolytic	73590-85-9		C <sub>17</sub> H <sub>19</sub> N <sub>3</sub> O <sub>2</sub> S
Uldazepam	Anxiolytic	28546-58-9		C <sub>18</sub> H <sub>15</sub> Cl <sub>2</sub> N <sub>3</sub> O
Ulifloxacin	Antibiotic	112984-60-8		C <sub>16</sub> H <sub>16</sub> FN <sub>3</sub> O <sub>3</sub> S
Umespiron	Antidepressant	107736-98-1		C <sub>28</sub> H <sub>40</sub> N <sub>4</sub> O <sub>5</sub>
Undecylenic Acid	Antifungal	112-38-9		C <sub>11</sub> H <sub>20</sub> O <sub>2</sub>
Unoprostone	Prostaglandin	120373-36-6		C <sub>22</sub> H <sub>38</sub> O <sub>5</sub>
Upenazime	Antihypertensive	95268-62-5		C <sub>14</sub> H <sub>30</sub> N <sub>4</sub> O <sub>2</sub>
Upidosin	Antihypertensive	152735-23-4		C <sub>31</sub> H <sub>33</sub> N <sub>3</sub> O <sub>4</sub>
Uracil	Antineoplastic	66-22-8	Y	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>
Uracil Mustard	Antineoplastic	66-75-1		C <sub>8</sub> H <sub>11</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>2</sub>
Urapidil	Antihypertensive	34661-75-1		C <sub>20</sub> H <sub>29</sub> N <sub>5</sub> O <sub>3</sub>
Urea	Diuretic	57-13-6		CH <sub>4</sub> N <sub>2</sub> O
Uredepa	Antineoplastic	302-49-8		C <sub>7</sub> H <sub>14</sub> N <sub>3</sub> O <sub>3</sub> P
Uredofos	Anthelminthic	52406-01-6		C <sub>19</sub> H <sub>25</sub> N <sub>4</sub> O <sub>6</sub> PS <sub>2</sub>
Urefibrate	Bone Resorption Inhibitor	38647-79-9		C <sub>15</sub> H <sub>12</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>4</sub>
Urethane	Antineoplastic	51-79-6		C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>
Ursodiol	Anticholelithogenic	128-13-2	Y	C <sub>24</sub> H <sub>40</sub> O <sub>4</sub>
Ursulcholic Acid	Anticholelithogenic	88426-32-8		C <sub>24</sub> H <sub>40</sub> O <sub>10</sub> S <sub>2</sub>
Utibapril	Antihypertensive	109683-61-6		C <sub>22</sub> H <sub>31</sub> N <sub>3</sub> O <sub>5</sub> S
Utibaprilat	Antihypertensive	109683-79-6		C <sub>20</sub> H <sub>27</sub> N <sub>3</sub> O <sub>5</sub> S
Vadocaine	Anesthetic	72005-58-4		C <sub>18</sub> H <sub>28</sub> N <sub>2</sub> O <sub>2</sub>
Valacyclovir	Antiviral	124832-26-4	Y	C <sub>13</sub> H <sub>20</sub> N <sub>6</sub> O <sub>4</sub>
Valategrast	Antihistamine	220847-86-9		C <sub>30</sub> H <sub>32</sub> Cl <sub>3</sub> N <sub>3</sub> O <sub>4</sub>
Valconazole	Antifungal	56097-80-4		C <sub>16</sub> H <sub>18</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
Valdecobix	Antiinflammatory	181695-72-7	Y	C <sub>16</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub> S
Valdetamide	Sedative	512-48-1		C <sub>9</sub> H <sub>17</sub> NO
Valdipromide	Analgesic	52061-73-1		C <sub>11</sub> H <sub>23</sub> NO
Valethamate Bromide	Antispasmodic	90-22-2		C <sub>19</sub> H <sub>32</sub> BrNO <sub>2</sub>
Valganciclovir	Antiviral	175865-60-8	Y	C <sub>14</sub> H <sub>22</sub> N <sub>6</sub> O <sub>5</sub>
Valnemulin	Antibacterial	101312-92-9		C <sub>31</sub> H <sub>54</sub> N <sub>2</sub> O <sub>8</sub> S
Valnoctamide	Anxiolytic	4171-13-5		C <sub>8</sub> H <sub>17</sub> NO
Valofane	Sedative	3258-51-3		C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub>
Valomaciclovir	Antiviral	195157-34-7		C <sub>15</sub> H <sub>24</sub> N <sub>6</sub> O <sub>4</sub>
Valopicitabine	Antineoplastic	640281-90-9		C <sub>15</sub> H <sub>24</sub> N <sub>4</sub> O <sub>6</sub>
Valperinol	Antihypertensive	64860-67-9		C <sub>16</sub> H <sub>27</sub> NO <sub>4</sub>
Valproate Pivoxil	Anticonvulsant	77372-61-3		C <sub>14</sub> H <sub>26</sub> O <sub>4</sub>
Valproic Acid	Anticonvulsant	99-66-1		C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>
Valpromide	Anticonvulsant	2430-27-5		C <sub>8</sub> H <sub>17</sub> NO
Valrocemide	Anticonvulsant	92262-58-3		C <sub>10</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>
Valrubicin	Antineoplastic	56124-62-0		C <sub>34</sub> H <sub>36</sub> F <sub>3</sub> NO <sub>13</sub>
Valsartan	Antihypertensive	137862-53-4	Y	C <sub>24</sub> H <sub>29</sub> N <sub>5</sub> O <sub>3</sub>
Valtorcitabine Dihydrochloride	Antiviral	380886-95-3		C <sub>14</sub> H <sub>22</sub> N <sub>4</sub> O <sub>5</sub>
Valtrate	Sedative	18296-44-1		C <sub>22</sub> H <sub>30</sub> O <sub>8</sub>
Vamicamide	Mydriatic	132373-81-0		C <sub>18</sub> H <sub>23</sub> N <sub>3</sub> O
Vandetanib	Ophthalmic	443913-73-3	Y	C <sub>22</sub> H <sub>24</sub> BrFN <sub>4</sub> O <sub>2</sub>
Vanepirim	Antibiotic	84854-86-4		C <sub>23</sub> H <sub>28</sub> N <sub>4</sub> O <sub>8</sub> S
Vanitolidide	Choleretic	17692-71-6		C <sub>12</sub> H <sub>15</sub> NO <sub>3</sub> S
Vanoxerine	Antidepressant	67469-69-6		C <sub>28</sub> H <sub>32</sub> F <sub>2</sub> N <sub>2</sub> O
Vanylidisulfamide	Antibiotic	119-85-7		C <sub>20</sub> H <sub>22</sub> N <sub>4</sub> O <sub>6</sub> S <sub>2</sub>
Vapiprost	Anticoagulant	85505-64-2		C <sub>30</sub> H <sub>39</sub> NO <sub>4</sub>
Vardenafil	Erectile Dysfunction	224785-90-4	Y	C <sub>23</sub> H <sub>32</sub> N <sub>6</sub> O <sub>4</sub> S
Varenicline Tartrate	Antidepressant	249296-44-4		C <sub>13</sub> H <sub>13</sub> N <sub>3</sub>
Varespladib Sodium	Antihypotensive	172732-68-2		C <sub>21</sub> H <sub>20</sub> N <sub>2</sub> O <sub>5</sub>
Vatalanib	Antineoplastic	212141-54-3		C <sub>20</sub> H <sub>15</sub> ClN <sub>4</sub>
Vatanidipine	Antiarrhythmic	116308-55-5		C <sub>41</sub> H <sub>42</sub> N <sub>4</sub> O <sub>6</sub>
Vebufloxacin	Antibiotic	79644-90-9		C <sub>19</sub> H <sub>22</sub> FN <sub>3</sub> O <sub>3</sub>
Vecuronium Bromide	Neuromuscular Blocking Agent	50700-72-6		C <sub>34</sub> H <sub>57</sub> BrN <sub>2</sub> O <sub>4</sub>
Vedaclidine	Antiparkinsonian	141575-50-0		C <sub>13</sub> H <sub>21</sub> N <sub>3</sub> S <sub>2</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Vedaprofen	Antiinflammatory	71109-09-6		C <sub>19</sub> H <sub>22</sub> O <sub>2</sub>
Velaresol	Immunomodulator	77858-21-0		C <sub>12</sub> H <sub>14</sub> O <sub>5</sub>
Velnacrine	Nootropic	124027-47-0		C <sub>13</sub> H <sub>14</sub> N <sub>2</sub> O
Venlafaxine	Antidepressant	93413-69-5	Y	C <sub>17</sub> H <sub>27</sub> NO <sub>2</sub>
Venritidine	Antilcerative	93064-63-2		C <sub>18</sub> H <sub>26</sub> N <sub>4</sub> O <sub>3</sub> S
Veradoline	Analgesic	82924-71-8		C <sub>20</sub> H <sub>26</sub> N <sub>2</sub> O <sub>2</sub>
Veralipride	Antipsychotic	66644-81-3		C <sub>17</sub> H <sub>25</sub> N <sub>3</sub> O <sub>5</sub> S
Verapamil	Antihypertensive	52-53-9	Y	C <sub>27</sub> H <sub>38</sub> N <sub>2</sub> O <sub>4</sub>
Verazide	Antibacterial	93-47-0		C <sub>15</sub> H <sub>15</sub> N <sub>3</sub> O <sub>3</sub>
Verilopam	Analgesic	68318-20-7		C <sub>20</sub> H <sub>26</sub> N <sub>2</sub> O <sub>2</sub>
Verlukast	Bronchodilator	120443-16-5		C <sub>26</sub> H <sub>27</sub> ClN <sub>2</sub> O <sub>3</sub> S <sub>2</sub>
Verofylline	Bronchodilator	66172-75-6		C <sub>12</sub> H <sub>18</sub> N <sub>4</sub> O <sub>2</sub>
Verteporfin	Antineoplastic	121310-58-5		C <sub>40</sub> H <sub>40</sub> N <sub>4</sub> O <sub>8</sub>
Vesnarinone	Cardiotonic	81840-15-5		C <sub>22</sub> H <sub>25</sub> N <sub>3</sub> O <sub>4</sub>
Vestipitant Mesylate	Antidepressant	334476-46-9		C <sub>23</sub> H <sub>24</sub> F <sub>7</sub> N <sub>3</sub> O
Vetrabutine	Antispasmodic	3735-45-3		C <sub>20</sub> H <sub>27</sub> NO <sub>2</sub>
Vicriviroc Maleate	Antiviral	306296-47-9		C <sub>28</sub> H <sub>38</sub> F <sub>3</sub> N <sub>5</sub> O <sub>2</sub>
Vidarabine	Antiviral	5536-17-4		C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>4</sub>
Vidarabine Phosphate	Antineoplastic	29984-33-6		C <sub>10</sub> H <sub>14</sub> N <sub>5</sub> O <sub>7</sub> P
Vigabatrin	Anticonvulsant	68506-86-5	Y	C <sub>6</sub> H <sub>11</sub> NO <sub>2</sub>
Vilazodone	Antidepressant	163521-12-8	Y	C <sub>26</sub> H <sub>27</sub> N <sub>5</sub> O <sub>2</sub>
Vildagliptin	Antidiabetic	274901-16-5	Y	C <sub>17</sub> H <sub>25</sub> N <sub>3</sub> O <sub>2</sub>
Viloxazine	Antidepressant	46817-91-8		C <sub>13</sub> H <sub>19</sub> NO <sub>3</sub>
Viminol	Analgesic	21363-18-8		C <sub>21</sub> H <sub>31</sub> ClN <sub>2</sub> O
Vinbarbital	Sedative	125-42-8		C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>
Vinblastine	Antineoplastic	865-21-4		C <sub>46</sub> H <sub>58</sub> N <sub>4</sub> O <sub>9</sub>
Vinburnine	Vasodilator	4880-88-0		C <sub>19</sub> H <sub>22</sub> N <sub>2</sub> O
Vincamine	Antineoplastic	1617-90-9		C <sub>21</sub> H <sub>26</sub> N <sub>2</sub> O <sub>3</sub>
Vincanol	Anesthetic	19877-89-5		C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> O
Vincantril	Unclassified	65285-58-7		C <sub>14</sub> H <sub>13</sub> ClN <sub>2</sub> O
Vincofos	Anthelmintic	17196-88-2		C <sub>11</sub> H <sub>21</sub> Cl <sub>2</sub> O <sub>4</sub> P
Vinconate	Nootropic	70704-03-9		C <sub>18</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>
Vincristine	Antineoplastic	57-22-7		C <sub>46</sub> H <sub>56</sub> N <sub>4</sub> O <sub>10</sub>
Vindeburnol	Nootropic	68779-67-9		C <sub>17</sub> H <sub>20</sub> N <sub>2</sub> O
Vindesine	Antineoplastic	53643-48-4		C <sub>43</sub> H <sub>55</sub> N <sub>5</sub> O <sub>7</sub>
Vinepidine Sulfate	Antineoplastic	68170-69-4		C <sub>46</sub> H <sub>56</sub> N <sub>4</sub> O <sub>9</sub>
Vinflunine	Antineoplastic	162652-95-1		C <sub>45</sub> H <sub>54</sub> F <sub>2</sub> N <sub>4</sub> O <sub>8</sub>
Vinformide	Unclassified	54022-49-0		C <sub>46</sub> H <sub>54</sub> N <sub>4</sub> O <sub>10</sub>
Vinfosiltine	Antineoplastic	123286-00-0		C <sub>51</sub> H <sub>72</sub> N <sub>5</sub> O <sub>10</sub> P
Vinglycinat Sulfate	Antineoplastic	865-24-7		C <sub>48</sub> H <sub>63</sub> N <sub>5</sub> O <sub>9</sub>
Vinleucinol	Antineoplastic	81571-28-0		C <sub>51</sub> H <sub>69</sub> N <sub>5</sub> O <sub>9</sub>
Vinleurosine Sulfate	Antineoplastic	23360-92-1		C <sub>46</sub> H <sub>56</sub> N <sub>4</sub> O <sub>9</sub>
Vinmegallate	Dermatologic	83482-77-3		C <sub>30</sub> H <sub>32</sub> N <sub>2</sub> O <sub>5</sub>
Vinorelbine	Antineoplastic	71486-22-1	Y	C <sub>45</sub> H <sub>54</sub> N <sub>4</sub> O <sub>8</sub>
Vinpocetine	Vasodilator	42971-09-5		C <sub>22</sub> H <sub>26</sub> N <sub>2</sub> O <sub>2</sub>
Vinpoline	Unclassified	57694-27-6		C <sub>23</sub> H <sub>30</sub> N <sub>2</sub> O <sub>3</sub>
Vinrosidine Sulfate	Antineoplastic	15228-71-4		C <sub>46</sub> H <sub>58</sub> N <sub>4</sub> O <sub>9</sub>
Vintoperol	Vasodilator	106498-99-1		C <sub>18</sub> H <sub>24</sub> N <sub>2</sub> O
Vinatriptol	Antineoplastic	81600-06-8		C <sub>56</sub> H <sub>68</sub> N <sub>6</sub> O <sub>9</sub>
Vinyl Ether	Anesthetic	109-93-3		C <sub>4</sub> H <sub>6</sub> O
Vinylbital	Sedative	2430-49-1		C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>
Vinzolidine Sulfate	Antineoplastic	67699-40-5		C <sub>48</sub> H <sub>58</sub> ClN <sub>5</sub> O <sub>9</sub>
Viomycin	Antibiotic	32988-50-4		C <sub>25</sub> H <sub>43</sub> N <sub>13</sub> O <sub>10</sub>
Viprostol	Vasodilator	73647-73-1		C <sub>23</sub> H <sub>36</sub> O <sub>5</sub>
Viqualine	Alcohol Deterrant	72714-74-0		C <sub>20</sub> H <sub>26</sub> N <sub>2</sub> O
Viquidil	Vasodilator	84-55-9		C <sub>20</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub>
Viroxime	Antiviral	63198-97-0		C <sub>17</sub> H <sub>18</sub> N <sub>4</sub> O <sub>3</sub> S
Visnadine	Vasodilator	477-32-7		C <sub>21</sub> H <sub>24</sub> O <sub>7</sub>
Visnafylline	Bronchodilator	17243-56-0		C <sub>25</sub> H <sub>29</sub> N <sub>5</sub> O <sub>7</sub>
Vofopitant	Antiemetic	168266-90-8		C <sub>21</sub> H <sub>23</sub> F <sub>3</sub> N <sub>6</sub> O
Voglibose	Antidiabetic	83480-29-9	Y	C <sub>10</sub> H <sub>21</sub> NO <sub>7</sub>
Volazocine	Analgesic	15686-68-7		C <sub>18</sub> H <sub>25</sub> N
Volpristin	Antibiotic	21102-49-8		C <sub>28</sub> H <sub>37</sub> N <sub>3</sub> O <sub>7</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Voriconazole	Antifungal	137234-62-9	Y	C <sub>16</sub> H <sub>14</sub> F <sub>3</sub> N <sub>5</sub> O
Vorinostat	Antineoplastic	149647-78-9	Y	C <sub>14</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub>
Vorozole	Antineoplastic	129731-10-8		C <sub>16</sub> H <sub>13</sub> ClN <sub>6</sub>
Voxergolide	Antiparkinsonian	89651-00-3		C <sub>16</sub> H <sub>20</sub> N <sub>2</sub> O <sub>5</sub>
Warfarin	Anticoagulant	81-81-2		C <sub>19</sub> H <sub>16</sub> O <sub>4</sub>
Xaliproden	Nootropic	135354-02-8		C <sub>24</sub> H <sub>22</sub> F <sub>3</sub> N
Xamoterol	Cardiotonic	81801-12-9		C <sub>16</sub> H <sub>25</sub> N <sub>3</sub> O <sub>5</sub>
Xanomeline	Cholinergic	131986-45-3		C <sub>14</sub> H <sub>23</sub> N <sub>3</sub> OS
Xanoxic Acid	Bronchodilator	33459-27-7		C <sub>17</sub> H <sub>14</sub> O <sub>5</sub>
Xanthiol	Unclassified	14008-71-0		C <sub>23</sub> H <sub>29</sub> ClN <sub>2</sub> OS
Xantifibrate	Antihyperlipidemic	2530-97-4		C <sub>13</sub> H <sub>21</sub> N <sub>5</sub> O <sub>4</sub>
Xantocillin	Antibiotic	580-74-5		C <sub>18</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>
Xemilofiban	Antianginal	149820-74-6	Y	C <sub>18</sub> H <sub>22</sub> N <sub>4</sub> O <sub>4</sub>
Xenalipin	Antihyperlipidemic	84392-17-6		C <sub>14</sub> H <sub>9</sub> F <sub>3</sub> O <sub>2</sub>
Xenazoic Acid	Antiviral	1174-11-4		C <sub>23</sub> H <sub>21</sub> NO <sub>4</sub>
Xenbucin	Antihyperlipidemic	959-10-4		C <sub>16</sub> H <sub>16</sub> O <sub>2</sub>
Xenipentone	Unclassified	55845-78-8		C <sub>17</sub> H <sub>16</sub> O
Xenthiorate	Unclassified	7009-79-2		C <sub>22</sub> H <sub>29</sub> NOS
Xenygloxal	Unclassified	1094-85-5		C <sub>16</sub> H <sub>14</sub> O <sub>6</sub>
Xenyhexenic Acid	Unclassified	95040-85-0	Y	C <sub>18</sub> H <sub>18</sub> O <sub>2</sub>
Xenytropium Bromide	Antispasmodic	511-55-7		C <sub>30</sub> H <sub>34</sub> BrNO <sub>3</sub>
Xibenolol	Antiarrhythmic	30187-90-7		C <sub>15</sub> H <sub>25</sub> NO <sub>2</sub>
Xibornol	Antibacterial	13741-18-9		C <sub>18</sub> H <sub>26</sub> O
Xidecaflur	Unclassified	13127-82-7		C <sub>22</sub> H <sub>45</sub> NO <sub>2</sub>
Xilobam	Muscle Relaxant	50528-97-7		C <sub>14</sub> H <sub>19</sub> N <sub>3</sub> O
Ximelagatran	Antithrombotic	192939-46-1		C <sub>24</sub> H <sub>35</sub> N <sub>5</sub> O <sub>5</sub>
Ximoprofen	Antiinflammatory	56187-89-4		C <sub>15</sub> H <sub>19</sub> NO <sub>3</sub>
Xinidamine	Analgesic	50264-78-3		C <sub>17</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>
Xinomiline	Unclassified	52832-91-4		C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O
Xipamide	Diuretic	14293-44-8		C <sub>15</sub> H <sub>15</sub> ClN <sub>2</sub> O <sub>4</sub> S
Xipranolol	Antihypertensive	19179-78-3		C <sub>23</sub> H <sub>33</sub> NO <sub>2</sub>
Xorphanol Mesylate	Analgesic	77287-89-9		C <sub>23</sub> H <sub>31</sub> NO
Xylamidine Tosylate	Antidepressant	6443-50-1		C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub>
Xylazine	Sedative	7361-61-7		C <sub>12</sub> H <sub>16</sub> N <sub>2</sub> S
Xylocoumarol	Anticoagulant	15301-97-0		C <sub>17</sub> H <sub>14</sub> O <sub>3</sub>
Xylometazoline	Decongestant	526-36-3		C <sub>16</sub> H <sub>24</sub> N <sub>2</sub>
Xyloxemine	Antitussive	1600-19-7		C <sub>23</sub> H <sub>33</sub> NO <sub>2</sub>
Yohimbic Acid	Erectile Dysfunction	522-87-2		C <sub>20</sub> H <sub>24</sub> N <sub>2</sub> O <sub>3</sub>
Yohimbine	Erectile Dysfunction	146-48-5		C <sub>21</sub> H <sub>26</sub> N <sub>2</sub> O <sub>3</sub>
Zabicipril	Antihypertensive	83059-56-7		C <sub>23</sub> H <sub>32</sub> N <sub>2</sub> O <sub>5</sub>
Zabiciprilat	Antihypertensive	90103-92-7		C <sub>21</sub> H <sub>28</sub> N <sub>2</sub> O <sub>5</sub>
Zabofloxacin	Antibiotic	219680-11-2	Y	C <sub>19</sub> H <sub>20</sub> FN <sub>5</sub> O <sub>4</sub>
Zacopride	Antiemetic	90182-92-6		C <sub>15</sub> H <sub>20</sub> ClN <sub>3</sub> O <sub>2</sub>
Zafirlukast	Bronchodilator	107753-78-6	Y	C <sub>31</sub> H <sub>33</sub> N <sub>3</sub> O <sub>6</sub> S
Zafuleptine	Antidepressant	59209-97-1		C <sub>17</sub> H <sub>26</sub> FNO <sub>2</sub>
Zalcitabine	Antiviral	7481-89-2	Y	C <sub>9</sub> H <sub>13</sub> N <sub>3</sub> O <sub>3</sub>
Zaldaride	Antidiarrheal	109826-26-8		C <sub>26</sub> H <sub>28</sub> N <sub>4</sub> O <sub>2</sub>
Zaleplon	Sedative	151319-34-5	Y	C <sub>17</sub> H <sub>15</sub> N <sub>5</sub> O
Zalospirone	Anxiolytic	114298-18-9		C <sub>24</sub> H <sub>29</sub> N <sub>5</sub> O <sub>2</sub>
Zaltidine	Antiulcerative	85604-00-8		C <sub>8</sub> H <sub>10</sub> N <sub>6</sub> S
Zaltoprofen	Antiinflammatory	74711-43-6		C <sub>17</sub> H <sub>14</sub> O <sub>3</sub> S
Zamifenacin	Mydriatic	127308-82-1		C <sub>27</sub> H <sub>29</sub> NO <sub>3</sub>
Zanamivir	Antiviral	139110-80-8		C <sub>12</sub> H <sub>20</sub> N <sub>4</sub> O <sub>7</sub>
Zanapezil	Nootropic	142852-50-4		C <sub>25</sub> H <sub>32</sub> N <sub>2</sub> O
Zankiren	Antihypertensive	138742-43-5		C <sub>35</sub> H <sub>55</sub> N <sub>5</sub> O <sub>6</sub> S <sub>2</sub>
Zanoterone	Steroid	107000-34-0		C <sub>23</sub> H <sub>32</sub> N <sub>2</sub> O <sub>3</sub> S
Zapizolam	Anxiolytic	64098-32-4		C <sub>15</sub> H <sub>9</sub> Cl <sub>2</sub> N <sub>5</sub>
Zaprinast	Antihistaminic	37762-06-4		C <sub>13</sub> H <sub>13</sub> N <sub>5</sub> O <sub>2</sub>
Zardaverine	Bronchodilator	101975-10-4		C <sub>12</sub> H <sub>10</sub> F <sub>2</sub> N <sub>2</sub> O <sub>3</sub>
Zatebradine	Antianginal	85175-67-3		C <sub>26</sub> H <sub>36</sub> N <sub>2</sub> O <sub>5</sub>
Zatoseptron Maleate	Antimigraine	123482-22-4		C <sub>19</sub> H <sub>25</sub> ClN <sub>2</sub> O <sub>2</sub>
Zelandopam	Antihypertensive	139233-53-7		C <sub>15</sub> H <sub>15</sub> NO <sub>4</sub>
Zenarestat	Antidiabetic	112733-06-9		C <sub>17</sub> H <sub>11</sub> BrClFN <sub>2</sub> O <sub>4</sub>

Table S1. Cont.

Common Name	Indication	CAS Number	Oral	Molecular Formula
Zenazocine Mesylate	Analgesic	68681-43-6		C <sub>23</sub> H <sub>35</sub> NO <sub>2</sub>
Zepastine	Antineoplastic	28810-23-3		C <sub>22</sub> H <sub>26</sub> N <sub>2</sub> O <sub>3</sub> S
Zeranol	Steroid	26538-44-3		C <sub>18</sub> H <sub>26</sub> O <sub>5</sub>
Zetidoline	Antipsychotic	51940-78-4		C <sub>16</sub> H <sub>22</sub> ClN <sub>3</sub> O
Zidamide	Antihypertensive	75820-08-5		C <sub>16</sub> H <sub>16</sub> ClN <sub>3</sub> O <sub>3</sub> S
Zidometacin	Antiinflammatory	62851-43-8		C <sub>19</sub> H <sub>16</sub> N <sub>4</sub> O <sub>4</sub>
Zidovudine	Antiviral	30516-87-1		C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>4</sub>
Zifrosilone	Antidote	132236-18-1		C <sub>11</sub> H <sub>13</sub> F <sub>3</sub> OSi
Zilantel	Anthelminthic	22012-72-2		C <sub>26</sub> H <sub>38</sub> N <sub>2</sub> O <sub>6</sub> P <sub>2</sub> S <sub>4</sub>
Zileuton	Antiinflammatory	111406-87-2		C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> S
Zilpaterol	Bronchodilator	119520-05-7		C <sub>14</sub> H <sub>19</sub> N <sub>3</sub> O <sub>2</sub>
Zimeldine	Antidepressant	56775-88-3		C <sub>16</sub> H <sub>17</sub> BrN <sub>2</sub>
Zimidoben	Unclassified	90697-56-6		C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>
Zindotrine	Bronchodilator	56383-05-2		C <sub>11</sub> H <sub>15</sub> N <sub>5</sub>
Zindoxifene	Antineoplastic	86111-26-4		C <sub>21</sub> H <sub>21</sub> NO <sub>4</sub>
Zinoconazole	Antifungal	84697-21-2		C <sub>15</sub> H <sub>11</sub> Cl <sub>3</sub> N <sub>4</sub> S
Zinterol	Bronchodilator	37000-20-7		C <sub>19</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub> S
Zinviroxime	Antiviral	72301-78-1		C <sub>17</sub> H <sub>18</sub> N <sub>4</sub> O <sub>3</sub> S
Zipeprol	Antitussive	34758-83-3		C <sub>23</sub> H <sub>32</sub> N <sub>2</sub> O <sub>3</sub>
Ziprasidone	Antipsychotic	146939-27-7	Y	C <sub>21</sub> H <sub>21</sub> ClN <sub>4</sub> OS
Zocainone	Unclassified	68876-74-4		C <sub>22</sub> H <sub>27</sub> NO <sub>3</sub>
Zofenopril Calcium	Antihypertensive	81872-10-8	Y	C <sub>22</sub> H <sub>23</sub> NO <sub>4</sub> S <sub>2</sub>
Zofenoprilat Arginine	Antihypertensive	75176-37-3		C <sub>15</sub> H <sub>19</sub> NO <sub>5</sub> S <sub>2</sub>
Zoficonazole	Antifungal	71097-23-9		C <sub>20</sub> H <sub>19</sub> Cl <sub>3</sub> N <sub>2</sub> O <sub>2</sub>
Zolamine	Antihistaminic	553-13-9		C <sub>15</sub> H <sub>21</sub> N <sub>3</sub> OS
Zolasartan	Antihypertensive	145781-32-4		C <sub>24</sub> H <sub>20</sub> BrClN <sub>6</sub> O <sub>3</sub>
Zolazepam	Sedative	31352-82-6		C <sub>15</sub> H <sub>15</sub> FN <sub>4</sub> O
Zoledronic Acid	Bone Resorption Inhibitor	118072-93-8		C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>7</sub> P <sub>2</sub>
Zolenzepine	Antiulcerative	78208-13-6		C <sub>19</sub> H <sub>24</sub> N <sub>6</sub> O <sub>2</sub>
Zolertine	Vasodilator	4004-94-8		C <sub>13</sub> H <sub>18</sub> N <sub>6</sub>
Zolimidine	Antiulcerative	1222-57-7		C <sub>14</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> S
Zoliprofen	Antiinflammatory	56355-17-0		C <sub>12</sub> H <sub>11</sub> NO <sub>3</sub> S
Zolmitriptan	Antimigraine	139264-17-8	Y	C <sub>16</sub> H <sub>21</sub> N <sub>3</sub> O <sub>2</sub>
Zoloperone	Antipsychotic	52867-74-0		C <sub>22</sub> H <sub>24</sub> FN <sub>3</sub> O <sub>3</sub>
Zolpidem	Sedative	82626-48-0	Y	C <sub>19</sub> H <sub>21</sub> N <sub>3</sub> O
Zomebazam	Anxiolytic	78466-70-3		C <sub>15</sub> H <sub>16</sub> N <sub>4</sub> O <sub>2</sub>
Zomepirac	Analgesic	33369-31-2		C <sub>15</sub> H <sub>14</sub> ClNO <sub>3</sub>
Zometapine	Antidepressant	51022-73-2		C <sub>14</sub> H <sub>15</sub> ClN <sub>4</sub>
Zonampanel	Antidepressant	210245-80-0		C <sub>13</sub> H <sub>9</sub> N <sub>5</sub> O <sub>6</sub>
Zoniclezole	Anticonvulsant	121929-20-2		C <sub>12</sub> H <sub>10</sub> ClN <sub>3</sub> O
Zoniporide	Cardiotonic	241800-98-6		C <sub>17</sub> H <sub>16</sub> N <sub>6</sub> O
Zonisamide	Anticonvulsant	68291-97-4		C <sub>8</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub> S
Zopiclone	Sedative	43200-80-2		C <sub>17</sub> H <sub>17</sub> ClN <sub>6</sub> O <sub>3</sub>
Zopolrestat	Antidiabetic	110703-94-1		C <sub>19</sub> H <sub>12</sub> F <sub>3</sub> N <sub>3</sub> O <sub>3</sub> S
Zorubicin	Antineoplastic	54083-22-6		C <sub>34</sub> H <sub>35</sub> N <sub>3</sub> O <sub>10</sub>
Zosuquidar Trihydrochloride	Antineoplastic	167354-41-8		C <sub>32</sub> H <sub>31</sub> F <sub>2</sub> N <sub>3</sub> O <sub>2</sub>
Zotepine	Antipsychotic	26615-21-4		C <sub>18</sub> H <sub>18</sub> ClNOS
Zoticasone	Antiinflammatory	678160-57-1		C <sub>25</sub> H <sub>30</sub> F <sub>2</sub> O <sub>6</sub> S
Zoxazolamine	Uricosuric	61-80-3		C <sub>7</sub> H <sub>5</sub> ClN <sub>2</sub> O
Zucapsaicin	Analgesic	25775-90-0		C <sub>18</sub> H <sub>27</sub> NO <sub>3</sub>
Zuclomiphene	Pituitary	15690-55-8		C <sub>26</sub> H <sub>28</sub> ClNO
Zuclopenthixol	Antipsychotic	53772-83-1		C <sub>22</sub> H <sub>25</sub> ClN <sub>2</sub> OS
Zylofuramine	Antidiabetic	3563-92-6		C <sub>14</sub> H <sub>21</sub> NO
Cetyl Myristate	Dermatologic	2599-01-1		C <sub>30</sub> H <sub>60</sub> O <sub>2</sub>
Cetyl Myristoleate	Dermatologic	64660-84-0		C <sub>30</sub> H <sub>58</sub> O <sub>2</sub>
Emtricitabine	Antineoplastic	143491-57-0	Y	C <sub>8</sub> H <sub>10</sub> FN <sub>3</sub> O <sub>3</sub> S
Metaraminol	Antihypotensive	54-49-9		C <sub>9</sub> H <sub>13</sub> NO <sub>2</sub>

“Y” represented the drug was administered orally.