

In silico Functional Profiling of Small Molecules and its Applications

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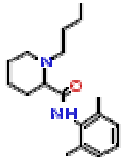
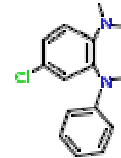
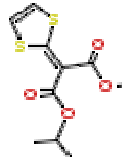
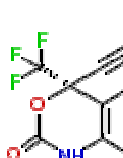
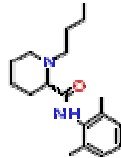
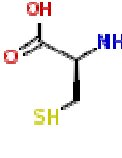
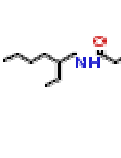
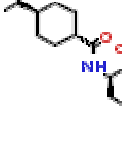
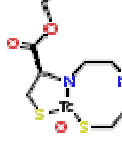
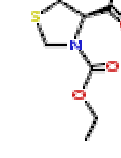
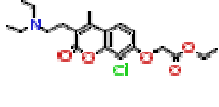
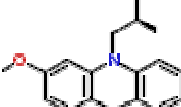
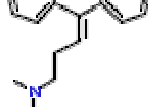
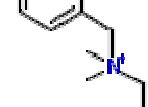
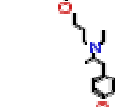
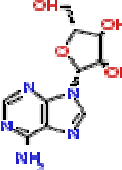
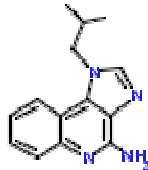
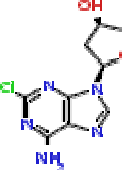
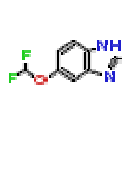
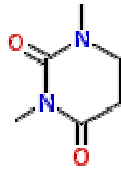
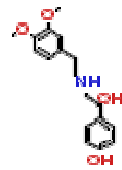
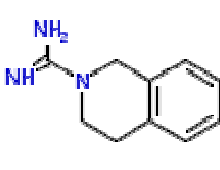
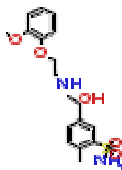
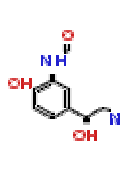
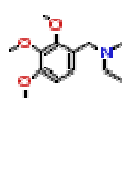
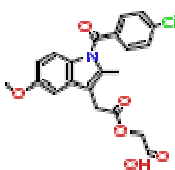
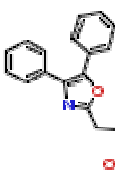
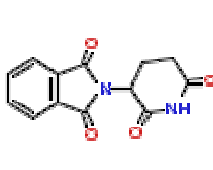
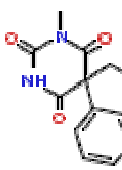
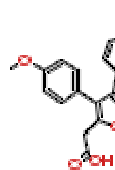
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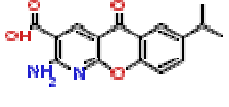
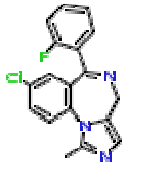
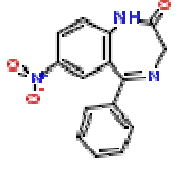
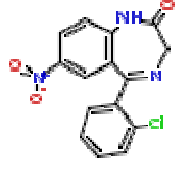
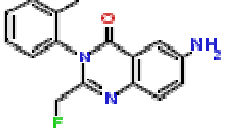
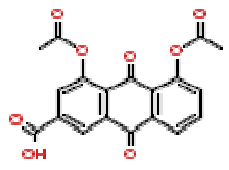
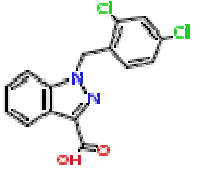
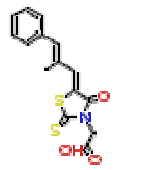
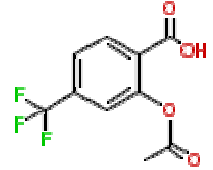
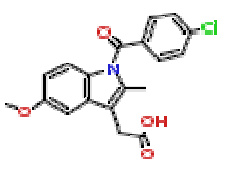
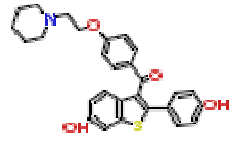
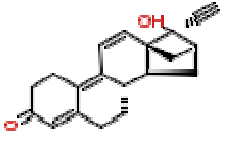
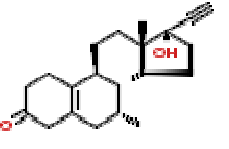
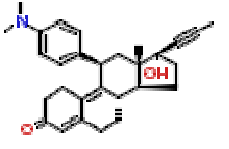
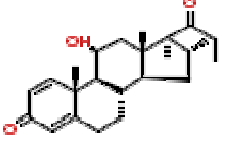
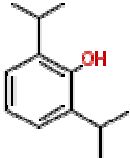
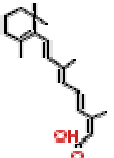
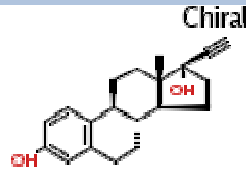
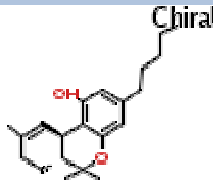
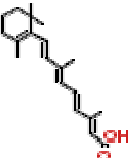
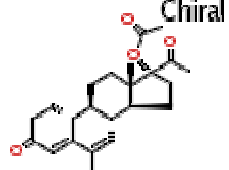
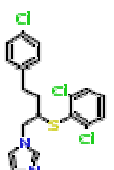
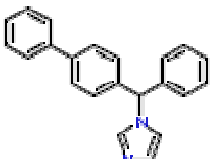
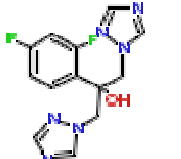
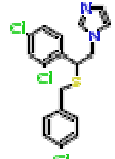
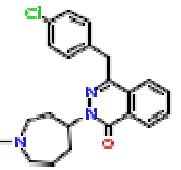
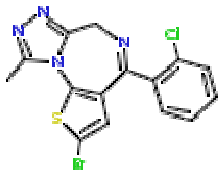
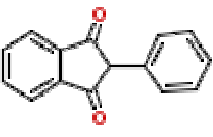
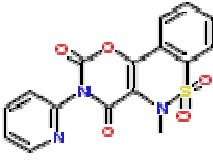
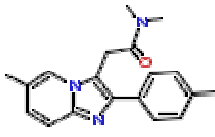
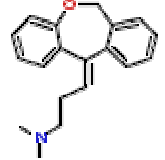
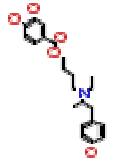
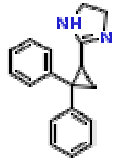
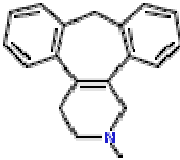
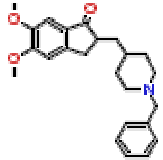
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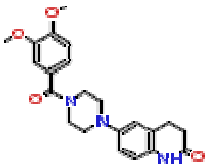
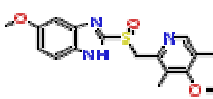
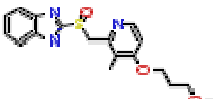
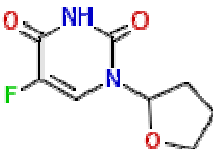
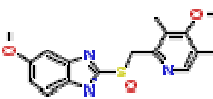
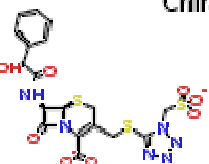
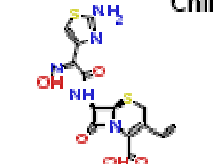
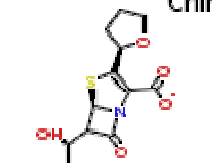
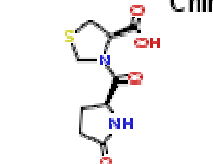
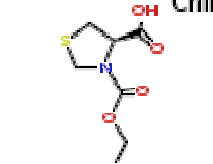
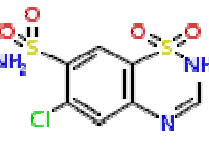
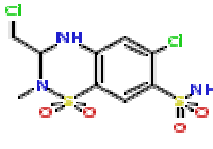
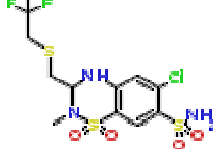
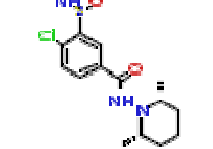
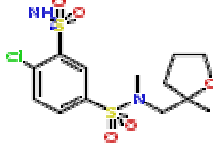
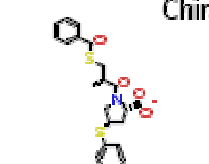
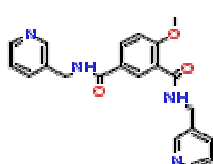
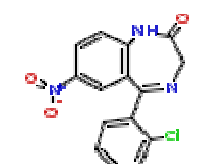
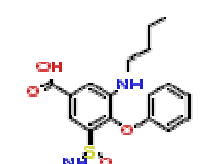
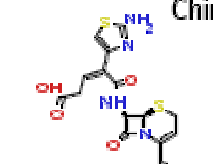
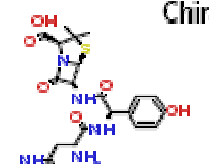
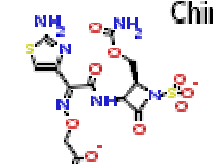
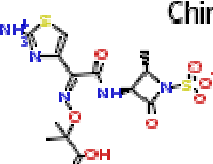
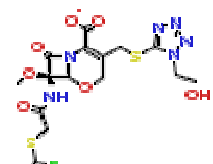
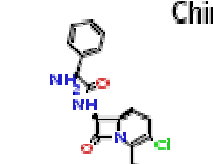
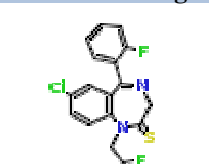
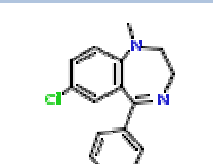
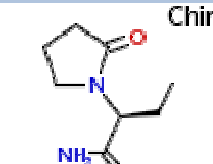
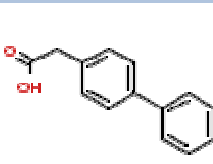
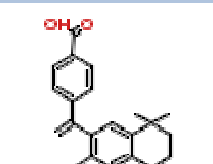
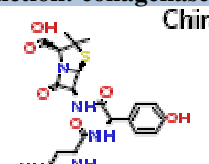
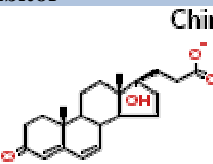
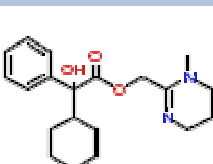
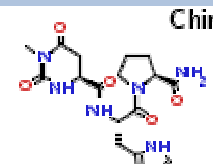
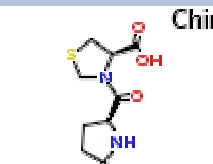
Page 2–20, Table S1 The structures and CAS numbers of five most positively predicted compounds for 70 molecular actions (A) and 55 therapeutic areas (B). The compounds are not annotated as positive for the functions in MDDR

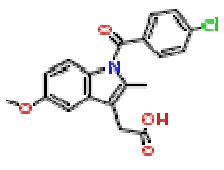
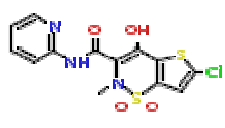
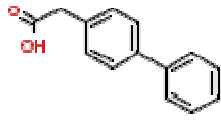
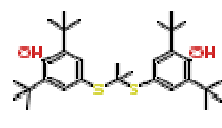
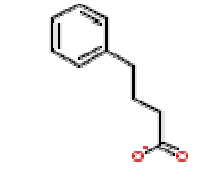
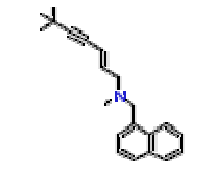
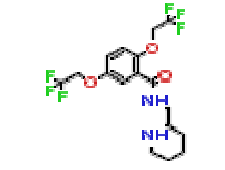
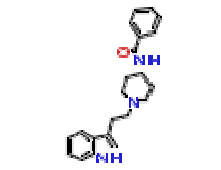
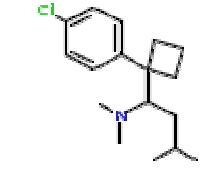
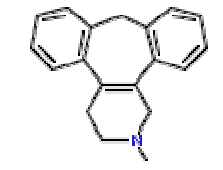
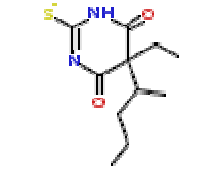
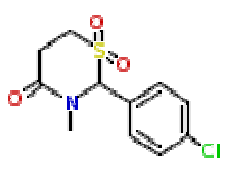
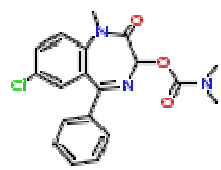
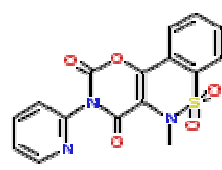
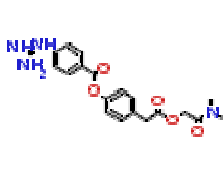
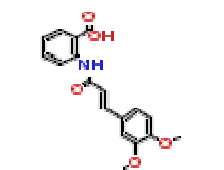
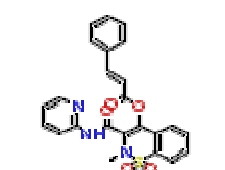
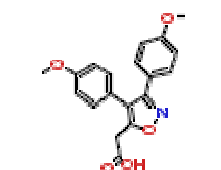
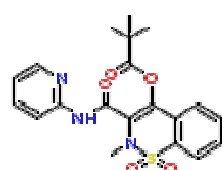
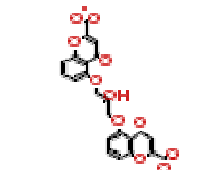
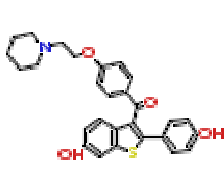
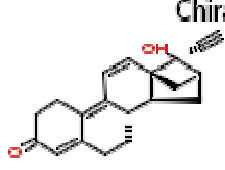
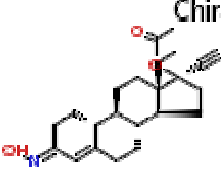
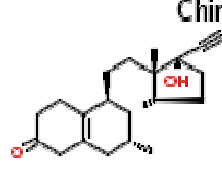
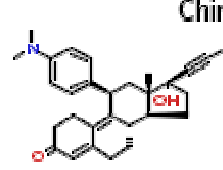
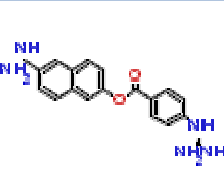
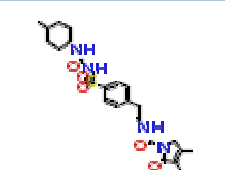
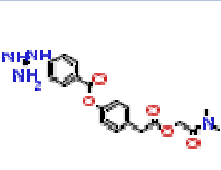
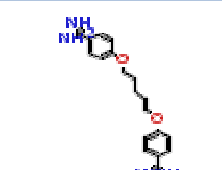
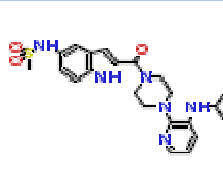
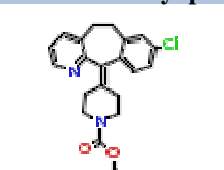
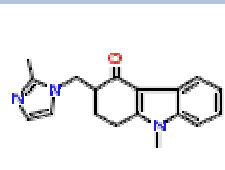
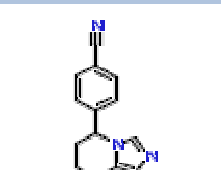
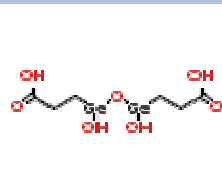
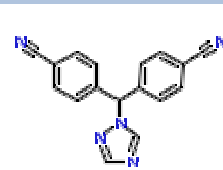
Table S1 The structures and CAS numbers of five most positively predicted compounds about 70 molecular actions (A) and 55 therapeutic areas (B). The compounds are not annotated as positive for the functions in MDDR

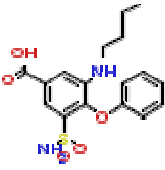
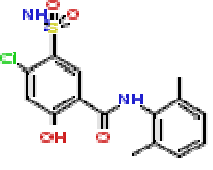
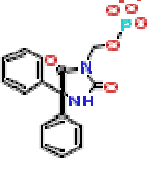
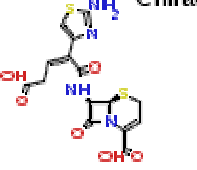
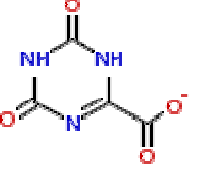
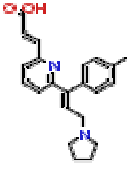
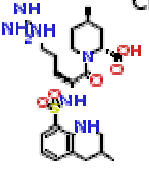
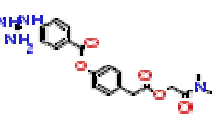
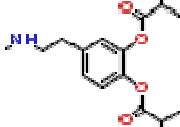
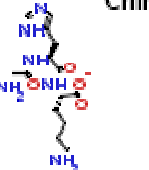
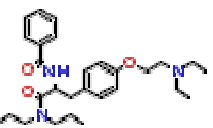
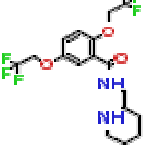
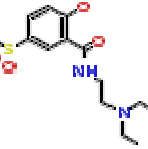
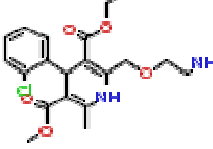
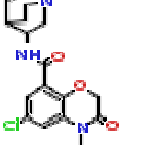
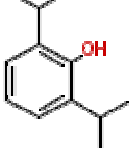
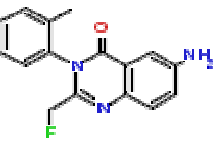
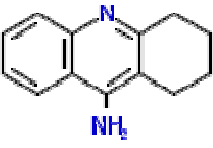
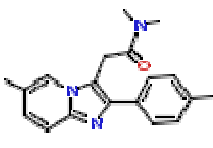
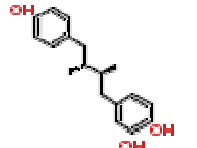
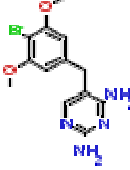
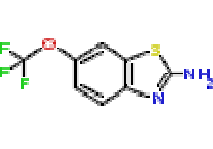
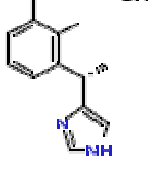
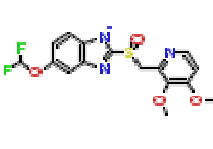
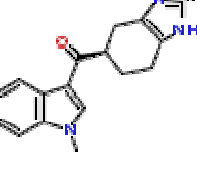
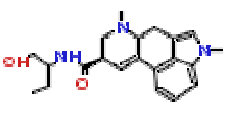
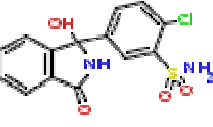
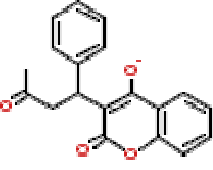
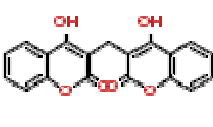
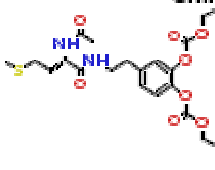
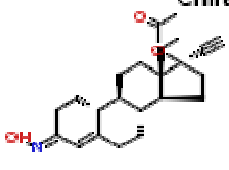
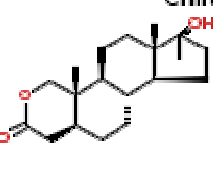
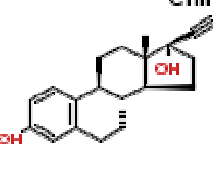
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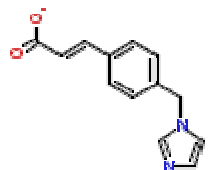
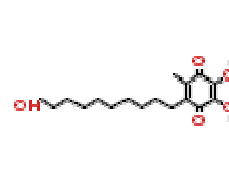
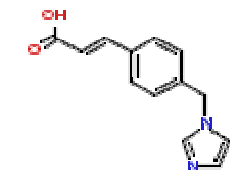
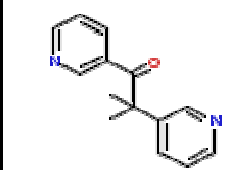
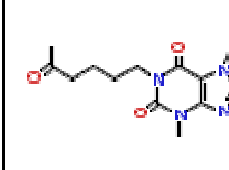
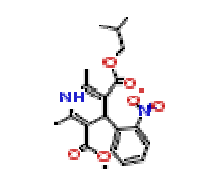
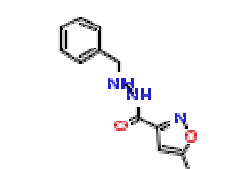
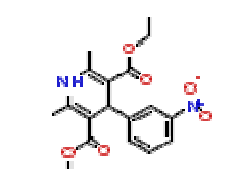
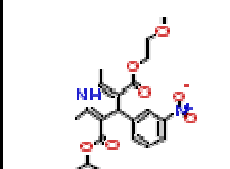
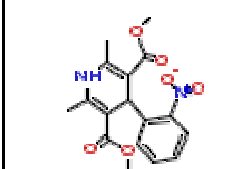
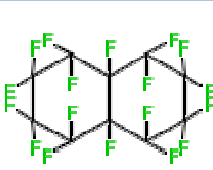
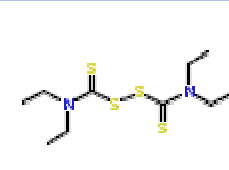
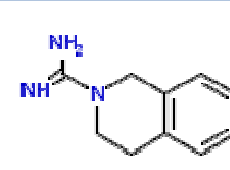
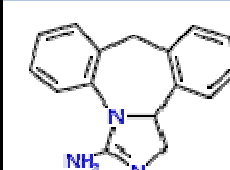
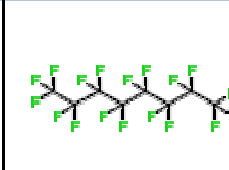
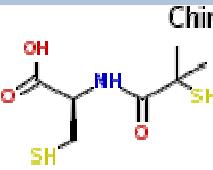
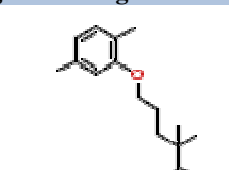
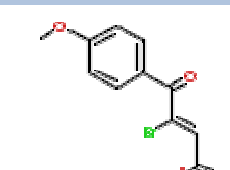
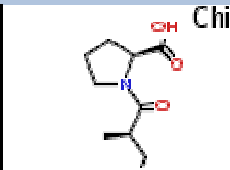
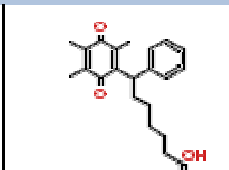
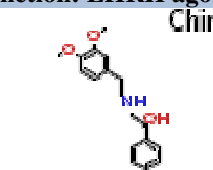
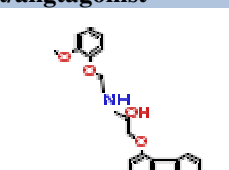
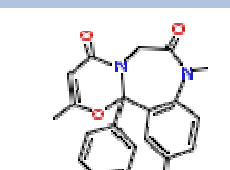
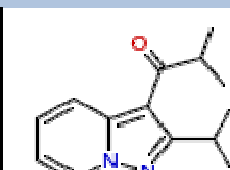
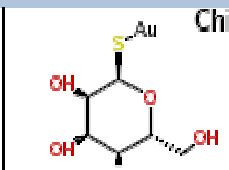
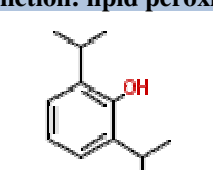
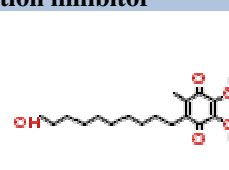
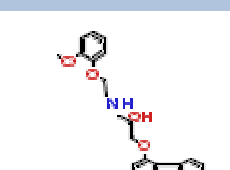
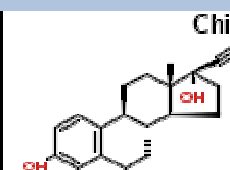
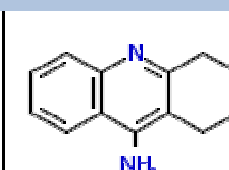
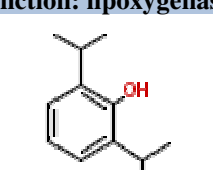
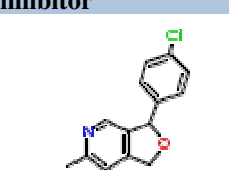
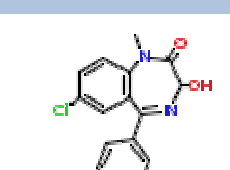
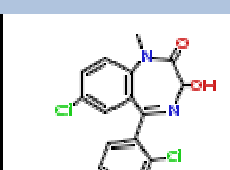
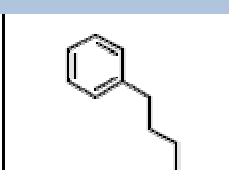
molecular actions				
function: ACAT inhibitor				
				
Rank 1 : 14252-80-3	Rank 2 : 22316-47-8	Rank 3 : 59937-28-9	Rank 4 : 154598-52-4	Rank 5 : 27262-47-1
function: ACE inhibitor				
				
Rank 1 : 65002-17-7	Rank 2 : 32838-28-1	Rank 3 : 105816-04-4	Rank 4 : 121281-41-2	Rank 5 : 122946-43-4
function: acetylcholinesterase inhibitor				
				
Rank 1 : 68206-94-0	Rank 2 : 60-99-1	Rank 3 : 1229-29-4	Rank 4 : 61-75-6	Rank 5 : 2753-45-9
function: adenosine agonist/antagonist				
				
Rank 1 : 58-61-7	Rank 2 : 99011-02-6	Rank 3 : 4291-63-8	Rank 4 : 102625-70-7	Rank 5 : 69-22-7
function: adrenoceptor agonist/antagonist				
				
Rank 1 : 71771-90-9	Rank 2 : 581-88-4	Rank 3 : 70958-86-0	Rank 4 : 73573-87-2	Rank 5 : 101477-54-7
function: aldose reductase inhibitor				
				
Rank 1 : 53164-05-9	Rank 2 : 21256-18-8	Rank 3 : 50-35-1	Rank 4 : 115-38-8	Rank 5 : 78967-07-4
function: AMPA receptor antagonist				

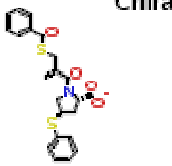
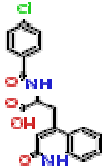
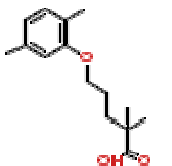
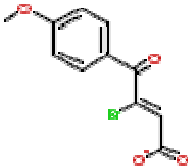
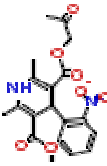
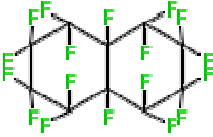
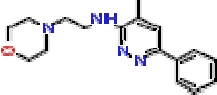
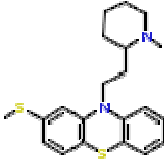
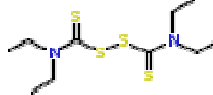
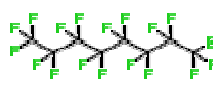
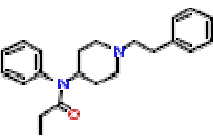
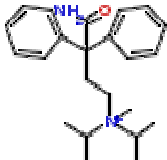
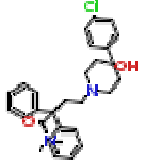
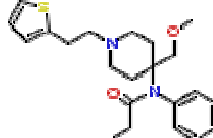
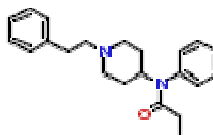
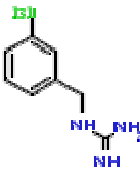
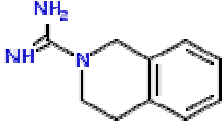
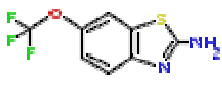
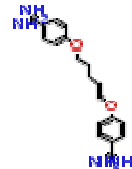
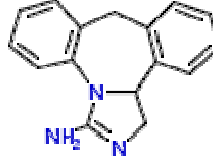
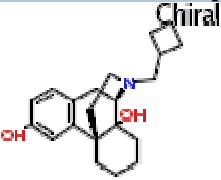
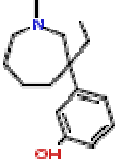
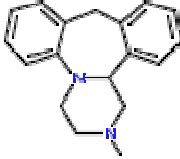
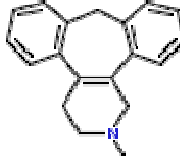
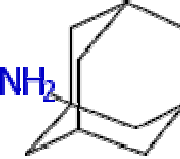
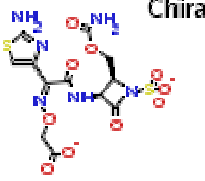
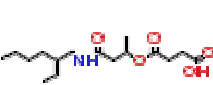
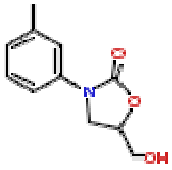
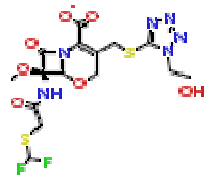
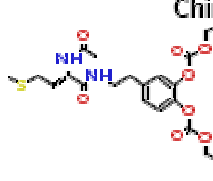
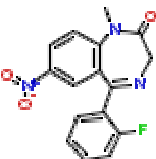
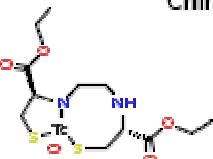
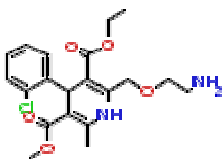
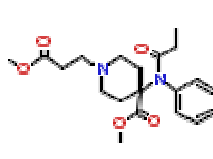
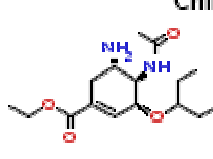
				
Rank 1 : 68302-57-8	Rank 2 : 59467-70-8	Rank 3 : 146-22-5	Rank 4 : 1622-61-3	Rank 5 : 56287-74-2
function: angiotensin 2 agonist/antagonist				
				
Rank 1 : 13739-02-1	Rank 2 : 50264-69-2	Rank 3 : 82159-09-9	Rank 4 : 322-79-2	Rank 5 : 53-86-1
function: antiestrogen				
				
Rank 1 : 82640-04-8	Rank 2 : 16320-04-0	Rank 3 : 5630-53-5	Rank 4 : 84371-65-3	Rank 5 : 49697-38-3
function: antioxidant				
				
Rank 1 : 2078-54-8	Rank 2 : 4759-48-2	Rank 3 : 57-63-6	Rank 4 : 1972-08-3	Rank 5 : 302-79-4
function: aromatase inhibitor				
				
Rank 1 : 58691-88-6	Rank 2 : 64872-77-1	Rank 3 : 60628-96-8	Rank 4 : 86386-73-4	Rank 5 : 61318-90-9
function: benzodiazepine				
				
Rank 1 : 58581-89-8	Rank 2 : 57801-81-7	Rank 3 : 83-12-5	Rank 4 : 90101-16-9	Rank 5 : 99294-93-6
function: Ca2+ channel blocker				
				
Rank 1 : 1229-29-4	Rank 2 : 2753-45-9	Rank 3 : 53267-01-9	Rank 4 : 57262-94-9	Rank 5 : 120011-70-3
function: cAMP phosphodiesterase inhibitor				

				
Rank 1 : 81840-15-5	Rank 2 : 73590-58-6	Rank 3 : 117976-90-6	Rank 4 : 17902-23-7	Rank 5 : 119141-88-7
function: carbapenem				
				
Rank 1 : 61270-78-8	Rank 2 : 91832-40-5	Rank 3 : 122547-49-3	Rank 4 : 121808-62-6	Rank 5 : 122946-43-4
function: carbonic anhydrase inhibitor				
				
Rank 1 : 569-57-3	Rank 2 : 135-07-9	Rank 3 : 346-18-9	Rank 4 : 636-54-4	Rank 5 : 7195-27-9
function: CCK				
				
Rank 1 : 81872-10-8	Rank 2 : 32828-81-2	Rank 3 : 1622-61-3	Rank 4 : 28395-03-1	Rank 5 : 97519-39-6
function: cephalosporin				
				
Rank 1 : 63358-49-6	Rank 2 : 86832-68-0	Rank 3 : 78110-38-0	Rank 4 : 92823-00-2	Rank 5 : 121961-22-6
function: cholinergic				
				
Rank 1 : 36735-22-5	Rank 2 : 2898-12-6	Rank 3 : 102767-28-2	Rank 4 : 5728-52-9	Rank 5 : 153559-49-0
function: collagenase inhibitor				
				
Rank 1 : 63358-49-6	Rank 2 : 2181-04-6	Rank 3 : 125-52-0	Rank 4 : 103300-74-9	Rank 5 : 121808-62-6
function: COX inhibitor				

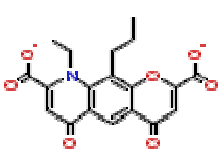
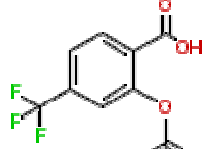
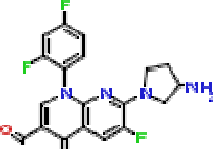
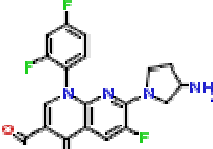
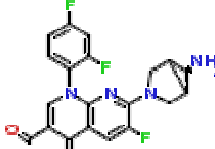
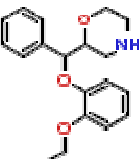
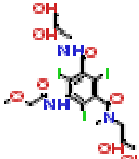
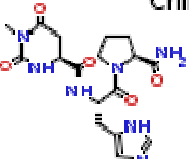
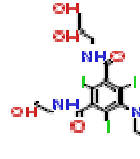
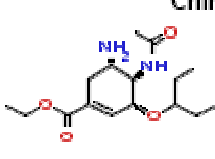
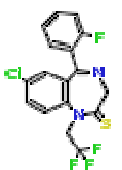
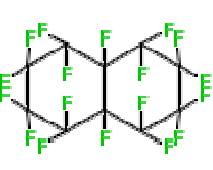
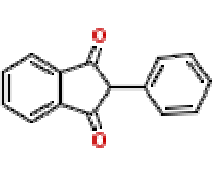
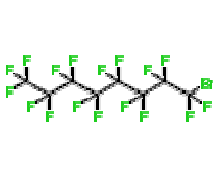
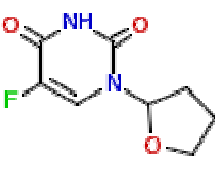
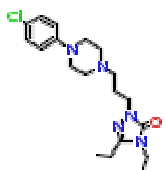
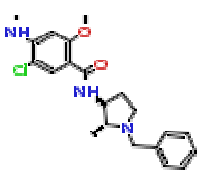
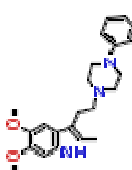
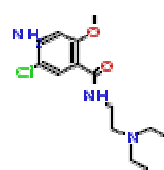
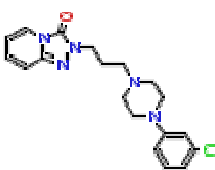
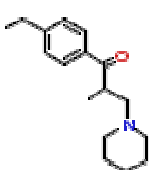
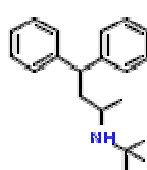
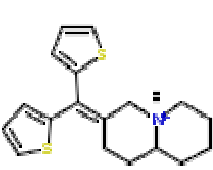
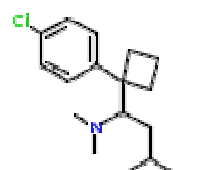
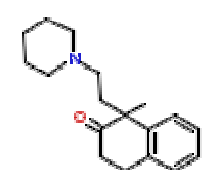
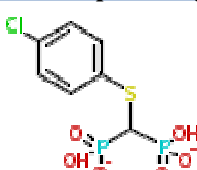
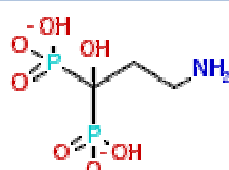
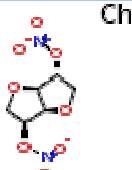
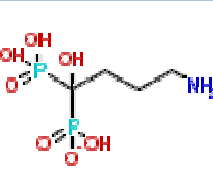
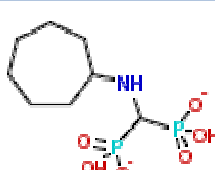
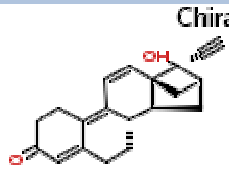
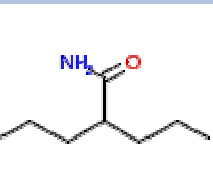
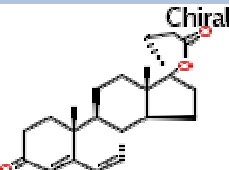
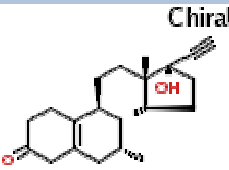
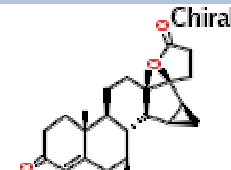
				
Rank 1 : 53-86-1	Rank 2 : 70374-39-9	Rank 3 : 5728-52-9	Rank 4 : 23288-49-5	Rank 5 : 1716-12-7
function: dopamine agonist/antagonist				
				
Rank 1 : 78628-80-5	Rank 2 : 54143-56-5	Rank 3 : 26844-12-2	Rank 4 : 84485-00-7	Rank 5 : 57262-94-9
function: elastase inhibitor				
				
Rank 1 : 71-73-8	Rank 2 : 80-77-3	Rank 3 : 36104-80-0	Rank 4 : 90101-16-9	Rank 5 : 59721-28-7
function: endothelin agonist/antagonist				
				
Rank 1 : 53902-12-8	Rank 2 : 87234-24-0	Rank 3 : 78967-07-4	Rank 4 : 87027-09-6	Rank 5 : 15826-37-6
function: estrogen				
				
Rank 1 : 82640-04-8	Rank 2 : 16320-04-0	Rank 3 : 35189-28-7	Rank 4 : 5630-53-5	Rank 5 : 84371-65-3
function: factor Xa inhibitor				
				
Rank 1 : 82956-11-4	Rank 2 : 93479-97-1	Rank 3 : 59721-28-7	Rank 4 : 100-33-4	Rank 5 : 148692-47-1
function: farnesyl protein transferase inhibitor				
				
Rank 1 : 79794-75-5	Rank 2 : 99614-02-5	Rank 3 : 102676-47-1	Rank 4 : 83172-76-3	Rank 5 : 112809-51-5
function: gastrin antagonist				

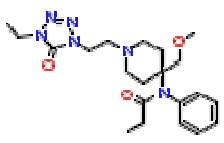
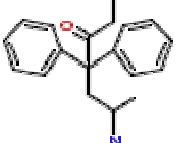
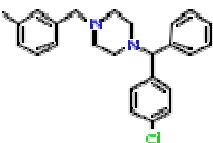
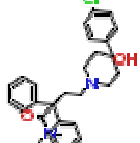
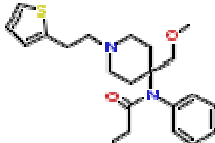
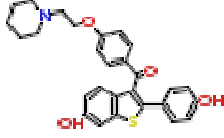
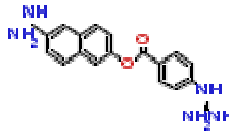
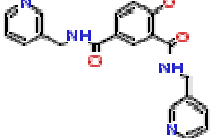
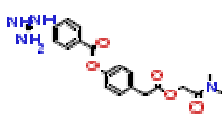
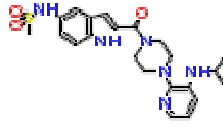
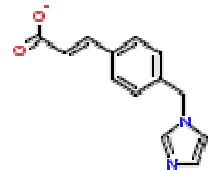
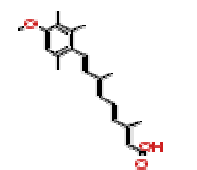
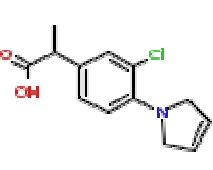
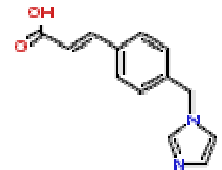
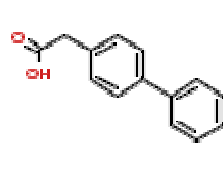
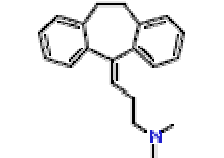
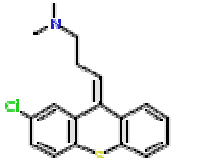
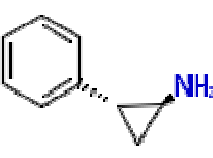
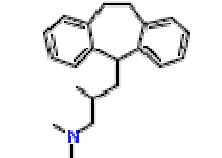
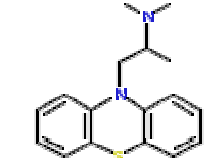
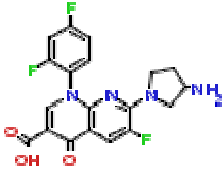
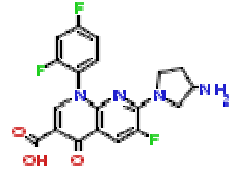
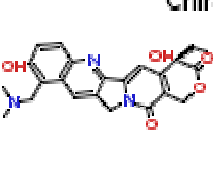
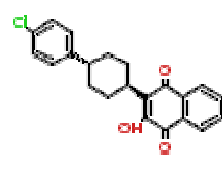
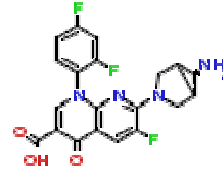
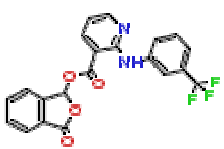
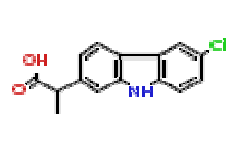
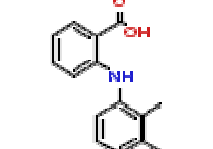
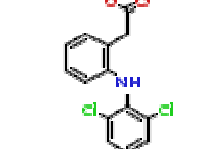
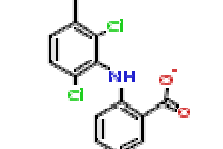
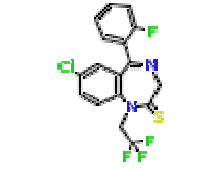
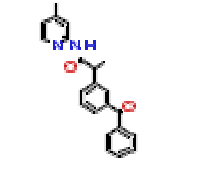
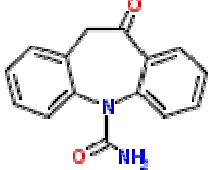
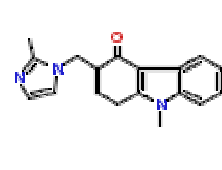
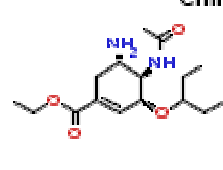
				
Rank 1 : 28395-03-1	Rank 2 : 14293-44-8	Rank 3 : 92134-98-0	Rank 4 : 97519-39-6	Rank 5 : 937-13-3
function: GP2b3a receptor antagonist				
				
Rank 1 : 87848-99-5	Rank 2 : 74863-84-6	Rank 3 : 59721-28-7	Rank 4 : 66195-31-1	Rank 5 : 130120-57-9
function: growth hormone release promoting agent				
				
Rank 1 : 55837-29-1	Rank 2 : 54143-56-5	Rank 3 : 51012-33-0	Rank 4 : 111470-99-6	Rank 5 : 123040-16-4
function: H+/K+ ATPase inhibitor				
				
Rank 1 : 2078-54-8	Rank 2 : 56287-74-2	Rank 3 : 321-64-2	Rank 4 : 99294-93-6	Rank 5 : 27686-84-6
function: histamine agonist/antagonist				
				
Rank 1 : 56518-41-3	Rank 2 : 1744-22-5	Rank 3 : 113775-47-6	Rank 4 : 102625-70-7	Rank 5 : 132036-88-5
function: HIV protease inhibitor				
				
Rank 1 : 129-49-7	Rank 2 : 77-36-1	Rank 3 : 129-06-6	Rank 4 : 66-76-2	Rank 5 : 74639-40-0
function: HMG-CoA reductase inhibitor				
				
Rank 1 : 35189-28-7	Rank 2 : 53-39-4	Rank 3 : 64218-02-6	Rank 4 : 57-63-6	Rank 5 : 661-19-8
function: IL-1 inhibitor				

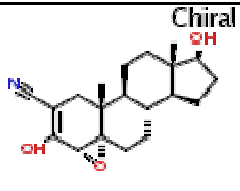
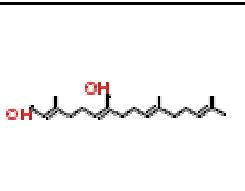
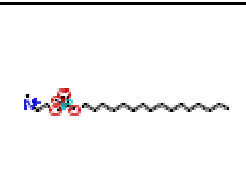
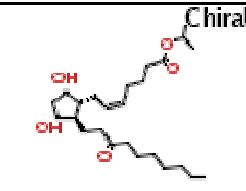
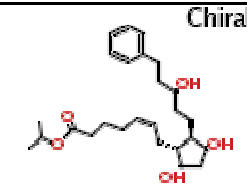
				
Rank 1 : 82571-53-7	Rank 2 : 58186-27-9	Rank 3 : 82571-53-7	Rank 4 : 54-36-4	Rank 5 : 6493-05-6
function: K+ channel activator				
				
Rank 1 : 63675-72-9	Rank 2 : 59-63-2	Rank 3 : 39562-70-4	Rank 4 : 66085-59-4	Rank 5 : 21829-25-4
function: K+ channel blocker				
				
Rank 1 : 306-94-5	Rank 2 : 97-77-8	Rank 3 : 581-88-4	Rank 4 : 80012-43-7	Rank 5 : 423-55-2
function: leukotriene agonist/antagonist				
				
Rank 1 : 65002-17-7	Rank 2 : 25812-30-0	Rank 3 : 21739-91-3	Rank 4 : 62571-86-2	Rank 5 : 103186-19-2
function: LHRH agonist/antagonist				
				
Rank 1 : 71771-90-9	Rank 2 : 72956-09-3	Rank 3 : 27223-35-4	Rank 4 : 50847-11-5	Rank 5 : 12192-57-3
function: lipid peroxidation inhibitor				
				
Rank 1 : 2078-54-8	Rank 2 : 58186-27-9	Rank 3 : 72956-09-3	Rank 4 : 57-63-6	Rank 5 : 321-64-2
function: lipoygenase inhibitor				
				
Rank 1 : 2078-54-8	Rank 2 : 89943-82-8	Rank 3 : 846-50-4	Rank 4 : 848-75-9	Rank 5 : 1716-12-7
function: MMP inhibitor				

 Rank 1 : 81872-10-8	 Rank 2 : 90098-04-7	 Rank 3 : 25812-30-0	 Rank 4 : 21739-91-3	 Rank 5 : 86780-90-7
function: muscarinic agonist/antagonist				
 Rank 1 : 306-94-5	 Rank 2 : 25953-17-7	 Rank 3 : 50-52-2	 Rank 4 : 97-77-8	 Rank 5 : 423-55-2
function: neurokinin agonist/antagonist				
 Rank 1 : 990-73-8	 Rank 2 : 71-81-8	 Rank 3 : 53179-11-6	 Rank 4 : 60561-17-3	 Rank 5 :
function: nitric oxide synthase inhibitor				
 Rank 1 : 77679-27-7	 Rank 2 : 581-88-4	 Rank 3 : 1744-22-5	 Rank 4 : 100-33-4	 Rank 5 : 80012-43-7
function: NMDA receptor antagonist				
 Rank 1 : 54965-23-0	 Rank 2 : 59263-76-2	 Rank 3 : 21535-47-7	 Rank 4 : 57262-94-9	 Rank 5 : 665-66-7
function: oxazolidinone				
 Rank 1 : 86832-68-0	 Rank 2 : 32838-28-1	 Rank 3 : 29218-27-7	 Rank 4 : 92823-00-2	 Rank 5 : 74639-40-0
function: oxytocin antagonist				
 Rank 1 : 1622-62-4	 Rank 2 : 121281-41-2	 Rank 3 : 111470-99-6	 Rank 4 : 132539-07-2	 Rank 5 : 196618-13-0
function: PAF analog/antagonist				

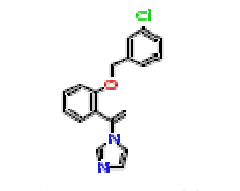
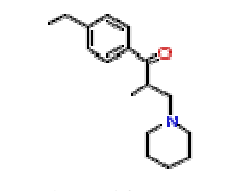
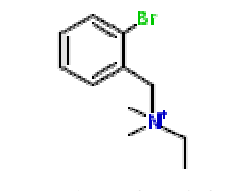
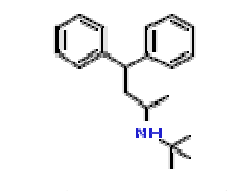
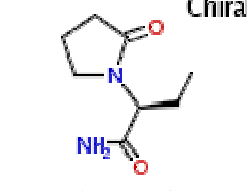
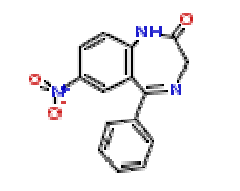
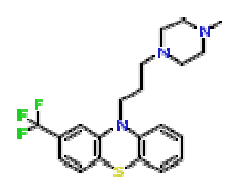
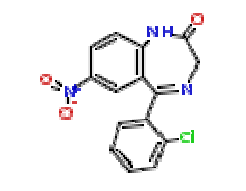
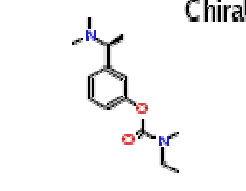
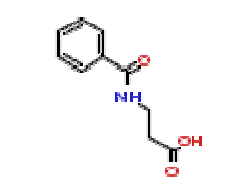
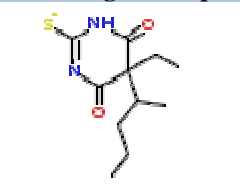
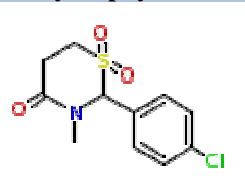
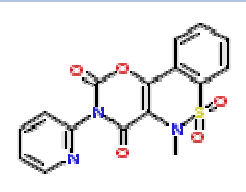
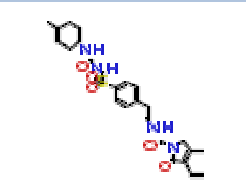
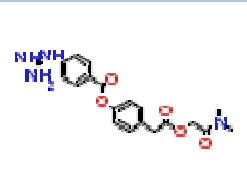
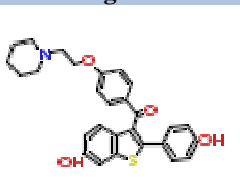
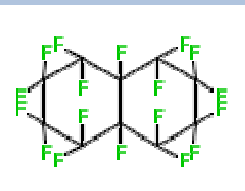
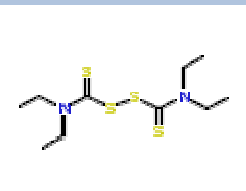
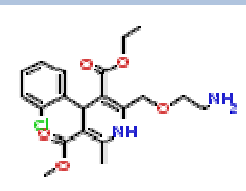
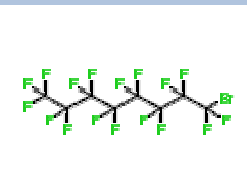
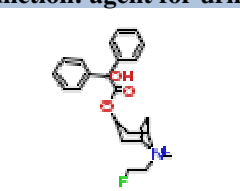
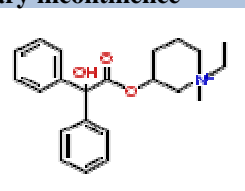
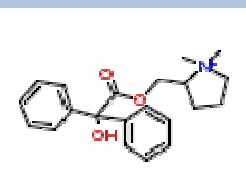
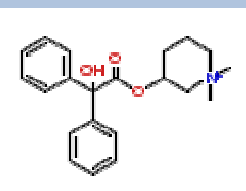
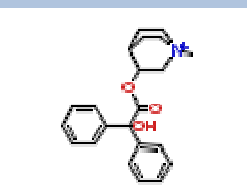
Rank 1 : 57801-81-7 Rank 2 : 88678-31-3 Rank 3 : 28911-01-5 Rank 4 : 29975-16-4 Rank 5 : 28981-97-7				
function: phosphodiesterase inhibitor				
				 Chiral
Rank 1 : 90101-16-9 Rank 2 : 70024-40-7 Rank 3 : 87234-24-0 Rank 4 : 87027-09-6 Rank 5 : 131741-08-7				
function: phospholipase inhibitor				
Rank 1 : 25812-30-0 Rank 2 : 22071-15-4 Rank 3 : 57469-78-0 Rank 4 : 106685-40-9 Rank 5 : 52-68-6				
function: PKC inhibitor				
Rank 1 : 70476-82-3 Rank 2 : 58-39-9 Rank 3 : 69-23-8 Rank 4 : 909-39-7 Rank 5 : 72275-67-3				
function: prolylendopeptidase inhibitor				
			 Chiral	
Rank 1 : 71-73-8 Rank 2 : 80-77-3 Rank 3 : 115-38-8 Rank 4 : 102767-28-2 Rank 5 : 77-41-8				
function: prostaglandin				
 Chiral	 Chiral	 Chiral	 Chiral	
Rank 1 : 64318-79-2 Rank 2 : 745-65-3 Rank 3 : 61849-14-7 Rank 4 : 60325-46-4 Rank 5 : 64218-02-6				
function: protease inhibitor				
			 Chiral	 Chiral
Rank 1 : 90101-16-9 Rank 2 : 665-66-7 Rank 3 : 81110-73-8 Rank 4 : 122946-43-4 Rank 5 : 196618-13-0				
function: quinolone				

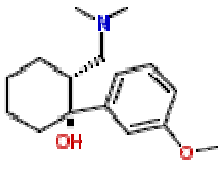
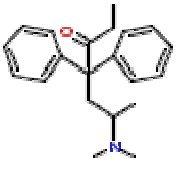
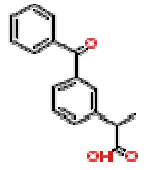
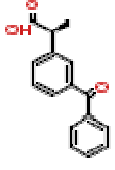
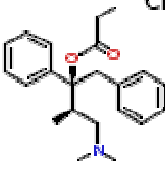
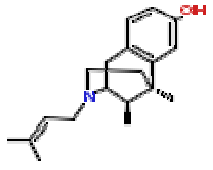
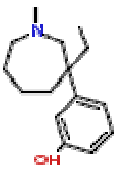
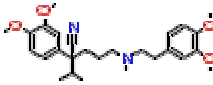
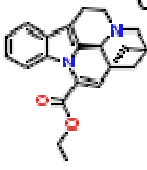
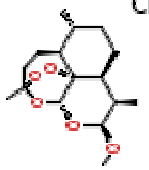
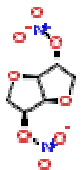
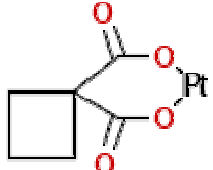
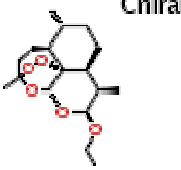
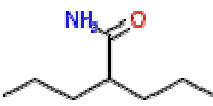
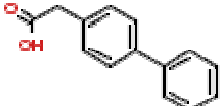
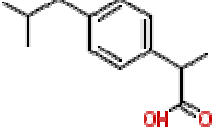
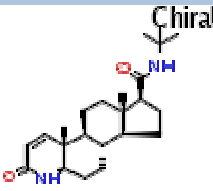
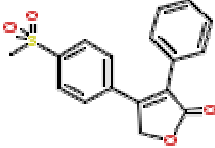
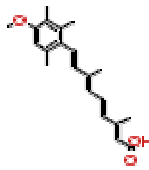
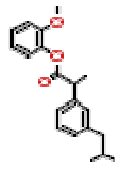
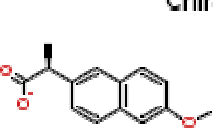
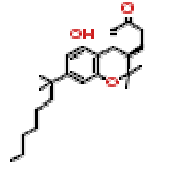
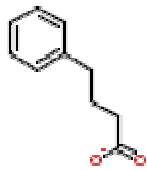
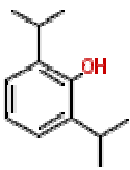
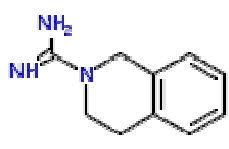
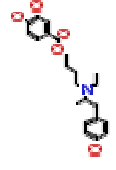
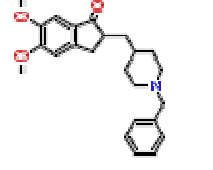
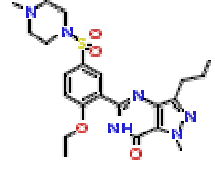
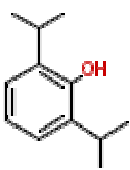
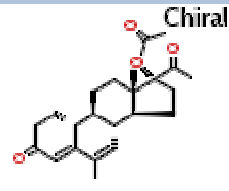
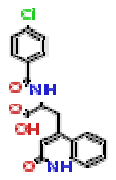
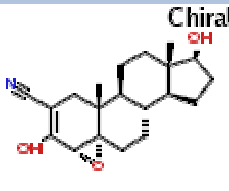
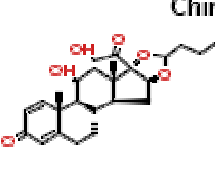
				
Rank 1 : 69049-73-6	Rank 2 : 322-79-2	Rank 3 : 104051-69-6	Rank 4 : 115964-29-9	Rank 5 : 147059-72-1
function: renin inhibitor				
				
Rank 1 : 71620-89-8	Rank 2 : 73334-07-3	Rank 3 : 103300-74-9	Rank 4 : 107793-72-6	Rank 5 : 196618-13-0
function: reverse transcriptase inhibitor				
				
Rank 1 : 36735-22-5	Rank 2 : 306-94-5	Rank 3 : 83-12-5	Rank 4 : 423-55-2	Rank 5 : 17902-23-7
function: serotonin agonist/antagonist				
				
Rank 1 : 57775-22-1	Rank 2 : 93664-94-9	Rank 3 : 153-87-7	Rank 4 : 54143-57-6	Rank 5 : 25332-39-2
function: sigma antagonist				
				
Rank 1 : 56839-43-1	Rank 2 : 7082-21-5	Rank 3 : 71731-58-3	Rank 4 : 84485-00-7	Rank 5 : 22443-11-4
function: squalene synthetase inhibitor				
				
Rank 1 : 89987-06-4	Rank 2 : 57248-88-1	Rank 3 : 87-33-2	Rank 4 : 66376-36-1	Rank 5 : 124351-85-5
function: steroid reductase inhibitor				
				
Rank 1 : 16320-04-0	Rank 2 : 2430-27-5	Rank 3 : 976-71-6	Rank 4 : 5630-53-5	Rank 5 : 67392-87-4
function: substance P antagonist				

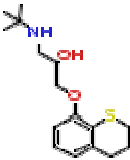
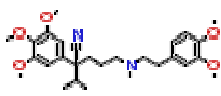
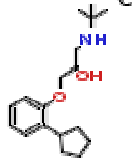
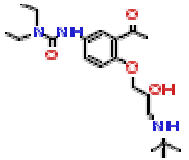
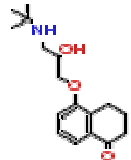
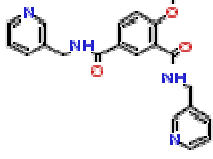
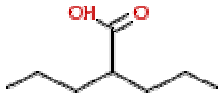
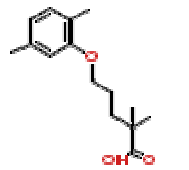
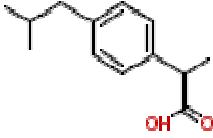
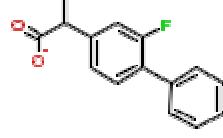
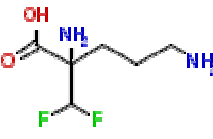
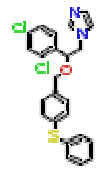
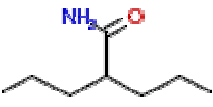
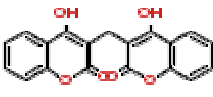
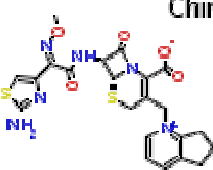
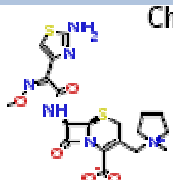
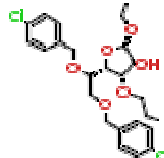
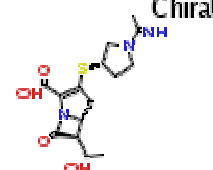
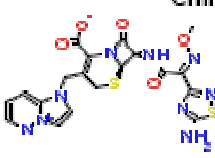
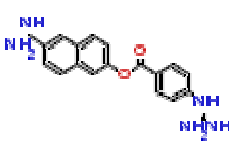
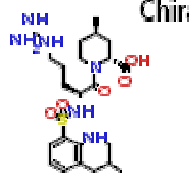
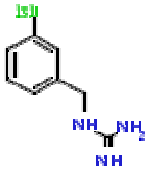
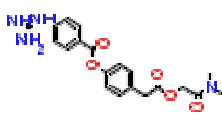
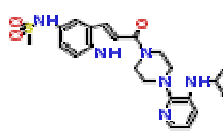
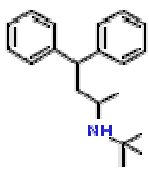
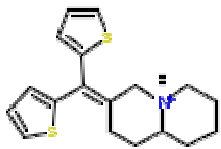
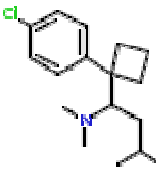
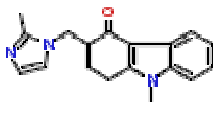
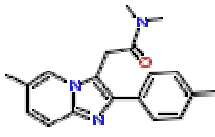
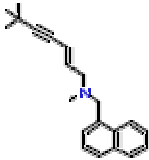
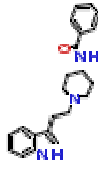
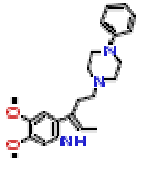
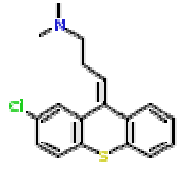
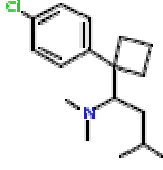
				
Rank 1 : 69049-06-5	Rank 2 : 1095-90-5	Rank 3 : 31884-77-2	Rank 4 : 53179-11-6	Rank 5 : 60561-17-3
function: thrombin inhibitor				
				
Rank 1 : 82640-04-8	Rank 2 : 82956-11-4	Rank 3 : 32828-81-2	Rank 4 : 59721-28-7	Rank 5 : 148692-47-1
function: thromboxane antagonist				
				
Rank 1 : 82571-53-7	Rank 2 : 55079-83-9	Rank 3 : 31793-07-4	Rank 4 : 82571-53-7	Rank 5 : 5728-52-9
function: TNF inhibitor				
				
Rank 1 : 549-18-8	Rank 2 : 113-59-7	Rank 3 : 13492-01-8	Rank 4 : 5585-73-9	Rank 5 : 58-33-3
function: topoisomerase inhibitor				
		 Chiral		
Rank 1 : 104051-69-6	Rank 2 : 115964-29-9	Rank 3 : 123948-87-8	Rank 4 : 95233-18-4	Rank 5 : 147059-72-1
function: tyrosine kinase inhibitor				
				
Rank 1 : 66898-62-2	Rank 2 : 53716-49-7	Rank 3 : 61-68-7	Rank 4 : 15307-79-6	Rank 5 : 6385-02-0
function: vasopressin antagonist				
				 Chiral
Rank 1 : 36735-22-5	Rank 2 : 60576-13-8	Rank 3 : 28721-07-5	Rank 4 : 99614-02-5	Rank 5 : 196618-13-0
function: vitamin D analog				

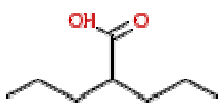
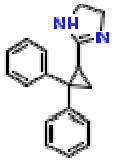
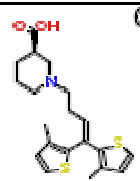
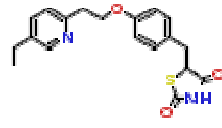
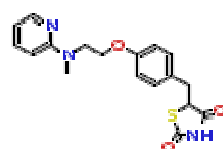
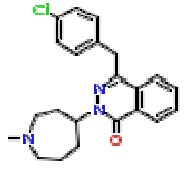
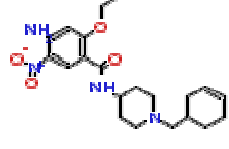
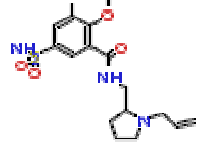
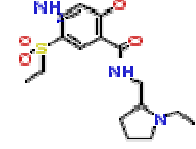
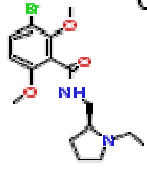
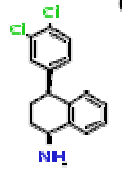
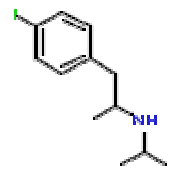
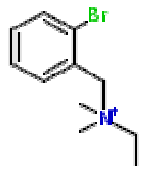
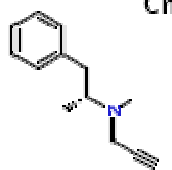
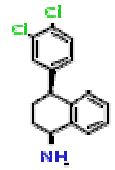
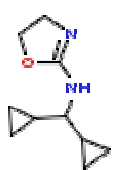
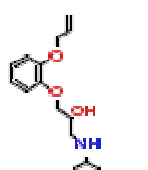
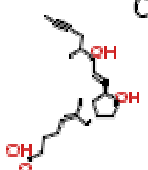
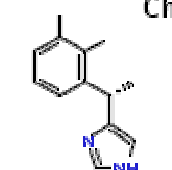
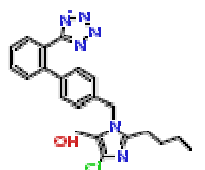
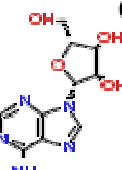
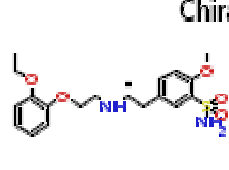
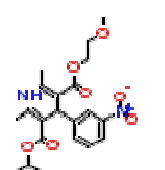
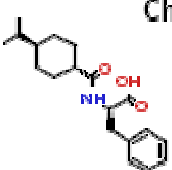
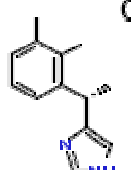
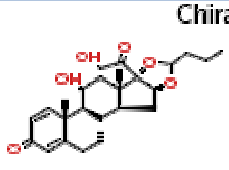
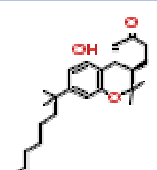
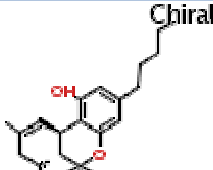
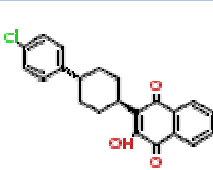
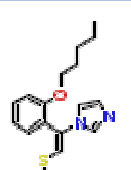
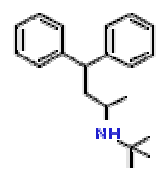
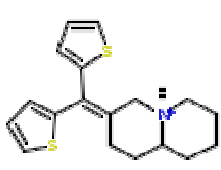
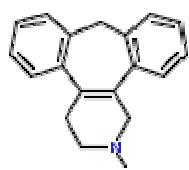
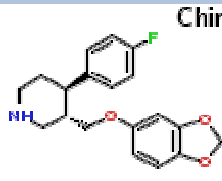
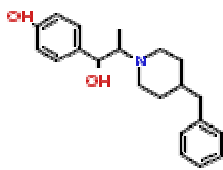
				
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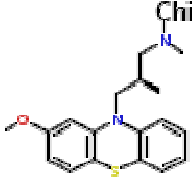
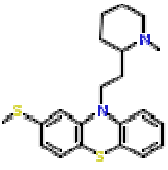
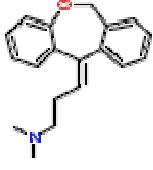
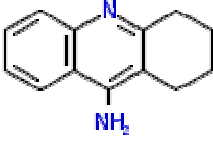
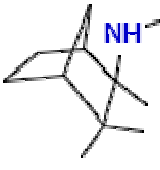
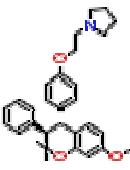
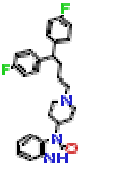
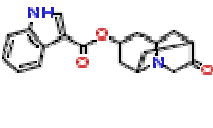
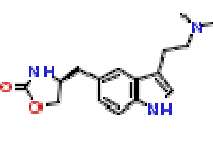
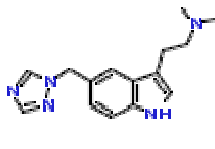
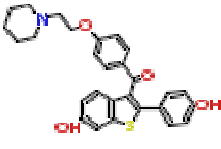
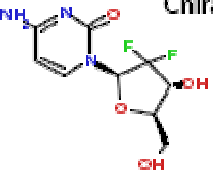
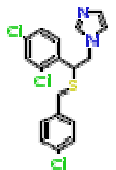
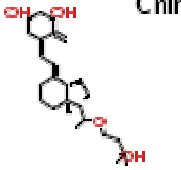
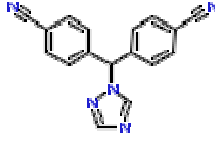
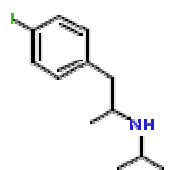
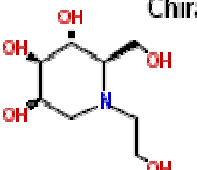
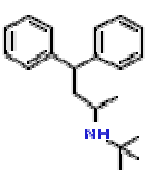
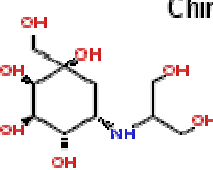
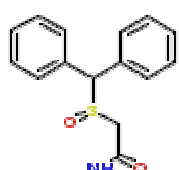
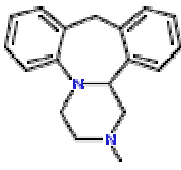
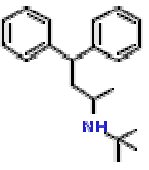
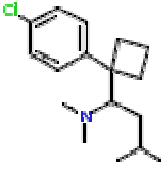
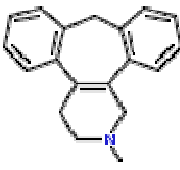
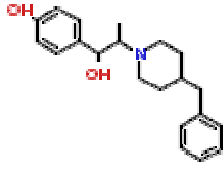
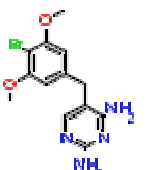
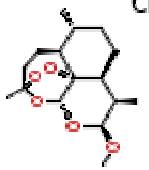
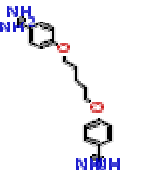
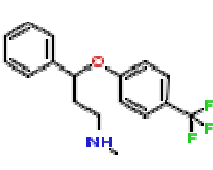
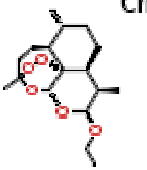
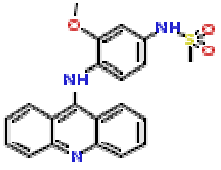
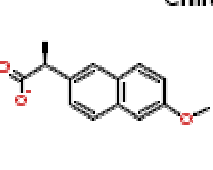
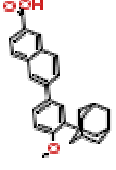
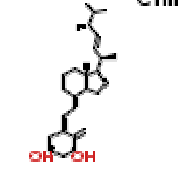
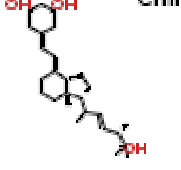
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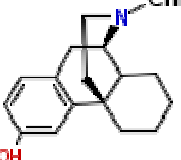
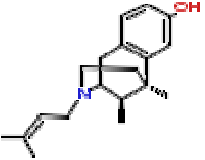
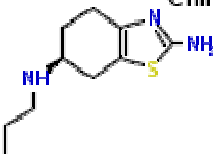
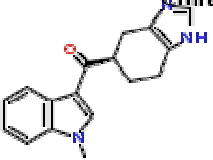
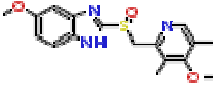
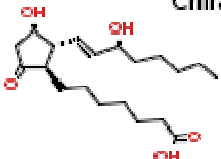
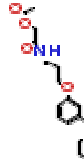
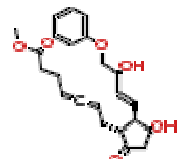
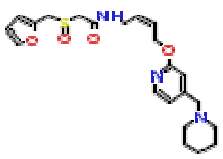
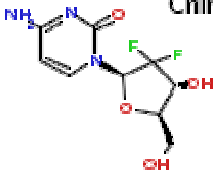
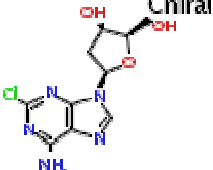
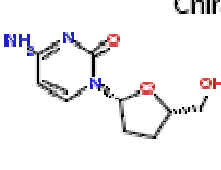
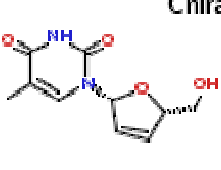
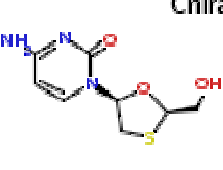
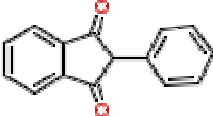
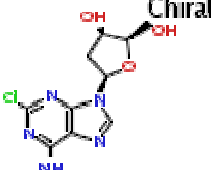
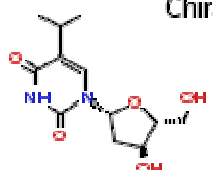
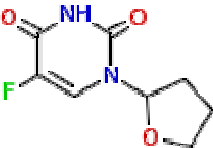
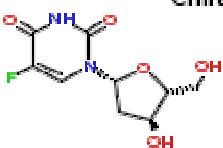
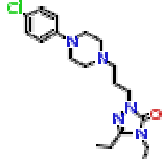
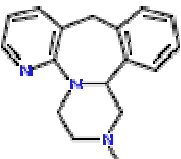
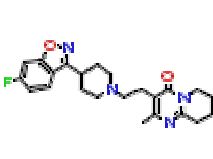
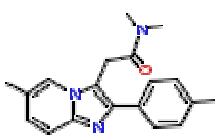
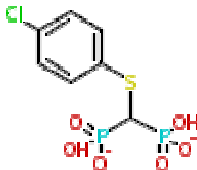
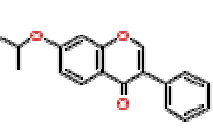
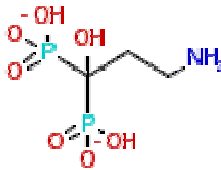
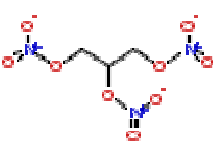
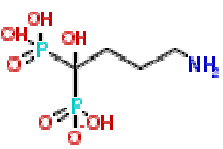
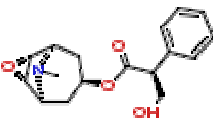
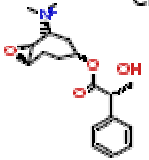
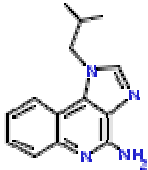
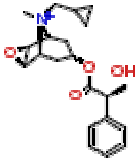
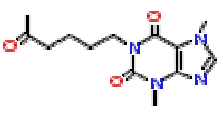
therapeutic areas				
function: agent for cognition disorders				
				
Rank 1 : 77174-66-4	Rank 2 : 56839-43-1	Rank 3 : 61-75-6	Rank 4 : 7082-21-5	Rank 5 : 102767-28-2
function: agent for pancreas disorders				
				
Rank 1 : 146-22-5	Rank 2 : 440-17-5	Rank 3 : 1622-61-3	Rank 4 : 123441-03-2	Rank 5 : 3440-28-6
function: agent for pulmonary emphysema				
				
Rank 1 : 71-73-8	Rank 2 : 80-77-3	Rank 3 : 90101-16-9	Rank 4 : 93479-97-1	Rank 5 : 59721-28-7
function: agent for restenosis				
				
Rank 1 : 82640-04-8	Rank 2 : 306-94-5	Rank 3 : 97-77-8	Rank 4 : 111470-99-6	Rank 5 : 423-55-2
function: agent for urinary incontinence				
				
Rank 1 : 63516-10-9	Rank 2 : 125-51-9	Rank 3 : 545-80-2	Rank 4 : 76-90-4	Rank 5 : 3485-62-9
function: analgesic non-opioid				

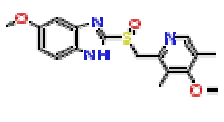
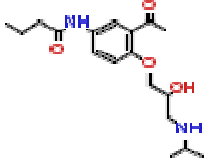
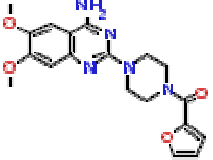
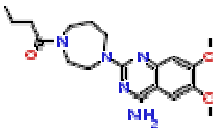
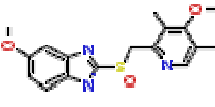
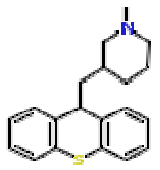
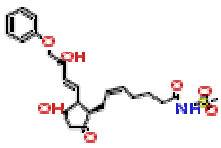
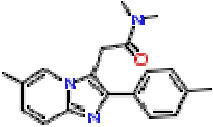
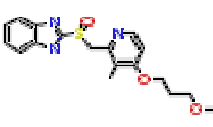
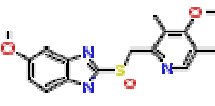
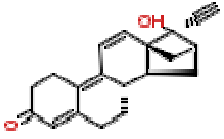
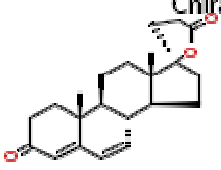
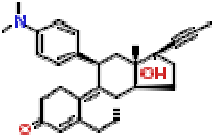
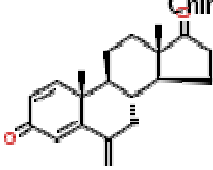
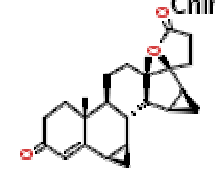
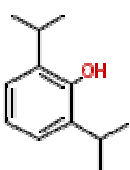
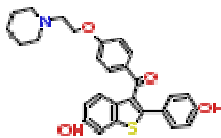
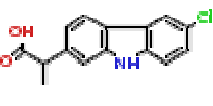
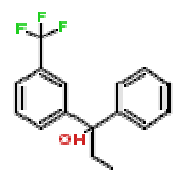
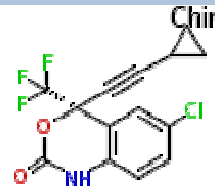
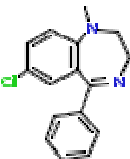
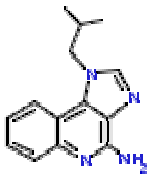
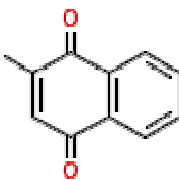
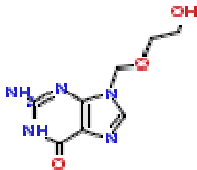
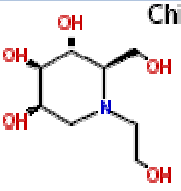
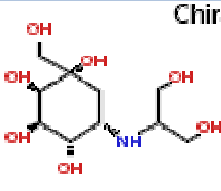
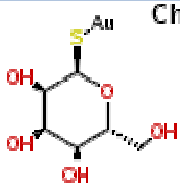
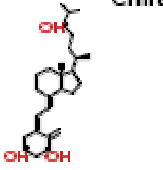
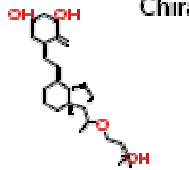
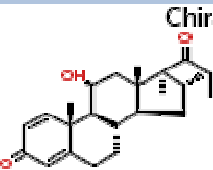
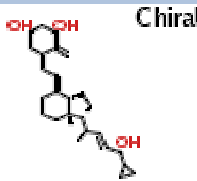
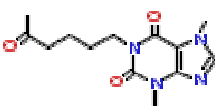
				 Chiral
Rank 1 : 22204-88-2 Rank 2 : 1095-90-5 Rank 3 : 57469-78-0 Rank 4 : 84-80-0 Rank 5 : 22161-81-5				
function: analgesic opioid				
 Chiral				 Chiral
Rank 1 : 1639-60-7 Rank 2 : 64024-15-3 Rank 3 : 59263-76-2 Rank 4 : 52-53-9 Rank 5 : 42971-09-5				
function: anthelmic				
	 Chiral	 Chiral		 Chiral
Rank 1 : 38260-01-4 Rank 2 : 71963-77-4 Rank 3 : 87-33-2 Rank 4 : 41575-94-4 Rank 5 : 75887-54-6				
function: antiacne				
			 Chiral	
Rank 1 : 2430-27-5 Rank 2 : 5728-52-9 Rank 3 : 15687-27-1 Rank 4 : 98319-26-7 Rank 5 : 162011-90-7				
function: antiallergic				
		 Chiral		
Rank 1 : 55079-83-9 Rank 2 : 66332-77-2 Rank 3 : 26159-34-2 Rank 4 : 51022-71-0 Rank 5 : 1716-12-7				
function: antianginal				
				
Rank 1 : 2078-54-8 Rank 2 : 581-88-4 Rank 3 : 2753-45-9 Rank 4 : 120011-70-3 Rank 5 : 139755-83-2				
function: antiangiogenic				
	 Chiral		 Chiral	 Chiral
Rank 1 : 2078-54-8 Rank 2 : 58691-88-6 Rank 3 : 90098-04-7 Rank 4 : 13647-35-3 Rank 5 : 51333-22-3				
function: antiarrhythmic				

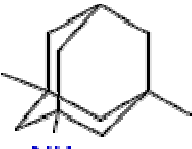
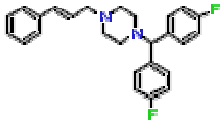
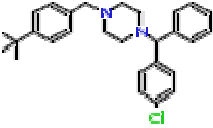
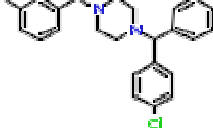
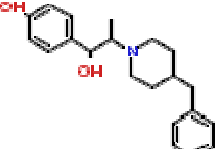
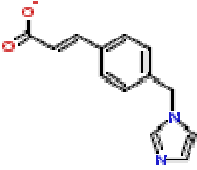
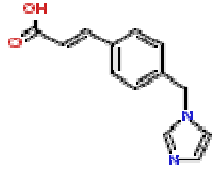
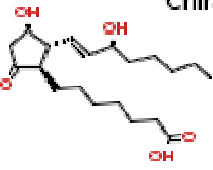
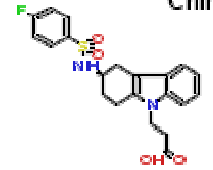
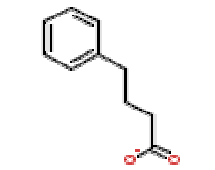
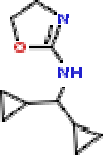
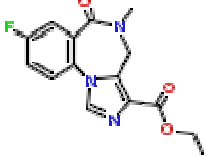
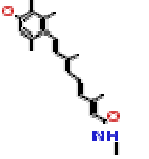
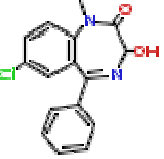
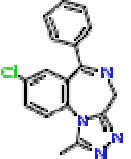
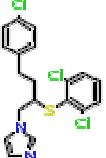
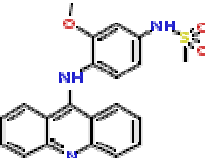
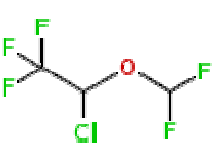
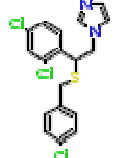
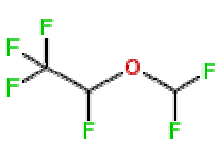
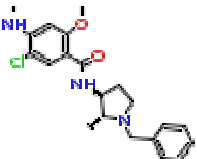
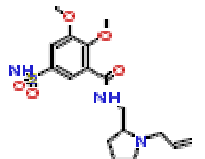
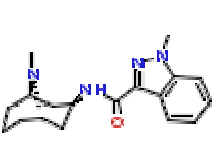
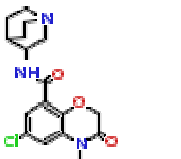
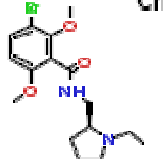
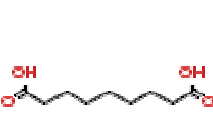
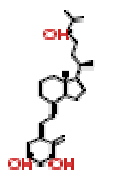
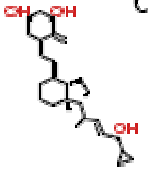
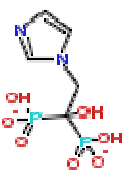
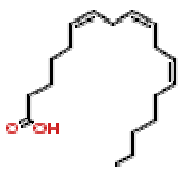
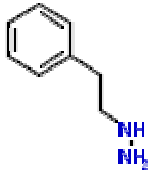
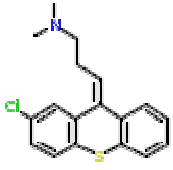
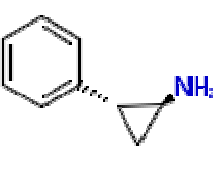
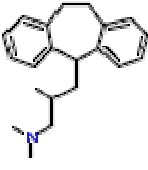
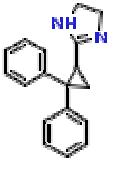
				
Rank 1 : 33580-30-2	Rank 2 : 16662-47-8	Rank 3 : 38363-32-5	Rank 4 : 57470-78-7	Rank 5 : 27912-14-7
function: antiarthritic				
				
Rank 1 : 32828-81-2	Rank 2 : 76584-70-8	Rank 3 : 25812-30-0	Rank 4 : 15687-27-1	Rank 5 : 5104-49-4
function: antibacterial				
				
Rank 1 : 96020-91-6	Rank 2 : 72479-26-6	Rank 3 : 2430-27-5	Rank 4 : 66-76-2	Rank 5 : 661-19-8
function: antibiotic				
				
Rank 1 : 84957-29-9	Rank 2 : 88040-23-7	Rank 3 : 29899-95-4	Rank 4 : 87726-17-8	Rank 5 : 113359-04-9
function: anticoagulant				
				
Rank 1 : 82956-11-4	Rank 2 : 74863-84-6	Rank 3 : 77679-27-7	Rank 4 : 59721-28-7	Rank 5 : 148692-47-1
function: anticonvulsant				
				
Rank 1 : 7082-21-5	Rank 2 : 71731-58-3	Rank 3 : 84485-00-7	Rank 4 : 99614-02-5	Rank 5 : 99294-93-6
function: antidepressant				
				
Rank 1 : 78628-80-5	Rank 2 : 26844-12-2	Rank 3 : 153-87-7	Rank 4 : 113-59-7	Rank 5 : 84485-00-7
function: antidiabetic				

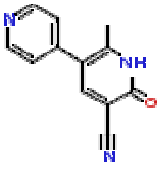
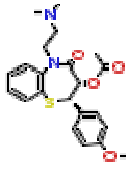
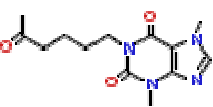
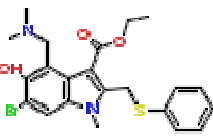
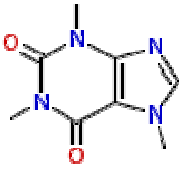
		 Chiral		 Chiral
Rank 1 : 76584-70-8	Rank 2 : 53267-01-9	Rank 3 : 115103-54-3	Rank 4 : 112529-15-4	Rank 5 : 155141-29-0
function: antiemetic				
	 Chiral			 Chiral
Rank 1 : 58581-89-8	Rank 2 : 66564-14-5	Rank 3 : 66644-81-3	Rank 4 : 71675-85-9	Rank 5 : 80125-14-0
function: antifungal				
 Chiral			 Chiral	 Chiral
Rank 1 : 79617-96-2	Rank 2 : 85068-76-4	Rank 3 : 61-75-6	Rank 4 : 14611-51-9	Rank 5 : 79617-96-2
function: antiglaucoma				
		 Chiral	 Chiral	
Rank 1 : 54187-04-1	Rank 2 : 6452-73-9	Rank 3 : 73873-87-7	Rank 4 : 113775-47-6	Rank 5 : 124750-99-8
function: antihypertensive				
 Chiral	 Chiral		 Chiral	 Chiral
Rank 1 : 58-61-7	Rank 2 : 80223-99-0	Rank 3 : 66085-59-4	Rank 4 : 105816-04-4	Rank 5 : 113775-47-6
function: antiinflammatory				
 Chiral		 Chiral		
Rank 1 : 51333-22-3	Rank 2 : 51022-71-0	Rank 3 : 1972-08-3	Rank 4 : 95233-18-4	Rank 5 : 111788-99-9
function: antiischemic				
			 Chiral	
Rank 1 : 7082-21-5	Rank 2 : 71731-58-3	Rank 3 : 57262-94-9	Rank 4 : 61869-08-7	Rank 5 : 23210-56-2
function: antimalarial				

 Rank 1 : 60-99-1	 Rank 2 : 50-52-2	 Rank 3 : 1229-29-4	 Rank 4 : 321-64-2	 Rank 5 : 826-39-1
function: antimigraine				
 Rank 1 : 31477-60-8	 Rank 2 : 2062-78-4	 Rank 3 : 115956-12-2	 Rank 4 : 139264-17-8	 Rank 5 : 144034-80-0
function: antineoplastic				
 Rank 1 : 82640-04-8	 Rank 2 : 95058-81-4	 Rank 3 : 61318-90-9	 Rank 4 : 103909-75-7	 Rank 5 : 112809-51-5
function: antiobesity				
 Rank 1 : 85068-76-4	 Rank 2 : 72432-03-2	 Rank 3 : 7082-21-5	 Rank 4 : 112653-29-9	 Rank 5 : 68693-11-8
function: antiparkinsonian				
 Rank 1 : 21535-47-7	 Rank 2 : 7082-21-5	 Rank 3 : 84485-00-7	 Rank 4 : 57262-94-9	 Rank 5 : 23210-56-2
function: antiprotozoal				
 Rank 1 : 56518-41-3	 Rank 2 : 71963-77-4	 Rank 3 : 100-33-4	 Rank 4 : 54910-89-3	 Rank 5 : 75887-54-6
function: antipsoriatic				
 Rank 1 : 51264-14-3	 Rank 2 : 26159-34-2	 Rank 3 : 106685-40-9	 Rank 4 : 54573-75-0	 Rank 5 : 131918-61-1
function: antipsychotic				

				
Rank 1 : 83366-66-9	Rank 2 : 6700-40-9	Rank 3 : 64024-15-3	Rank 4 : 104632-26-0	Rank 5 : 132036-88-5
function: antiulcerative				
				
Rank 1 : 73590-58-6	Rank 2 : 745-65-3	Rank 3 : 78628-28-1	Rank 4 : 73121-56-9	Rank 5 : 118288-08-7
function: antiviral				
				
Rank 1 : 95058-81-4	Rank 2 : 4291-63-8	Rank 3 : 7481-89-2	Rank 4 : 3056-17-5	Rank 5 : 134678-17-4
function: antiviral AIDS				
				
Rank 1 : 83-12-5	Rank 2 : 4291-63-8	Rank 3 : 60136-25-6	Rank 4 : 17902-23-7	Rank 5 : 50-91-9
function: anxiolytic				
				
Rank 1 : 57775-22-1	Rank 2 : 83366-66-9	Rank 3 : 61337-67-5	Rank 4 : 106266-06-2	Rank 5 : 99294-93-6
function: bone resorption inhibitor				
				
Rank 1 : 89987-06-4	Rank 2 : 35212-22-7	Rank 3 : 57248-88-1	Rank 4 : 55-63-0	Rank 5 : 66376-36-1
function: bronchodilator				
				
Rank 1 : 51-34-3	Rank 2 : 155-41-9	Rank 3 : 99011-02-6	Rank 4 : 51598-60-8	Rank 5 : 6493-05-6
function: cardiotonic				

				 Chiral
Rank 1 : 73590-58-6	Rank 2 : 34381-68-5	Rank 3 : 19237-84-4	Rank 4 : 52712-76-2	Rank 5 : 119141-88-7
function: gastric antisecretory				
	 Chiral			 Chiral
Rank 1 : 7081-40-5	Rank 2 : 60325-46-4	Rank 3 : 99294-93-6	Rank 4 : 117976-90-6	Rank 5 : 119141-88-7
function: hair growth promoter				
 Chiral	 Chiral	 Chiral	 Chiral	 Chiral
Rank 1 : 16320-04-0	Rank 2 : 976-71-6	Rank 3 : 84371-65-3	Rank 4 : 107868-30-4	Rank 5 : 67392-87-4
function: hypolipidemic				
				 Chiral
Rank 1 : 2078-54-8	Rank 2 : 82640-04-8	Rank 3 : 53716-49-7	Rank 4 : 56430-99-0	Rank 5 : 154598-52-4
function: immunomodulator				
				
Rank 1 : 2898-12-6	Rank 2 : 84-80-0	Rank 3 : 99011-02-6	Rank 4 : 863-61-6	Rank 5 : 58-27-5
function: immunostimulant				
	 Chiral	 Chiral	 Chiral	
Rank 1 : 59277-89-3	Rank 2 : 72432-03-2	Rank 3 : 112653-29-9	Rank 4 : 12192-57-3	Rank 5 : 661-19-8
function: immunosuppressant				
 Chiral	 Chiral	 Chiral	 Chiral	
Rank 1 : 93129-94-3	Rank 2 : 103909-75-7	Rank 3 : 49697-38-3	Rank 4 : 112828-00-9	Rank 5 : 6493-05-6
function: neural injury inhibitor				

 Rank 1 : 19982-08-2	 Rank 2 : 30484-77-6	 Rank 3 : 129-74-8	 Rank 4 : 31884-77-2	 Rank 5 : 23210-56-2
function: platelet antiaggregatory				
 Rank 1 : 82571-53-7	 Rank 2 : 82571-53-7	 Rank 3 : 745-65-3	 Rank 4 : 116649-85-5	 Rank 5 : 1716-12-7
function: sedative/hypnotic				
 Rank 1 : 54187-04-1	 Rank 2 : 78755-81-4	 Rank 3 : 56281-36-8	 Rank 4 : 846-50-4	 Rank 5 : 28981-97-7
function: signal transduction inhibitor				
 Rank 1 : 64872-77-1	 Rank 2 : 51264-14-3	 Rank 3 : 26675-46-7	 Rank 4 : 61318-90-9	 Rank 5 : 57041-67-5
function: stimulant peristaltic				
 Rank 1 : 93664-94-9	 Rank 2 : 66644-81-3	 Rank 3 : 109889-09-0	 Rank 4 : 123040-16-4	 Rank 5 : 80125-14-0
function: treatment for osteoporosis				
 Rank 1 : 123-99-9	 Rank 2 : 93129-94-3	 Rank 3 : 112828-00-9	 Rank 4 : 118072-93-8	 Rank 5 : 506-26-3
function: treatment for septic shock				
 Rank 1 : 156-51-4	 Rank 2 : 113-59-7	 Rank 3 : 13492-01-8	 Rank 4 : 5585-73-9	 Rank 5 : 53267-01-9
function: vasodilator				

 Rank 1 : 78415-72-2	Chiral  Rank 2 : 42399-41-7	 Rank 3 : 6493-05-6	 Rank 4 : 131707-23-8	 Rank 5 : 69-22-7
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