

Supplementary Materials: Small Molecule Docking Supports Broad and Narrow Spectrum Potential for the Inhibition of the Novel Antibiotic Target Bacterial Pth1

Paul P. Ferguson, W. Blake Holloway, William N. Setzer, Hana McFeeters and Robert L. McFeeters

			10	20	30	40	50
E. coli	(2PTH)	-----	T I K L I V G L A N P G A E Y A A T R H N A G A W F V D L L A E R L R A P L R E E A K F F G Y T S R				
S. typhi.	(4P7B)	-----	A I K L I V G L A N P G A E Y A A T R H N A G A W Y V D L L A E R L R A P L R E E P K F F G Y T S R				
P. aeru.	(4FYJ)	-----	T A V Q L I V G L G N P G P E Y D Q T R H N A G A L F V E R L A H A Q G V S L V A D R K Y F G L V G K				
A. baum.	(4FOP)	-----	M S N I S L I V G L G N P G S E Y A Q T R H N A G F W F V E Q L A D K Y G I T L K N D P K F H G I S G R G				
B. thai.	(3V2I)	MG T L E A Q T Q G P G S M I K L I V G L G N P G A E Y T A T R H N A G F W L V D Q L A R E A G A T L R D E R R F H G F Y A K					
F. tula.	(3NEA)	S S G L V P R G S H - M P K I K M I I G L G N I G K E Y Q D T R H N V G E W F I A K I A Q D N N Q S F S S N P K L N C N L A K					
M. tube.	(2Z2I)	-----	M A E P L L V V G L G N P G A N Y A R T R H N L G F V V A D L L A A R L G A K F K A H K R S G A E V A T				
M. smeg.	(3KJZ)	-----	M A E P L L V V G L G N P G P T Y A K T R H N L G F M V A D V L A G R I G S A F K V H K K S G A E V V T				

	60	70	80	90	100	110	120
V T L G G E D V R L L V P T T F M N L S G K A V A A M A S F F R I N P D E I L V A H D E L D L P P G V A K F K L G G G H G G H N G L K D I I S K L G N N							
I T L E G E D V R L L V P T T F M N L S G K A V G A M A S F Y R I Q P D E I L V A H D E L D L P P G V A K F K L G G G H G G H N G L K D I I S K L G N N							
F S H Q G K D V R L L I P T T Y M N R S G Q S V A A L A G F F R I A P D A I L V A H D E L D M P P G V A K L K T G G G H G G H N G L R D I I A Q L G N Q							
N I E G H D V R L L L P M T Y M N R S G Q S V V P F S K F Y Q I A P E A I L I A H D E L D M N P G V I R L K T G G G H G G H N G L R D I V P H I G P -							
A R L Y G E E V H L L E P Q T Y M N R S G Q S V V A L A H F F K I L P N E I L V A H D E L D L P P G V A K L K L G G G S G G H N G L K D I S A H L S S Q							
V S I D Y N N V V L V F P T T Y M N N S G L A V S K V A N F Y K I A P A E I L V V H D E L D I D S G E I R L K K G G G H G G H N G L R S I N Q H L G T N							
G R S A G R S L V L A K P R C Y M N E S G R Q I G P L A K F Y S V A P A N I I V I H D D L D L E F G R I R L K I G G G E G G H N G L R S V V A A L G T K							
G R L A G T T V V L A K P R I S M N E S G R Q V G P L A K F Y S V P P Q Q I V V I H D E L D I D F G R I R L K L G G G E G G H N G L R S V A S A L G T K							

	130	140	150	160	170	180	190	200
P N F H R L R I G I G H P - - - - -								
P N F H R L R V G I G H P - - - - -								
N S F H R L R L G I G H P - - - - -								
- N F H R L R I G I G H P - - - - -								
- Q Y W R L R I G I G H P R D M I P E S A R A G A K P D V A N F V L K P P R K E E Q D V I D A A I E R A L A V M P A V V K G E T E R A M M Q L H R N G A -								
- D Y L R L R I G I G H P - - - - -								
- D F Q R V R I G I G R P - - - - -								
- N F H R V R I G V G R P - - - - -								

Figure S1. Amino Acid Sequence Alignment of Pth1s. Number corresponds to *E. coli* Pth1.

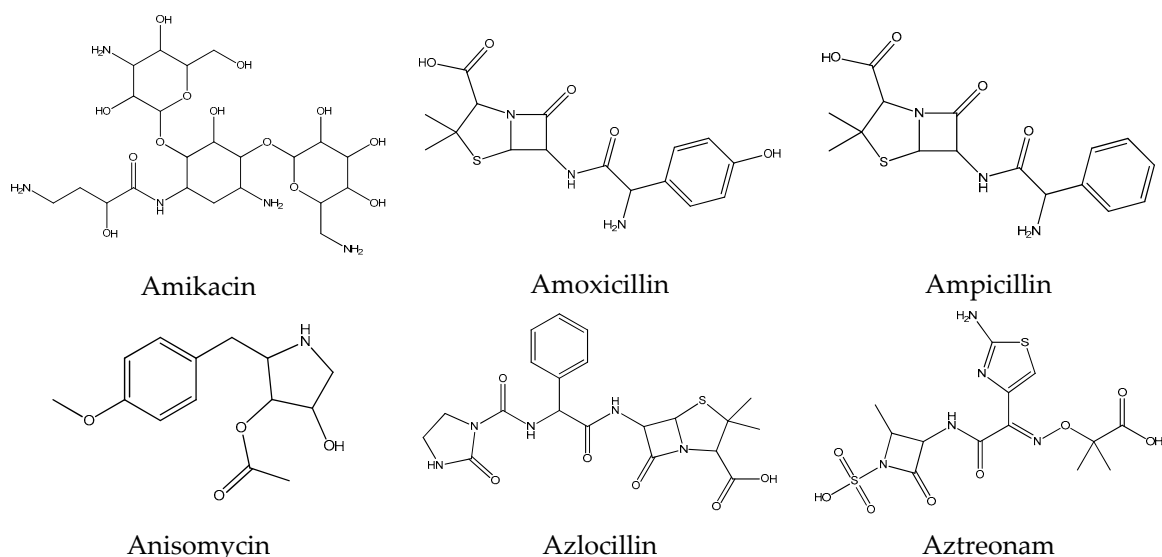
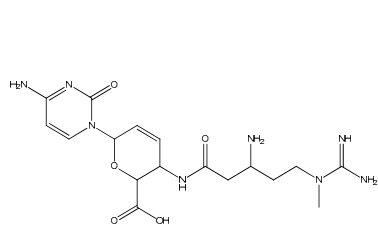
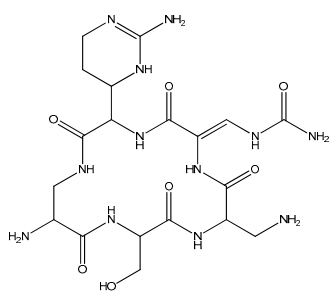


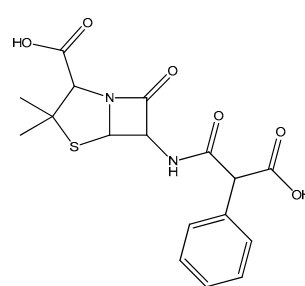
Figure S2. Cont.



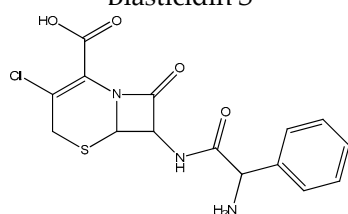
Blastidicin S



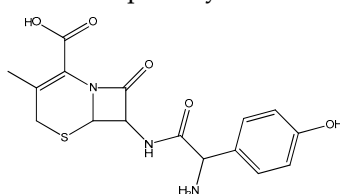
Capreomycin



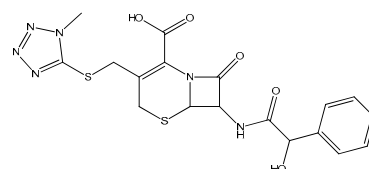
Carbenicillin



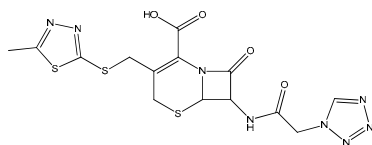
Cefaclor



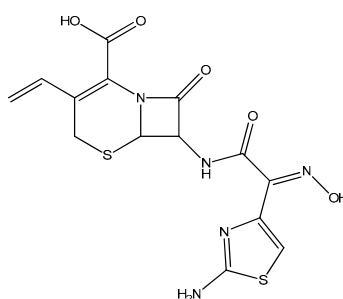
Cefadroxil



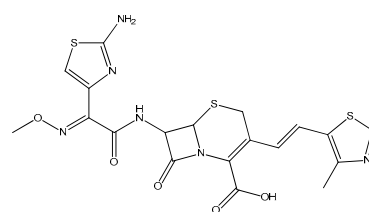
Cefamandole



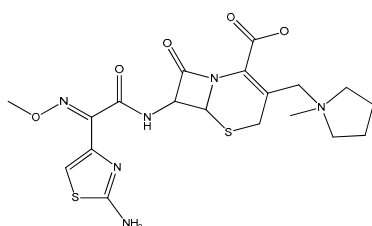
Cefazolin



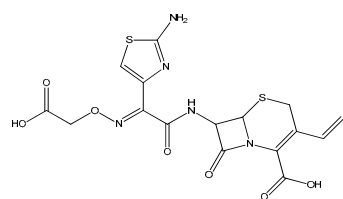
Cefdinir



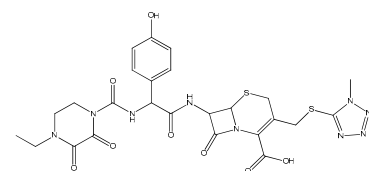
Cefditoren



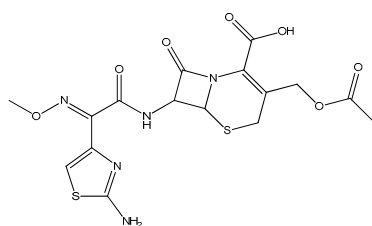
Cefepime



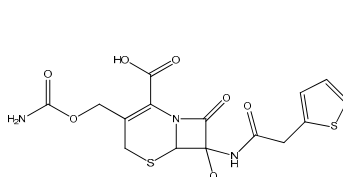
Cefixime



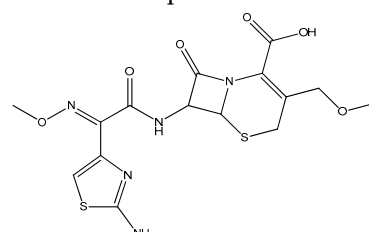
Cefoperazone



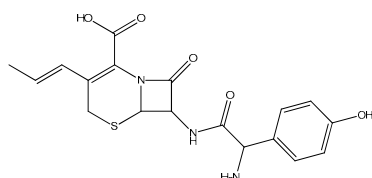
Cefotaxime



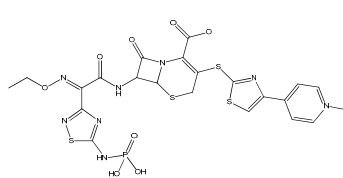
Cefoxitin



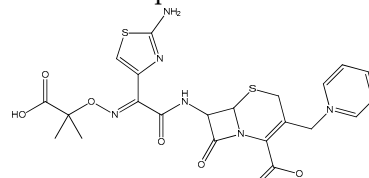
Cefpodoxime



Cefprozil

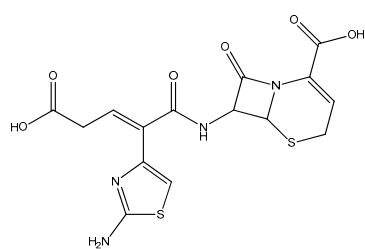


Ceftaroline fosamil

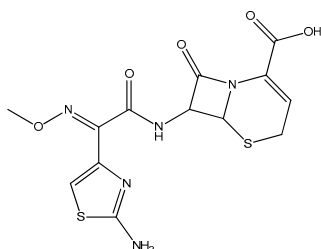


Ceftazidime

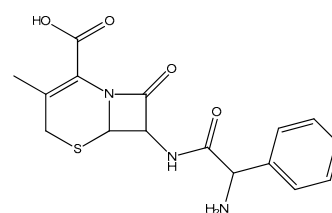
Figure S2. Cont.



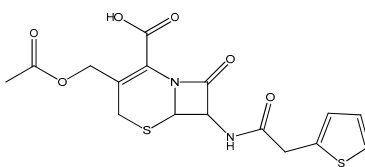
Cefitibuten



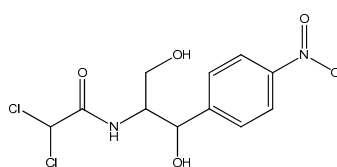
Ceftizoxime



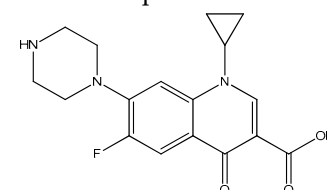
Cephalexin



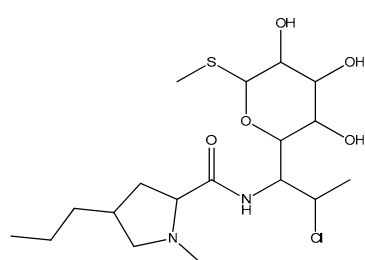
Cephalothin



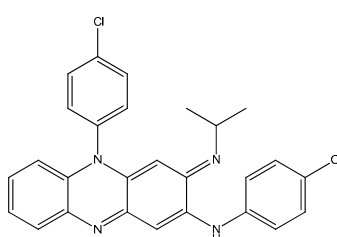
Chloramphenicol



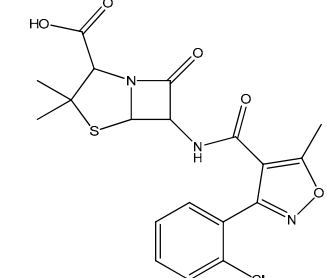
Ciprofloxacin



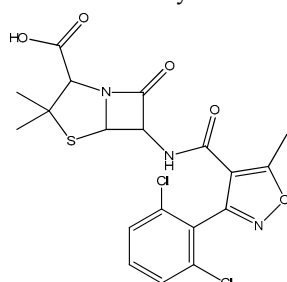
Clindamycin



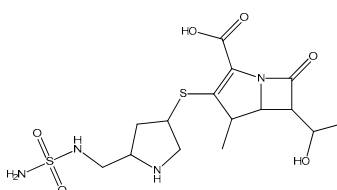
Clofazimine



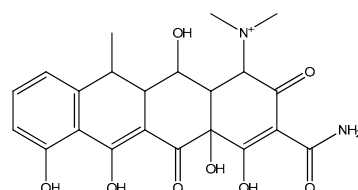
Cloxacillin



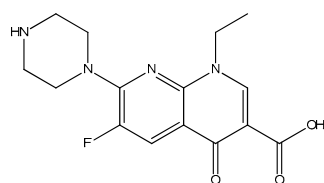
Dicloxacillin



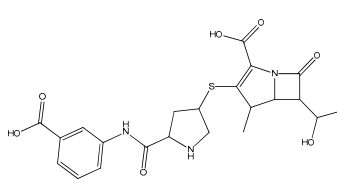
Doripenem



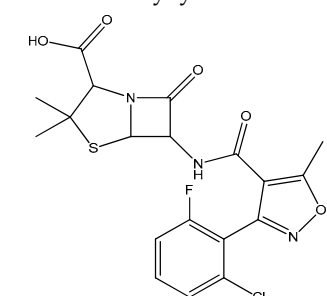
Doxycycline



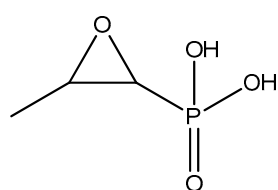
Enoxacin



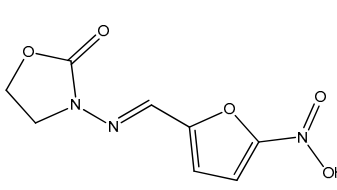
Ertapenem



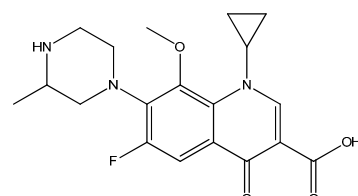
Flucloxacillin



Fosfomycin

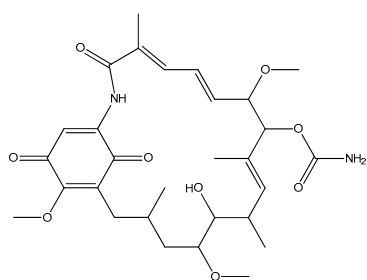


Furazolidone

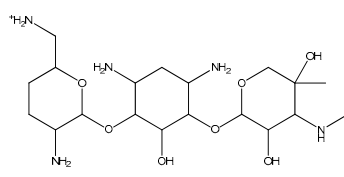


Gatifloxacin

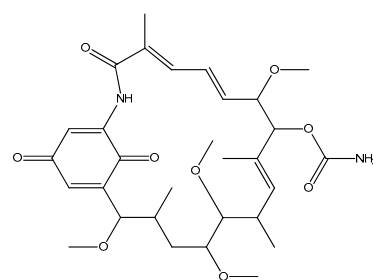
Figure S2. Cont.



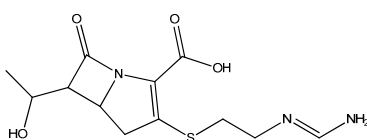
Geldanamycin



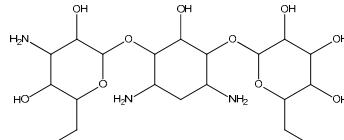
Gentamicin C



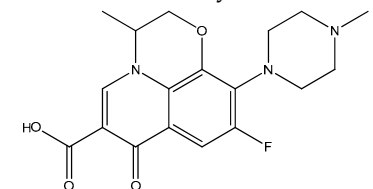
Herbimycin



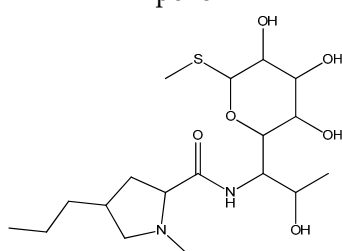
Imipenem



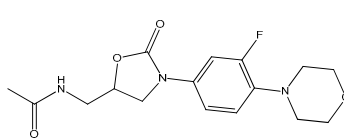
Kanamycin



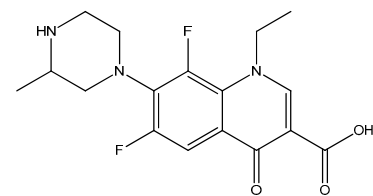
Levofloxacin



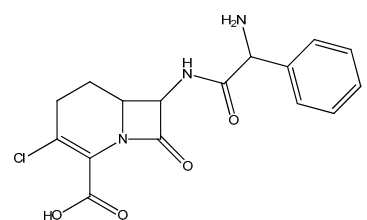
Lincomycin



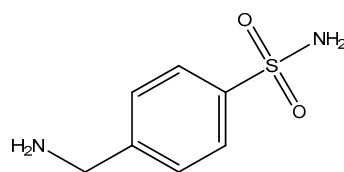
Linezolid



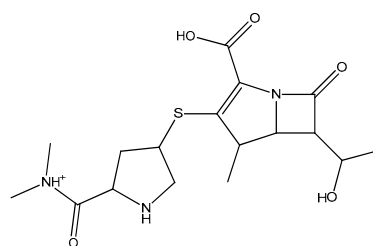
Lomefloxacin



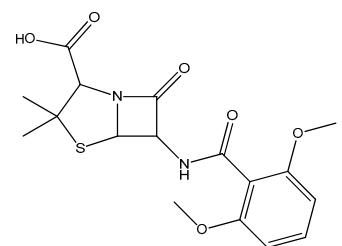
Loracarbef



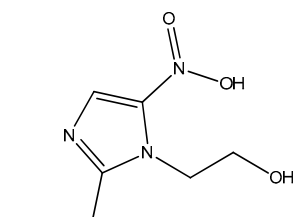
Mafenide



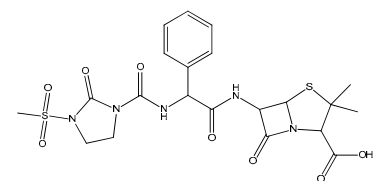
Meropenem



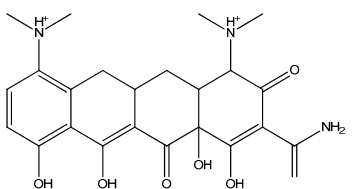
Methicillin



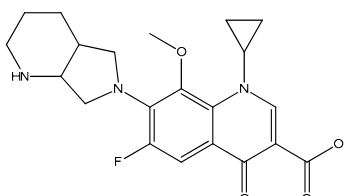
Metronidazole



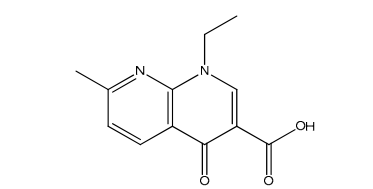
Mezlocillin



Minocycline

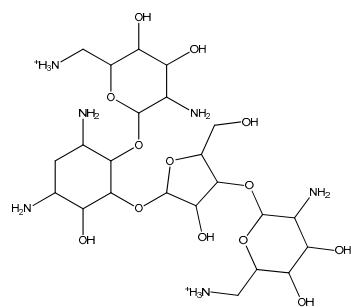


Moxifloxacin

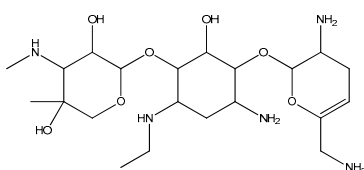


Nalidixic acid

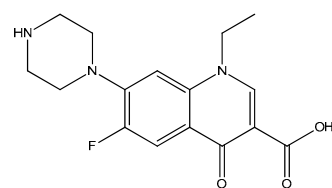
Figure S2. Cont.



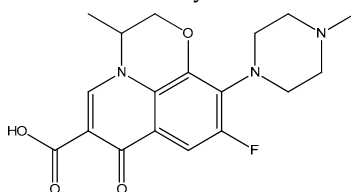
Neomycin



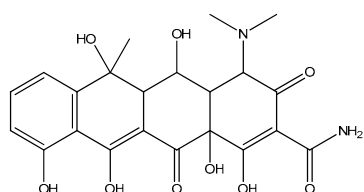
Netilmicin



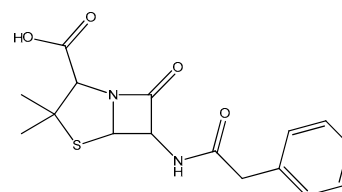
Norfloxacin



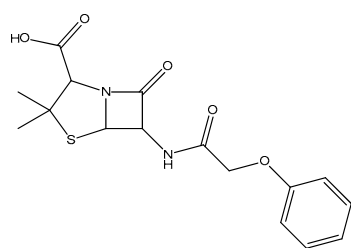
Ofloxacin



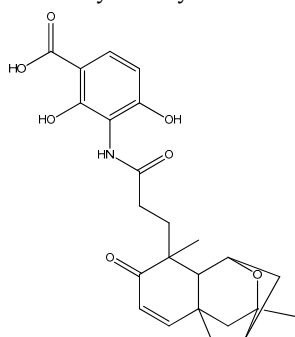
Oxytetracycline



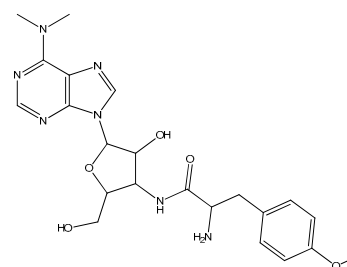
Penicillin G



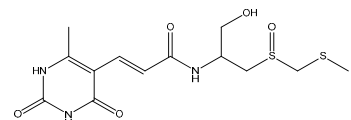
Penicillin V



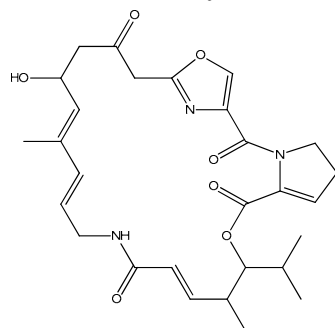
Platensimycin



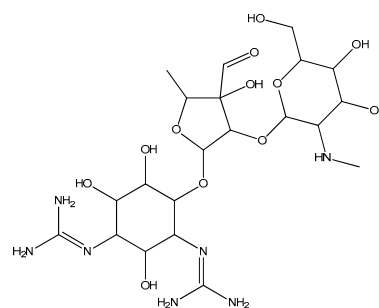
Puromycin



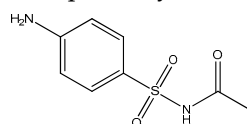
Sparsomycin



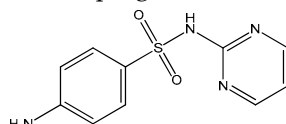
Streptogramin A



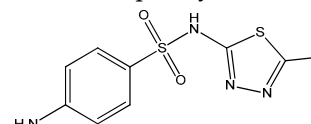
Streptomycin



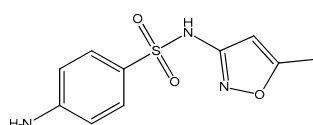
Sulfacetamide



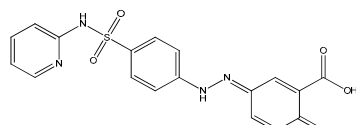
Sulfadiazine



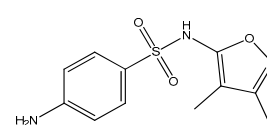
Sulfamethizole



Sulfamethoxazole

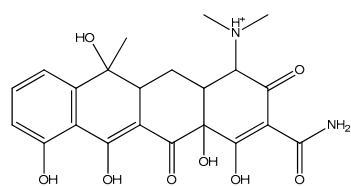


Sulfasalazine

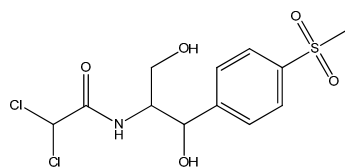


Sulfisoxazole

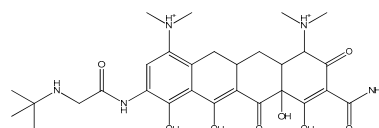
Figure S2. Cont.



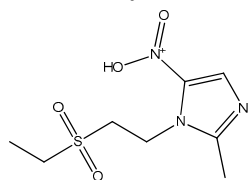
Tetracycline



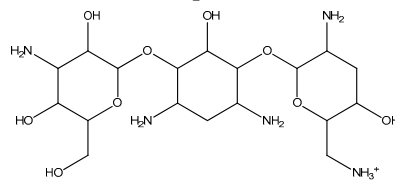
Thiamphenicol



Tigecycline



Tinidazole



Tobramycin

Figure S2. Antibiotic ligands examined in this work.