Supplementary Information (SI) for Natural Product Reports.
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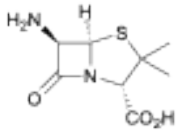
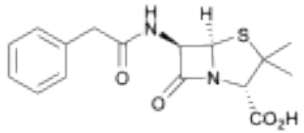
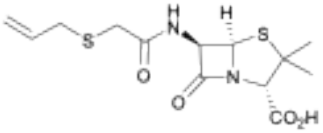
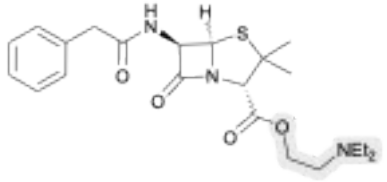
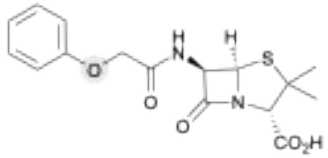
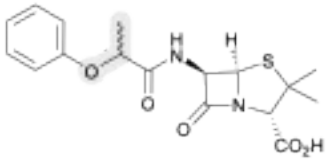
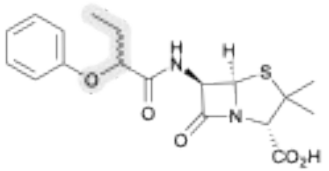
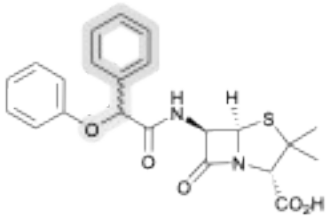
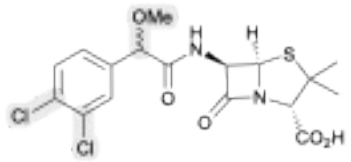
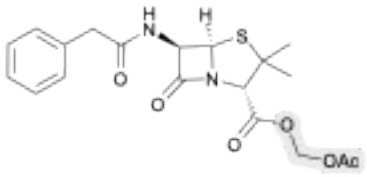
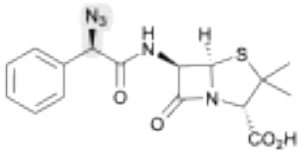
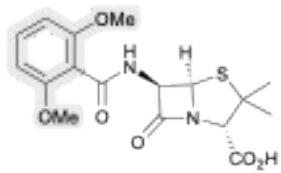
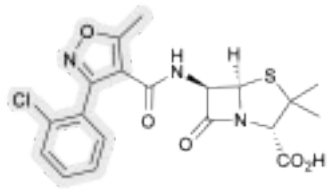
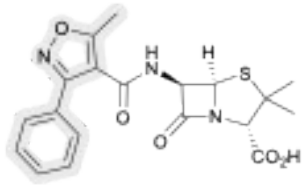
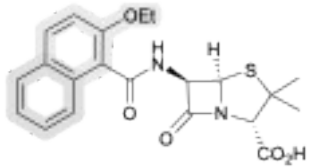
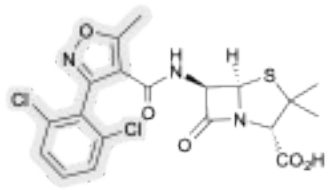
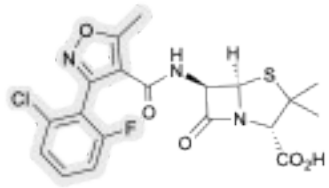
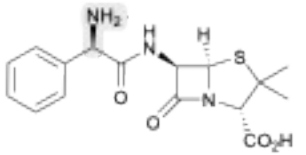
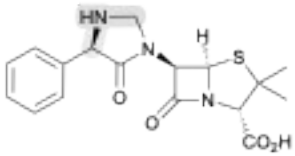
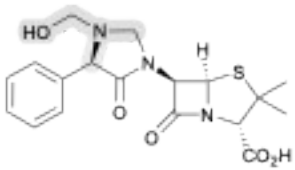
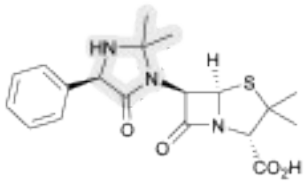
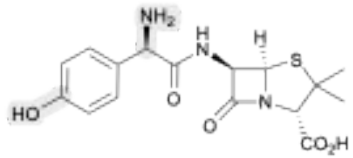
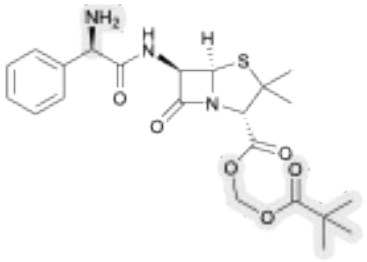
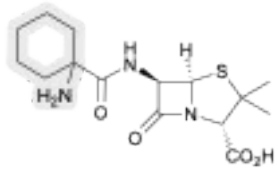
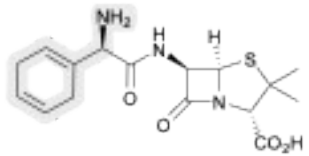
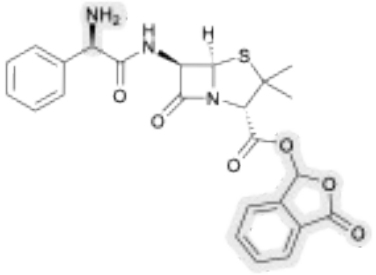
Name	#	Chemdraw	SMILES	InChI	InChIKey
6-aminopenicillanic acid	**6-APA**		N[C@H](C1=O)[C@](SC2(C)C)([H])N1[C@H]2C(O)=O	InChI=1S/C8H12N2O3S/c1-8(2)4(7(12)13)10-5(11)3(9)6(10)14-8/h3-4,6H,9H2,1-2H3,(H,12,13)/t3-,4+,6-/m1/s1	NGHVIOIJCVXTGV-ALEPSDHESA-N
penicillin G	**2.01**		O=C(CC1=CC=CC=C1)N[C@H](C2=O)[C@](SC3(C)C)([H])N2[C@H]3C(O)=O	InChI=1S/C16H18N2O4S/c1-16(2)12(15(21)22)18-13(20)11(14(18)23-16)17-10(19)8-9-6-4-3-5-7-9/h3-7,11-12,14H,8H2,1-2H3,(H,17,19)(H,21,22)/t11-,12+,14-/m1/s1	JGSARLDLIJGVTE-MBNYWOFBSA-N
penicillin O	**2.02**		O=C(CSCC=C)N[C@H](C1=O)[C@](SC2(C)C)([H])N1[C@H]2C(O)=O	InChI=1S/C13H18N2O4S2/c1-4-5-20-6-7(16)14-8-10(17)15-9(12(18)19)13(2,3)21-11(8)15/h4,8-9,11H,1,5-6H2,2-3H3,(H,14,16)(H,18,19)/t8-,9+,11-/m1/s1	QULKGELYPOJSLP-WCABBAIRSA-N
penethamate	**2.03**		O=C(CC1=CC=CC=C1)N[C@H](C2=O)[C@](SC3(C)C)([H])N2[C@H]3C(OCCN(CC)CC)=O	InChI=1S/C22H31N3O4S/c1-5-24(6-2)12-13-29-21(28)18-22(3,4)30-20-17(19(27)25(18)20)23-16(26)14-15-10-8-7-9-11-15/h7-11,17-18,20H,5-6,12-14H2,1-4H3,(H,23,26)/t17-,18+,20-/m1/s1	AFKRZUUZFWTBCC-WSTZPKSXSA-N
penicillin V	**2.04**		O=C(COC1=CC=CC=C1)N[C@H](C2=O)[C@](SC3(C)C)([H])N2[C@H]3C(O)=O	InChI=1S/C16H18N2O5S/c1-16(2)12(15(21)22)18-13(20)11(14(18)24-16)17-10(19)8-23-9-6-4-3-5-7-9/h3-7,11-12,14H,8H2,1-2H3,(H,17,19)(H,21,22)/t11-,12+,14-/m1/s1	BPLBGHOLXOTWMN-MBNYWOFBSA-N

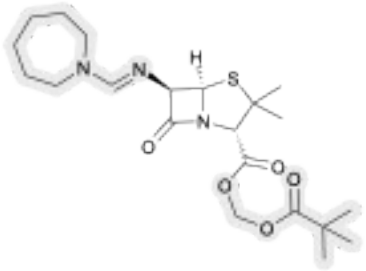
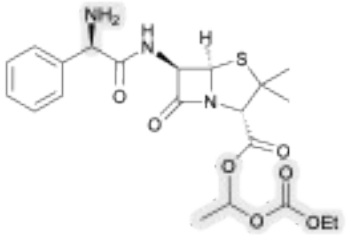
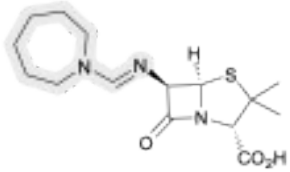
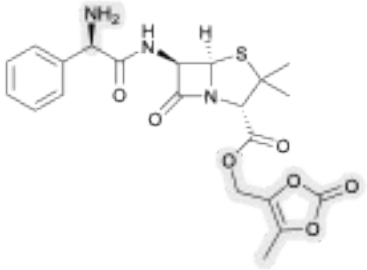
Name	#	Chemdraw	SMILES	InChI	InChIKey
phenethicillin	**2.05**		O=C(C(C)OC1=CC=CC=C1)N[C@H](C2=O)[C@](SC3(C)C)([H])N2[C@H]3C(O)=O	InChI=1S/C17H20N2O5S/c1-9(24-10-7-5-4-6-8-10)13(20)18-11-14(21)19-12(16(22)23)17(2,3)25-15(11)19/h4-9,11-12,15H,1-3H3,(H,18,20)(H,22,23)/t9?,11-,12+,15-/m1/s1	NONJJLVGHLVQQM-JHXYUMNGSA-N
propicillin	**2.06**		O=C(C(CC)OC1=CC=CC=C1)N[C@H](C2=O)[C@](SC3(C)C)([H])N2[C@H]3C(O)=O	InChI=1S/C18H22N2O5S/c1-4-11(25-10-8-6-5-7-9-10)14(21)19-12-15(22)20-13(17(23)24)18(2,3)26-16(12)20/h5-9,11-13,16H,4H2,1-3H3,(H,19,21)(H,23,24)/t11?,12-,13+,16-/m1/s1	HOCWPKXKMNXINF-XQERAMJGSA-N
phenbenicillin	**2.07**		O=C(C(C1=CC=CC=C1)OC2=CC=CC=C2)N[C@H](C3=O)[C@](SC4(C)C)([H])N3[C@H]4C(O)=O	InChI=1S/C22H22N2O5S/c1-22(2)17(21(27)28)24-19(26)15(20(24)30-22)23-18(25)16(13-9-5-3-6-10-13)29-14-11-7-4-8-12-14/h3-12,15-17,20H,1-2H3,(H,23,25)(H,27,28)/t15-,16?,17+,20-/m1/s1	VZPPEUOYDWPUKO-MQWDNKACSA-N
clometocillin	**2.08**		O=C(C(OC)C1=CC=C(Cl)C(Cl)=C1)N[C@H](C2=O)[C@](SC3(C)C)([H])N2[C@H]3C(O)=O	InChI=1S/C17H18Cl2N2O5S/c1-17(2)12(16(24)25)21-14(23)10(15(21)27-17)20-13(22)11(26-3)7-4-5-8(18)9(19)6-7/h4-6,10-12,15H,1-3H3,(H,20,22)(H,24,25)/t10-,11?,12+,15-/m1/s1	JKXQBIZCQJLVOS-GSNLGQFWSA-N

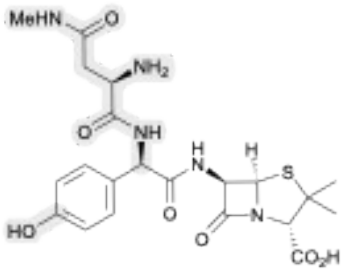
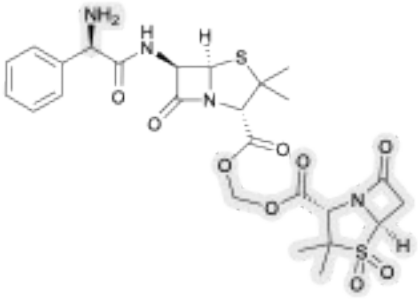
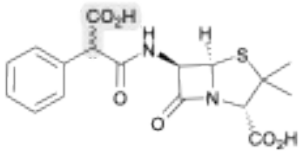
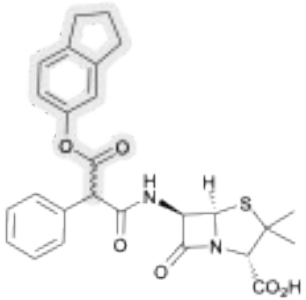
Name	#	Chemdraw	SMILES	InChI	InChIKey
penamecillin	**2.09**		O=C(CC1=CC=CC=C1)N[C@H](C2=O)[C@](SC3(C)C)([H])N2[C@H]3C(OCOC(C)=O)=O	InChI=1S/C19H22N2O6S/c1-11(22)26-10-27-18(25)15-19(2,3)28-17-14(16(24)21(15)17)20-13(23)9-12-7-5-4-6-8-12/h4-8,14-15,17H,9-10H2,1-3H3,(H,20,23)/t14-,15+,17-/m1/s1	NLOOMWLTUVBWAW-HLLBOEOZSA-N
azidocillin	**2.10**		O=C([C@H](N=[N+]=[N-])C1=CC=CC=C1)N[C@H](C2=O)[C@](SC3(C)C)([H])N2[C@H]3C(O)=O	InChI=1S/C16H17N5O4S/c1-16(2)11(15(24)25)21-13(23)10(14(21)26-16)18-12(22)9(19-20-17)8-6-4-3-5-7-8/h3-7,9-11,14H,1-2H3,(H,18,22)(H,24,25)/t9-,10+,11-,14+/m0/s1	ODFHGIPNGIAMDK-BBGACYKPSA-N
methicillin	**2.11**		O=C(C1=C(OC)C=CC=C1OC)N[C@H](C2=O)[C@](SC3(C)C)([H])N2[C@H]3C(O)=O	InChI=1S/C17H20N2O6S/c1-17(2)12(16(22)23)19-14(21)11(15(19)26-17)18-13(20)10-8(24-3)6-5-7-9(10)25-4/h5-7,11-12,15H,1-4H3,(H,18,20)(H,22,23)/t11-,12+,15-/m1/s1	RJQXTJLFIWVMTO-TYNCELHUSA-N
cloxacillin	**2.12**		O=C(C1=C(C)ON=C1C2=C(C=CC=C2)Cl)N[C@H](C3=O)[C@](SC4(C)C)([H])N3[C@H]4C(O)=O	InChI=1S/C19H18ClN3O5S/c1-8-11(12(22-28-8)9-6-4-5-7-10(9)20)15(24)21-13-16(25)23-14(18(26)27)19(2,3)29-17(13)23/h4-7,13-14,17H,1-3H3,(H,21,24)(H,26,27)/t13-,14+,17-/m1/s1	LQOLIRLGBULYKD-JKIFEVAISA-N
oxacillin	**2.13**		O=C(C1=C(C)ON=C1C2=CC=CC=C2)N[C@H](C3=O)[C@](SC4(C)C)([H])N3[C@H]4C(O)=O	InChI=1S/C19H19N3O5S/c1-9-11(12(21-27-9)10-7-5-4-6-8-10)15(23)20-13-16(24)22-14(18(25)26)19(2,3)28-17(13)22/h4-8,13-14,17H,1-3H3,(H,20,23)(H,25,26)/t13-,14+,17-/m1/s1	UWYHMGVUTGAWSP-JKIFEVAISA-N

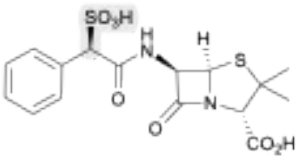
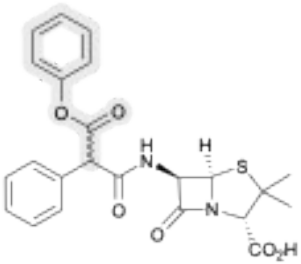
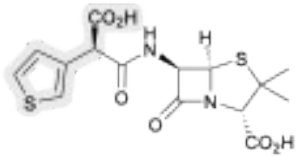
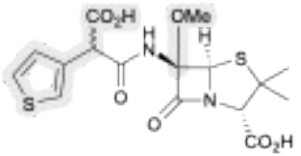
Name	#	Chemdraw	SMILES	InChI	InChIKey
nafcillin	**2.14**		O=C(C1=C(OCC)C=CC2=C1C=CC=C2)N[C@H](C3=O)[C@](SC4(C)C)([H])N3[C@H]4C(O)=O	InChI=1S/C21H22N2O5S/c1-4-28-13-10-9-11-7-5-6-8-12(11)14(13)17(24)22-15-18(25)23-16(20(26)27)21(2,3)29-19(15)23/h5-10,15-16,19H,4H2,1-3H3,(H,22,24)(H,26,27)/t15-,16+,19-/m1/s1	GPXLMGHLHQJAGZ-JTDSTZFVSA-N
dicloxacillin	**2.15**		O=C(C1=C(C)ON=C1C2=C(C=CC=C2Cl)Cl)N[C@H](C3=O)[C@](SC4(C)C)([H])N3[C@H]4C(O)=O	InChI=1S/C19H17Cl2N3O5S/c1-7-10(12(23-29-7)11-8(20)5-4-6-9(11)21)15(25)22-13-16(26)24-14(18(27)28)19(2,3)30-17(13)24/h4-6,13-14,17H,1-3H3,(H,22,25)(H,27,28)/t13-,14+,17-/m1/s1	YFAGHNZHGGCZAX-JKIFEVAISA-N
flucloxacillin	**2.16**		O=C(C1=C(C)ON=C1C2=C(C=CC=C2F)Cl)N[C@H](C3=O)[C@](SC4(C)C)([H])N3[C@H]4C(O)=O	InChI=1S/C19H17ClFN3O5S/c1-7-10(12(23-29-7)11-8(20)5-4-6-9(11)21)15(25)22-13-16(26)24-14(18(27)28)19(2,3)30-17(13)24/h4-6,13-14,17H,1-3H3,(H,22,25)(H,27,28)/t13-,14+,17-/m1/s1	UIOFUWFRIANQPC-JKIFEVAISA-N
ampicillin	**2.17**		CC(C)(S[C@@]1([C@@H]2NC([C@@H](C3=CC=CC=C3)N)=O)[H])[C@@H](N1C2=O)C(O)=O	InChI=1S/C16H19N3O4S/c1-16(2)11(15(22)23)19-13(21)10(14(19)24-16)18-12(20)9(17)8-6-4-3-5-7-8/h3-7,9-11,14H,17H2,1-2H3,(H,18,20)(H,22,23)/t9-,10-,11+,14-/m1/s1	AVKUERGKIZMTKX-NJBDSQKTSA-N

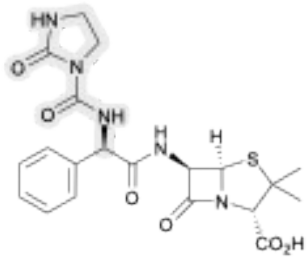
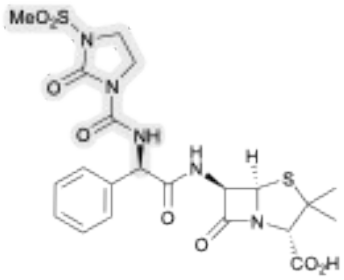
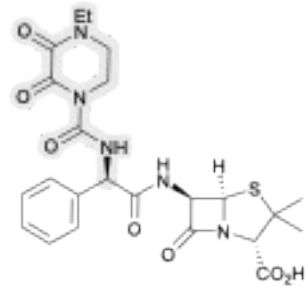
Name	#	Chemdraw	SMILES	InChI	InChIKey
metampicillin	**2.18a**		CC(C)(S[C@@]1([C@@H]2N3C([C@@H](C4=CC=CC=C4)NC3)=O)[H])[C@@H](N1C2=O)C(O)=O	InChI=1S/C17H19N3O4S/c1-17(2)12(16(23)24)20-14(22)11(15(20)25-17)19-8-18-10(13(19)21)9-6-4-3-5-7-9/h3-7,10-12,15,18H,8H2,1-2H3,(H,23,24)/t10-,11-,12+,15-/m1/s1	GEIXZQNCZIMALB-MCYUEQNJSA-N
metampicillin	**2.18b**		CC(C)(S[C@@]1([C@@H]2N3C([C@@H](C4=CC=CC=C4)N(CO)C3)=O)[H])[C@@H](N1C2=O)C(O)=O	InChI=1S/C18H21N3O5S/c1-18(2)13(17(25)26)21-15(24)12(16(21)27-18)20-8-19(9-22)11(14(20)23)10-6-4-3-5-7-10/h3-7,11-13,16,22H,8-9H2,1-2H3,(H,25,26)/t11-,12-,13+,16-/m1/s1	UWCDPMDKHWAOIL-NFFDBFGFSA-N
hetacillin	**2.19**		O=C1[C@@H](N2C([C@@H](C3=CC=CC=C3)NC2(C)C)=O)[C@]4([H])N1[C@H](C(C)(S4)C)C(O)=O	InChI=1S/C19H23N3O4S/c1-18(2)13(17(25)26)21-15(24)12(16(21)27-18)22-14(23)11(20-19(22,3)4)10-8-6-5-7-9-10/h5-9,11-13,16,20H,1-4H3,(H,25,26)/t11-,12-,13+,16-/m1/s1	DXVUYOAEDJXBPY-NFFDBFGFSA-N
amoxicillin	**2.20**		CC(C)(S[C@@]1([C@@H]2NC([C@@H](C3=CC=C(O)C=C3)N)=O)[H])[C@@H](N1C2=O)C(O)=O	InChI=1S/C16H19N3O5S/c1-16(2)11(15(23)24)19-13(22)10(14(19)25-16)18-12(21)9(17)7-3-5-8(20)6-4-7/h3-6,9-11,14,20H,17H2,1-2H3,(H,18,21)(H,23,24)/t9-,10-,11+,14-/m1/s1	LSQZJLSUYDQPKJ-NJBDSQKTSA-N

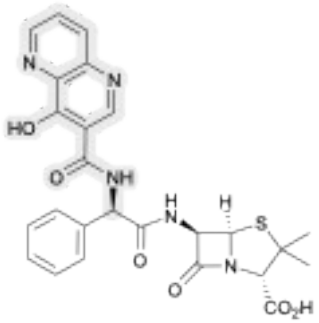
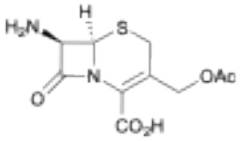
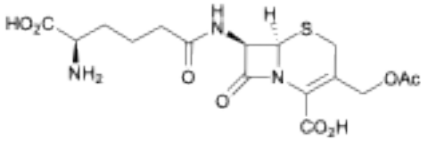
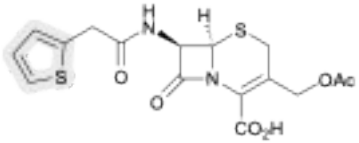
Name	#	Chemdraw	SMILES	InChI	InChIKey
ampicillin pivoxil	**2.21**		O=C(OCOC(C(C)(C)C)=O)[C@H](N1C2=O)C(C)(S[C@@]1([C@@H]2NC([C@@H](C3=CC=CC=C3)N)=O)[H])C	InChI=1S/C22H29N3O6S/c1-21(2,3)20(29)31-11-30-19(28)15-22(4,5)32-18-14(17(27)25(15)18)24-16(26)13(23)12-9-7-6-8-10-12/h6-10,13-15,18H,11,23H2,1-5H3,(H,24,26)/t13-,14-,15+,18-/m1/s1	ZEMIJUDPLILVNQ-ZXFNITATSA-N
ciclacillin	**2.22**		O=C(C1(CCCCC1)N)N[C@H](C2=O)[C@](SC3(C)C)([H])N2[C@H]3C(O)=O	InChI=1S/C15H23N3O4S/c1-14(2)9(12(20)21)18-10(19)8(11(18)23-14)17-13(22)15(16)6-4-3-5-7-15/h8-9,11H,3-7,16H2,1-2H3,(H,17,22)(H,20,21)/t8-,9+,11-/m1/s1	HGBLNBBNRORJKI-WCABBAIRSA-N
epicillin	**2.23**		CC(C)(S[C@@]1([C@@H]2NC([C@@H](C3=CCC=CC3)N)=O)[H])[C@@H](N1C2=O)C(O)=O	InChI=1S/C16H21N3O4S/c1-16(2)11(15(22)23)19-13(21)10(14(19)24-16)18-12(20)9(17)8-6-4-3-5-7-8/h3-4,7,9-11,14H,5-6,17H2,1-2H3,(H,18,20)(H,22,23)/t9-,10-,11+,14-/m1/s1	RPBAFSBGYDKNRG-NJBDSQKTSA-N
talampicillin	**2.24**		CC(C)(S[C@@]1([C@@H]2NC([C@@H](C3=CC=CC=C3)N)=O)[H])[C@@H](N1C2=O)C(OC4C5=CC=CC=C5C(O4)=O)=O	InChI=1S/C24H23N3O6S/c1-24(2)17(22(31)33-23-14-11-7-6-10-13(14)21(30)32-23)27-19(29)16(20(27)34-24)26-18(28)15(25)12-8-4-3-5-9-12/h3-11,15-17,20,23H,25H2,1-2H3,(H,26,28)/t15-,16-,17+,20-,23?/m1/s1	SOROUYSPFADXSN-SUWVAFIASA-N

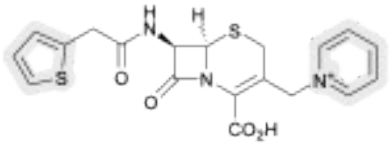
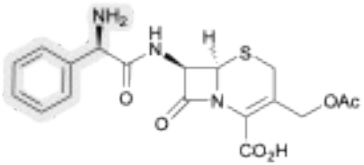
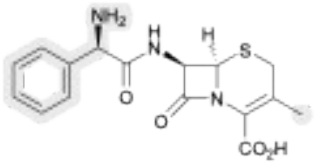
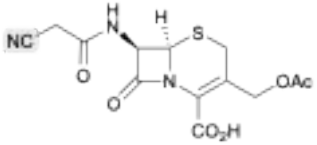
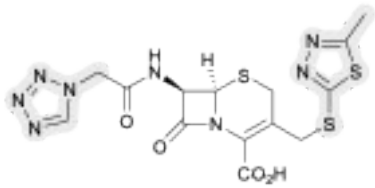
Name	#	Chemdraw	SMILES	InChI	InChIKey
pivmecillinam	**2.25**		O=C([C@@H]1N2[C@@](SC1(C)C)([H])[C@@H](C2=O)/N=C/N3CCCCCC3)OCOC(C(C)(C)C)=O	InChI=1S/C21H33N3O5S/c1-20(2,3)19(27)29-13-28-18(26)15-21(4,5)30-17-14(16(25)24(15)17)22-12-23-10-8-6-7-9-11-23/h12,14-15,17H,6-11,13H2,1-5H3/b22-12+/t14-,15+,17-/m1/s1	NPGNOVNWUSPMDP-UTEPHESZSA-N
bacampicillin	**2.26**		O=C(OC(C)OC(OCC)=O)[C@H](N1C2=O)C(C)(S[C@@]1([C@@H]2NC([C@@H](C3=CC=CC=C3)N)=O)[H])C	InChI=1S/C21H27N3O7S/c1-5-29-20(28)31-11(2)30-19(27)15-21(3,4)32-18-14(17(26)24(15)18)23-16(25)13(22)12-9-7-6-8-10-12/h6-11,13-15,18H,5,22H2,1-4H3,(H,23,25)/t11?,13-,14-,15+,18-/m1/s1	PFOLLRNADZZWEX-FFGRCDKISA-N
mecillinam	**2.27**		O=C1[C@@H](/N=C/N2CCCCCC2)[C@](SC3(C)C)([H])N1[C@H]3C(O)=O	InChI=1S/C15H23N3O3S/c1-15(2)11(14(20)21)18-12(19)10(13(18)22-15)16-9-17-7-5-3-4-6-8-17/h9-11,13H,3-8H2,1-2H3,(H,20,21)/b16-9+/t10-,11+,13-/m1/s1	BWWVAEOLVKTZFQ-ISVUSNJMSA-N
ampicillin medoxomil	**2.28**		O=C(OCC1=C(OC(O1)=O)C)[C@H](N2C3=O)C(C)(S[C@@]2([C@@H]3NC([C@@H](C4=CC=CC=C4)N)=O)[H])C	InChI=1S/C21H23N3O7S/c1-10-12(31-20(28)30-10)9-29-19(27)15-21(2,3)32-18-14(17(26)24(15)18)22-16(25)13(23)11-7-5-4-6-8-11/h4-8,13-15,18H,9,22H2,1-3H3,(H,23,25)/t13-,14-,15+,18-/m1/s1	ZKUKMWMSYCIYRD-ZXFNITATSA-N

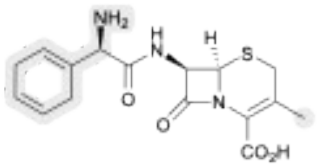
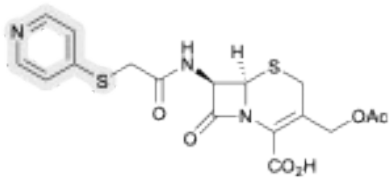
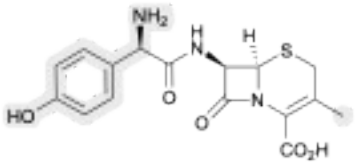
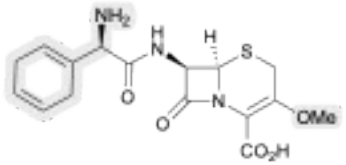
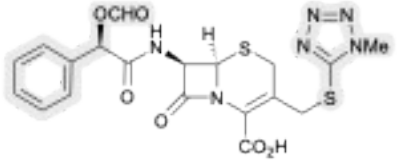
Name	#	Chemdraw	SMILES	InChI	InChIKey
aspoxicillin	**2.29**		OC(C=C1)=CC=C1[C@@H](NC([C@H](N)CC(NC)=O)=O)C(N[C@H]2[C@]3([H])N(C2=O)[C@H](C(C)(S3)C)C(O)=O)=O	InChI=1S/C21H27N5O7S/c1-21(2)15(20(32)33)26-18(31)14(19(26)34-21)25-17(30)13(9-4-6-10(27)7-5-9)24-16(29)11(22)8-12(28)23-3/h4-7,11,13-15,19,27H,8,22H2,1-3H3,(H,23,28)(H,24,29)(H,25,30)(H,32,33)/t11-,13-,14-,15+,19-/m1/s1	BHELIUBJHYAEDK-OAIUPTLZSA-N
sultamicillin	**2.30**		O=C(OCOC([C@H]1C(C)(S(=O)([C@@]2(CC(N21)=O)[H])=O)C)=O)[C@H](N3C4=O)C(C)(S[C@@]3([C@@H]4NC([C@@H](C5=CC=CC=C5)N)=O)[H])C	InChI=1S/C25H30N4O9S2/c1-24(2)17(29-20(32)16(21(29)39-24)27-19(31)15(26)12-8-6-5-7-9-12)22(33)37-11-38-23(34)18-25(3,4)40(35,36)14-10-13(30)28(14)18/h5-9,14-18,21H,10-11,26H2,1-4H3,(H,27,31)/t14-,15-,16-,17+,18+,21-/m1/s1	OPYGFNJSCUDTBT-PMLPCWDUSA-N
carbenicillin	**2.31**		O=C(C(C(O)=O)C1=CC=CC=C1)N[C@H](C2=O)[C@](SC3(C)C)([H])N2[C@H]3C(O)=O	InChI=1S/C17H18N2O6S/c1-17(2)11(16(24)25)19-13(21)10(14(19)26-17)12(20)9(15(22)23)8-6-4-3-5-7-8/h3-7,9-11,14H,1-2H3,(H,18,20)(H,22,23)(H,24,25)/t9?,10-,11+,14-/m1/s1	FPPNZSSZRUTDAP-UWFZAAFLSA-N
carbenicillin indanyl	**2.32**		O=C(C(C(OC1=CC=C2CCCC2=C1)=O)C3=CC=CC=C3)N[C@H](C4=O)[C@](SC5(C)C)([H])N4[C@H]5C(O)=O	InChI=1S/C26H26N2O6S/c1-26(2)20(24(31)32)28-22(30)19(23(28)35-26)27-21(29)18(15-7-4-3-5-8-15)25(33)34-17-12-11-14-9-6-10-16(14)13-17/h3-5,7-8,11-13,18-20,23H,6,9-10H2,1-2H3,(H,27,29)(H,31,32)/t18?,19-,20+,23-/m1/s1	JIRBAUWICKGBFE-MNRDOXJOSA-N

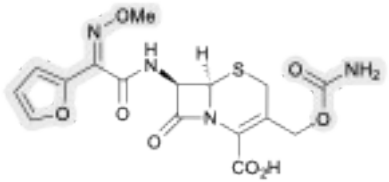
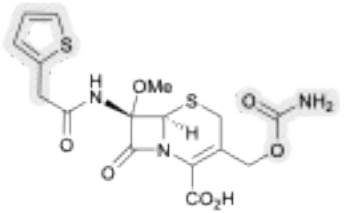
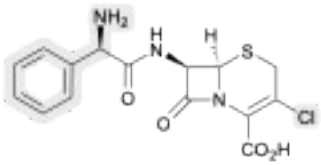
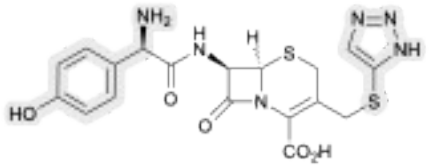
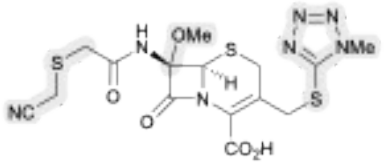
Name	#	Chemdraw	SMILES	InChI	InChIKey
sulbenicillin	**2.33**		O=C([C@@H](C1=CC=CC=C1)S(=O)(O)=O)N[C@H](C2=O)[C@](SC3(C)C)([H])N2[C@H]3C(O)=O	InChI=1S/C16H18N2O7S2/c1-16(2)11(15(21)22)18-13(20)9(14(18)26-16)17-12(19)10(27(23,24)25)8-6-4-3-5-7-8/h3-7,9-11,14H,1-2H3,(H,17,19)(H,21,22)(H,23,24,25)/t9-,10-,11+,14-/m1/s1	JETQIUPBHQNHNZ-NJBDSQKTSA-N
carbenicillin phenyl	**2.34**		O=C(C(C(OC1=CC=CC=C1)=O)C2=CC=CC=C2)N[C@H](C3=O)[C@](SC4(C)C)([H])N3[C@H]4C(O)=O	InChI=1S/C23H22N2O6S/c1-23(2)17(21(28)29)25-19(27)16(20(25)32-23)24-18(26)15(13-9-5-3-6-10-13)22(30)31-14-11-7-4-8-12-14/h3-12,15-17,20H,1-2H3,(H,24,26)(H,28,29)/t15?,16-,17+,20-/m1/s1	NZDASSHFKWDBBU-KVMCETHSSA-N
ticarcillin	**2.35**		O=C([C@H](C(O)=O)C1=CSC=C1)N[C@H](C2=O)[C@](SC3(C)C)([H])N2[C@H]3C(O)=O	InChI=1S/C15H16N2O6S2/c1-15(2)9(14(22)23)17-11(19)8(12(17)25-15)16-10(18)7(13(20)21)6-3-4-24-5-6/h3-5,7-9,12H,1-2H3,(H,16,18)(H,20,21)(H,22,23)/t7-,8-,9+,12-/m1/s1	OHKOGUYZJXTSFX-KZFFXBSXSA-N
temocillin	**2.36**		O=C(C(C(O)=O)C1=CSC=C1)N[C@@](C2=O)(OC)[C@](SC3(C)C)([H])N2[C@H]3C(O)=O	InChI=1S/C16H18N2O7S2/c1-15(2)9(12(22)23)18-13(24)16(26-3,14(18)27-15)17-10(19)8(11(20)21)7-4-5-26-6-7/h4-6,8-9,14H,1-3H3,(H,17,19)(H,20,21)(H,22,23)/t8?,9-,14+,16-/m0/s1	BVCKFLJARNKCSS-DWPRYXJFSA-N

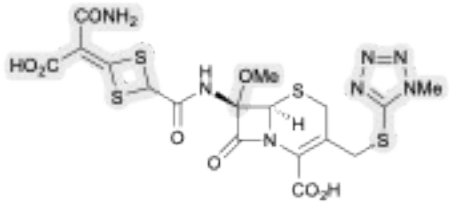
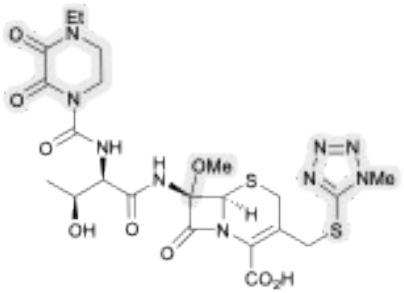
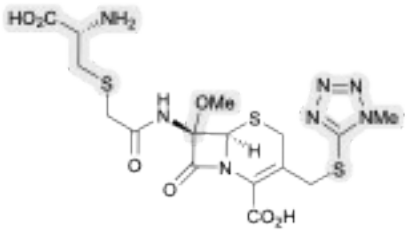
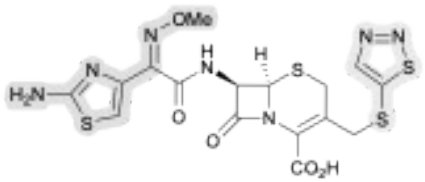
Name	#	Chemdraw	SMILES	InChI	InChIKey
azlocillin	**2.37**		O=C([C@H](NC(N1CCNC1=O)=O)C2=CC=CC=C2)N[C@H]3[C@]4([H])N(C3=O)[C@H](C(C)(S4)C)C(O)=O	InChI=1S/C20H23N5O6S/c1-20(2)13(17(28)29)25-15(27)12(16(25)32-20)22-14(26)11(10-6-4-3-5-7-10)23-19(31)24-9-8-21-18(24)30/h3-7,11-13,16H,8-9H2,1-2H3,(H,21,30)(H,22,26)(H,23,31)(H,28,29)/t11-,12-,13+,16-/m1/s1	JTWOMNBEOCYFNV-NFFDBFGFSA-N
mezlocillin	**2.38**		O=C([C@H](NC(N1CCN(C1=O)S(=O)(C)=O)=O)C2=CC=CC=C2)N[C@H]3[C@]4([H])N(C3=O)[C@H](C(C)(S4)C)C(O)=O	InChI=1S/C21H25N5O8S2/c1-21(2)14(18(29)30)26-16(28)13(17(26)35-21)22-15(27)12(11-7-5-4-6-8-11)23-19(31)24-9-10-25(20(24)32)36(3,33)34/h4-8,12-14,17H,9-10H2,1-3H3,(H,22,27)(H,23,31)(H,29,30)/t12-,13-,14+,17-/m1/s1	YPBATNHYBCGSSN-VWPFQQQWSA-N
piperacillin	**2.39**		O=C([C@H](NC(N1CCN(C(C1=O)=O)CC)=O)C2=CC=CC=C2)N[C@H]3[C@]4([H])N(C3=O)[C@H](C(C)(S4)C)C(O)=O	InChI=1S/C23H27N5O7S/c1-4-26-10-11-27(19(32)18(26)31)35-13(12-8-6-5-7-9-12)16(29)24-14-17(30)28-15(21(33)34)23(2,3)36-20(14)28/h5-9,13-15,20H,4,10-11H2,1-3H3,(H,24,29)(H,25,35)(H,33,34)/t13-,14-,15+,20-/m1/s1	IVBHGBMCVLDMKU-GXNBUGAJSA-N

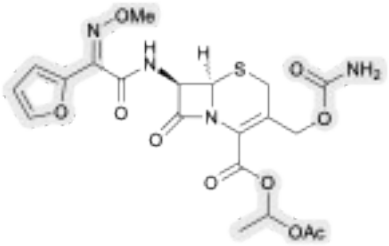
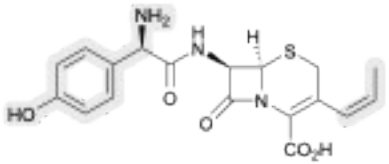
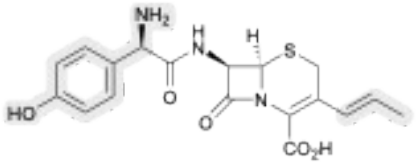
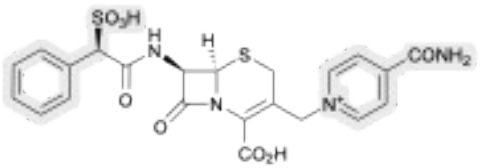
Name	#	Chemdraw	SMILES	InChI	InChIKey
apalcillin	**2.40**		O=C(N[C@H]1[C@]2([H])N(C1=O)[C@H](C(C)(S2)C)C(O)=O)[C@H](NC(C(C=N3)=C(O)C4=C3C=CC=N4)=O)C5=CC=CC=C5	InChI=1S/C25H23N5O6S/c1-25(2)19(24(35)36)30-22(34)17(23(30)37-25)29-21(33)15(12-7-4-3-5-8-12)28-20(32)13-11-27-14-9-6-10-26-16(14)18(13)31/h3-11,15,17,19,23H,1-2H3,(H,27,31)(H,28,32)(H,29,33)(H,35,36)/t15-,17-,19+,23-/m1/s1	XMQVYNAURODYCQ-SLFBBCNNSA-N
7-aminocephalosporanic acid	**7-ACA**		N[C@H](C1=O)[C@]2([H])N1C(C(O)=O)=C(COC(C)=O)CS2	InChI=1S/C10H12N2O5S/c1-4(13)17-2-5-3-18-9-6(11)8(14)12(9)7(5)10(15)16/h6,9H,2-3,11H2,1H3,(H,15,16)/t6-,9-/m1/s1	HSHGZXNAXBPPDL-HZGVNTEJSA-N
cephalosporin C	**2.41**		N[C@@H](C(O)=O)CCCC(N[C@H](C1=O)[C@]2([H])N1C(C(O)=O)=C(COC(C)=O)CS2)=O	InChI=1S/C16H21N3O8S/c1-7(20)27-5-8-6-28-14-11(13(22)19(14)10(8)16(25)26)18-10(21)4-2-3-9(17)15(23)24/h9,11,14H,2-6,17H2,1H3,(H,18,21)(H,23,24)(H,25,26)/t9-,11-,14-/m1/s1	HOKIDJSKDBPKTQ-GLXFQSAKSA-N
cefalotin	**2.42**		O=C(CC1=CC=CS1)N[C@H]2[C@]3([H])N(C(C(O)=O)=C(COC(C)=O)CS3)C2=O	InChI=1S/C16H16N2O6S2/c1-8(19)24-6-9-7-26-15-12(14(21)18(15)13(9)16(22)23)17-11(20)5-10-3-2-4-25-10/h2-4,12,15H,5-7H2,1H3,(H,17,20)(H,22,23)/t12-,15-/m1/s1	XIURVHNZVLADCM-IUODEOHRSA-N

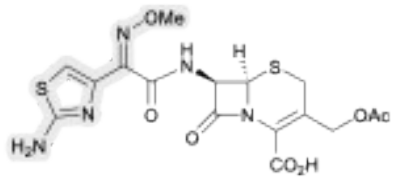
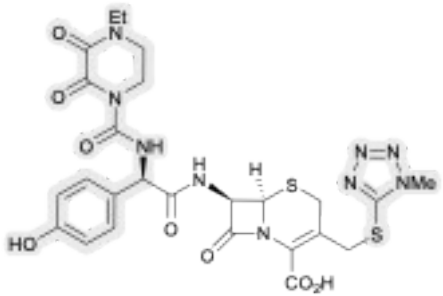
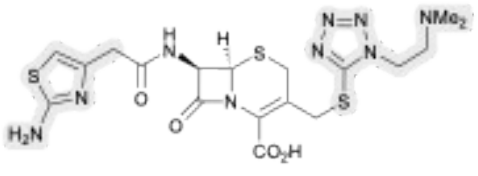
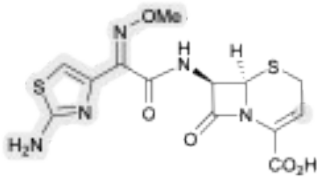
Name	#	Chemdraw	SMILES	InChI	InChIKey
cefaloridine	**2.43**		O=C1N2C(C(O)=O)=C(C[N+]3=CC=CC=C3)CS[C@]2([H])[C@@H]1NC(CC4=CC=CS4)=O	InChI=1S/C19H17N3O4S2/c23-14(9-13-5-4-8-27-13)20-15-17(24)22-16(19(25)26)12(11-28-18(15)22)10-21-6-2-1-3-7-21/h1-8,15,18H,9-11H2,(H-,20,23,25,26)/p+1/t15-,18-/m1/s1	CZTQZXZIADLWOZ-CRAIPNDOSA-O
cefaloglycin	**2.44**		N[C@H](C1=CC=CC=C1)C(N[C@H](C2=O)[C@]3([H])N2C(C(O)=O)=C(COC(C)=O)CS3)=O	InChI=1S/C18H19N3O6S/c1-9(22)27-7-11-8-28-17-13(16(24)21(17)14(11)18(25)26)20-15(23)12(19)10-5-3-2-4-6-10/h2-6,12-13,17H,7-8,19H2,1H3,(H,20,23)(H,25,26)/t12-,13-,17-/m1/s1	FUBBGQLTSCSAON-PBFPGSCMSA-N
cefalexin	**2.45**		O=C1N2[C@@](SCC(C)=C2C(O)=O)([H])[C@@H]1NC([C@@H](C3=CC=CC=C3)N)=O	InChI=1S/C16H17N3O4S/c1-8-7-24-15-11(14(21)19(15)12(8)16(22)23)18-13(20)10(17)9-5-3-2-4-6-9/h2-6,10-11,15H,7,17H2,1H3,(H,18,20)(H,22,23)/t10-,11-,15-/m1/s1	ZAIPMKNFIOOWCQ-UEKVPHQBSA-N
cefacetrile	**2.46**		O=C(CC#N)N[C@H](C1=O)[C@]2([H])N1C(C(O)=O)=C(COC(C)=O)CS2	InChI=1S/C13H13N3O6S/c1-6(17)22-4-7-5-23-12-9(15-8(18)2-3-14)11(19)16(12)10(7)13(20)21/h9,12H,2,4-5H2,1H3,(H,15,18)(H,20,21)/t9-,12-/m1/s1	RRYMAQUWDLIUPV-BXKDBHETSA-N
cefazolin	**2.47**		O=C(CN1C=NN=N1)N[C@H](C2=O)[C@]3([H])N2C(C(O)=O)=C(CSC4=NN=C(S4)C)CS3	InChI=1S/C14H14N8O4S3/c1-6-17-18-14(29-6)28-4-7-3-27-12-9(11(24)22(12)10(7)13(25)26)16-8(23)2-21-5-15-19-20-21/h5,9,12H,2-4H2,1H3,(H,16,23)(H,25,26)/t9-,12-/m1/s1	MLYYVTUWGNIJIB-BXKDBHETSA-N

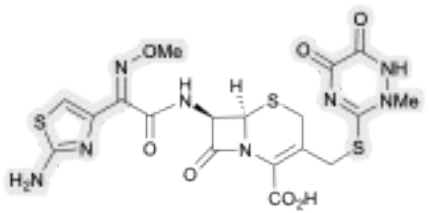
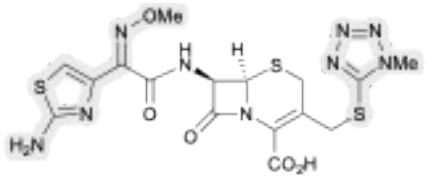
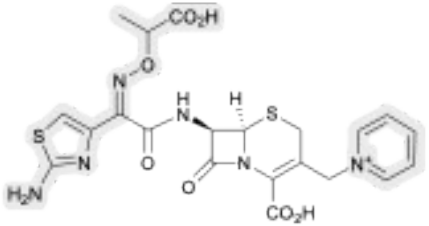
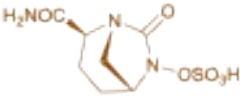
Name	#	Chemdraw	SMILES	InChI	InChIKey
cefradine	**2.48**		O=C1N2[C@@](SCC(C)=C2C(O)=O)([H])[C@@H]1NC([C@@H](C3=CCC=CC3)N)=O	InChI=1S/C16H19N3O4S/c1-8-7-24-15-11(14(21)19(15)12(8)16(22)23)18-13(20)10(17)9-5-3-2-4-6-9/h2-3,6,10-11,15H,4-5,7,17H2,1H3,(H,18,20)(H,22,23)/t10-,11-,15-/m1/s1	RDLPVSKMFDYCOR-UEKVPHQBSA-N
cefapirin	**2.49**		O=C(CSC1=CC=NC=C1)N[C@H](C2=O)[C@]3([H])N2C(C(O)=O)=C(COC(C)=O)CS3	InChI=1S/C17H17N3O6S2/c1-9(21)26-6-10-7-28-16-13(15(23)20(16)14(10)17(24)25)19-12(22)8-27-11-2-4-18-5-3-11/h2-5,13,16H,6-8H2,1H3,(H,19,22)(H,24,25)/t13-,16-/m1/s1	UQLLWWBDSUHNEB-CZUORRHYSA-N
cefadroxil	**2.50**		N[C@H](C1=CC=C(C=C1)O)C(N[C@H](C2=O)[C@]3([H])N2C(C(O)=O)=C(C)CS3)=O	InChI=1S/C16H17N3O5S/c1-7-6-25-15-11(14(22)19(15)12(7)16(23)24)18-13(21)10(17)8-2-4-9(20)5-3-8/h2-5,10-11,15,20H,6,17H2,1H3,(H,18,21)(H,23,24)/t10-,11-,15-/m1/s1	BOEGTKLJZSQCCD-UEKVPHQBSA-N
cefroxadine	**2.51**		N[C@H](C1=CCC=CC1)C(N[C@H](C2=O)[C@]3([H])N2C(C(O)=O)=C(OC)CS3)=O	InChI=1S/C16H19N3O5S/c1-24-9-7-25-15-11(14(21)19(15)12(9)16(22)23)18-13(20)10(17)8-5-3-2-4-6-8/h2-3,6,10-11,15H,4-5,7,17H2,1H3,(H,18,20)(H,22,23)/t10-,11-,15-/m1/s1	RDMOROXKXONCAL-UEKVPHQBSA-N
cefamandole nafate	**2.52**		O=C([C@@H](C1=CC=CC=C1)OC=O)N[C@H](C2=O)[C@]3([H])N2C(C(O)=O)=C(CSC4=NN=NN4C)CS3	InChI=1S/C19H18N6O6S2/c1-24-19(21-22-23-24)34-8-11-7-32-17-12(16(28)25(17)13(11)18(30)31)20-15(27)14(26)9-2-4-10(29)5-3-9/h2-6,12,14,17H,7-8H2,1H3,(H,20,27)(H,29,30)/t12-,14-,17-/m1/s1	RRJHESVQVSRQEX-SUYBPPKGSA-N

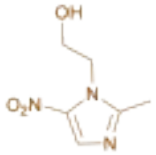
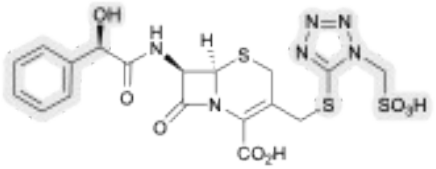
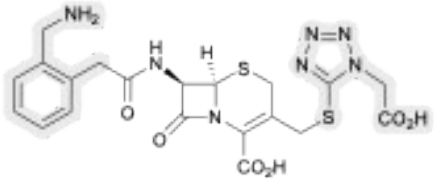
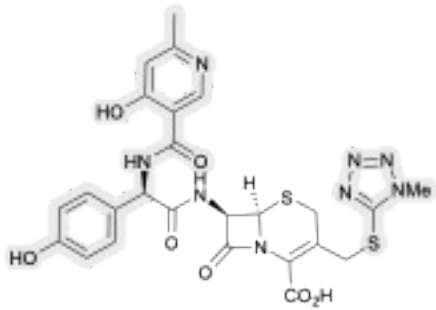
Name	#	Chemdraw	SMILES	InChI	InChIKey
cefuroxime	**2.53**		O=C(/C(C1=CC=CO1)=N\OC)N[C@H](C2=O)[C@]3([H])N2C(C(O)=O)=C(COC(N)=O)CS3	InChI=1S/C16H16N4O8S/c1-26-19-9(8-3-2-4-27-8)12(21)18-10-13(22)20-11(15(23)24)7(5-28-16(17)25)6-29-14(10)20/h2-4,10,14H,5-6H2,1H3,(H2,17,25)(H,18,21)(H,23,24)/b19-9-/t10-,14-/m1/s1	JFPVXVDWJQMJEE-IZRZKJBUSA-N
cefoxitin	**2.54**		O=C(CC1=CC=CS1)N[C@]2([C@]3([H])N(C(C(O)=O)=C(CS3)COC(N)=O)C2=O)OC	InChI=1S/C16H17N3O7S2/c1-25-16(18-10(20)5-9-3-2-4-27-9)13(23)19-11(12(21)22)8(6-26-15(17)24)7-28-14(16)19/h2-4,14H,5-7H2,1H3,(H2,17,24)(H,18,20)(H,21,22)/t14-,16+/m1/s1	WZOZEZRFJCJXNZ-ZBFHGGJFSA-N
cefaclor	**2.55**		O=C1N2[C@@](SCC(Cl)=C2C(O)=O)([H])[C@@H]1NC([C@@H](C3=CC=CC=C3)N)=O	InChI=1S/C15H14ClN3O4S/c16-8-6-24-14-10(13(21)19(14)11(8)15(22)23)18-12(20)9(17)7-4-2-1-3-5-7/h1-5,9-10,14H,6,17H2,(H,18,20)(H,22,23)/t9-,10-,14-/m1/s1	QYIYFLOTGYLRGG-GPCCPHFNSA-N
cefatrizine	**2.56**		N[C@H](C1=CC=C(C=C1)O)C(N[C@H](C2=O)[C@]3([H])N2C(C(O)=O)=C(CSC4=CN=NN4)CS3)=O	InChI=1S/C18H18N6O5S2/c19-12(8-1-3-10(25)4-2-8)15(26)21-13-16(27)24-14(18(28)29)9(7-31-17(13)24)6-30-11-5-20-23-22-11/h1-5,12-13,17,25H,6-7,19H2,(H,21,26)(H,28,29)(H,20,22,23)/t12-,13-,17-/m1/s1	UOCJDOLVGGIYIQ-PBFPGSCMSA-N
cefmetazole	**2.57**		O=C(CSCC#N)N[C@]1([C@]2([H])N(C(C(O)=O)=C(CS2)CSC3=NN=NN3C)C1=O)OC	InChI=1S/C15H17N7O5S3/c1-21-14(18-19-20-21)30-6-8-5-29-13-15(27-2,17-9(23)7-28-4-3-16)12(26)22(13)10(8)11(24)25/h13H,4-7H2,1-2H3,(H,17,23)(H,24,25)/t13-,15+/m1/s1	SNBUBQHDYVFSQF-HIFRSBDPSA-N

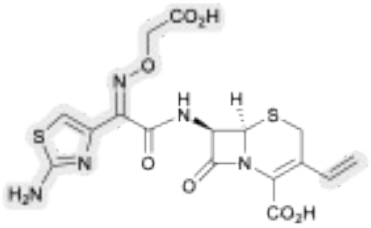
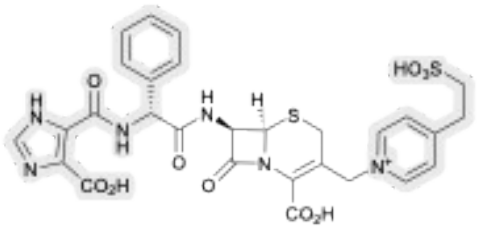
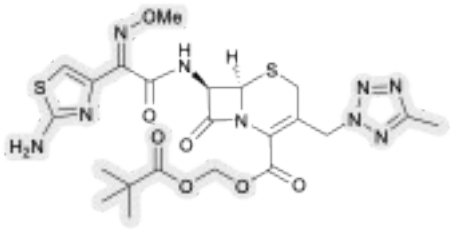
Name	#	Chemdraw	SMILES	InChI	InChIKey
cefotetan	**2.58**		O=C(C1S/C(S1)=C(C(O)=O)\C(N)=O)N[C@]2([C@]3([H])N(C(C(O)=O)=C(CS3)CSC4=NN=NN4C)C2=O)OC	InChI=1S/C17H17N7O8S4/c1-23-16(20-21-22-23)34-4-5-33-15-17(32-2,14(31)24(15)7(5)11(29)30)19-9(26)13-35-12(36-13)6(8(18)25)10(27)28/h13,15H,3-4H2,1-2H3,(H2,18,25)(H,19,26)(H,27,28)(H,29,30)/b12-6-/t13?,15-,17+/m1/s1	SRZNHPXWXCNNDU-IXOPCIAXSA-N
cefbuperazone	**2.59**		O=C([C@H](NC(N1CCN(C(C1=O)=O)CC)=O)[C@H](C)O)N[C@]2([C@]3([H])N(C(C(O)=O)=C(CS3)CSC4=NN=NN4C)C2=O)OC	InChI=1S/C22H29N9O9S2/c1-5-29-6-7-30(16(35)15(29)34)20(39)23-12(10(2)32)14(33)24-22(40-4)18(38)31-13(17(36)37)11(8-41-19(22)31)9-42-21-25-26-27-28(21)3/h10,12,19,32H,5-9H2,1-4H3,(H,23,39)(H,24,33)(H,36,37)/t10-,12+,19+,22-/m0/s1	SMSRCGPDNDCXFR-CYWZMYCQSA-N
cefminox	**2.60**		N[C@H](CSCC(N[C@]1([C@]2([H])N(C(C(O)=O)=C(CS2)CSC3=NN=NN3C)C1=O)OC)=O)C(O)=O	InChI=1S/C16H21N7O7S3/c1-22-15(19-20-21-22)33-4-7-3-32-14-16(30-2,13(29)23(14)10(7)12(27)28)18-9(24)6-31-5-8(17)11(25)26/h8,14H,3-6,17H2,1-2H3,(H,18,24)(H,25,26)(H,27,28)/t8-,14-,16+/m1/s1	JSDXOWVAHXDYCU-VXSYNFHWSA-N
cefuzonam	**2.61**		O=C(/C(C1=CSC(N)=N1)=N\OC)N[C@H](C2=O)[C@]3([H])N2C(C(O)=O)=C(CSC4=CN=NS4)CS3	InChI=1S/C16H15N7O5S4/c1-28-21-9(7-5-31-16(17)19-7)12(24)20-10-13(25)23-11(15(26)27)6(4-30-14(10)23)3-29-8-2-18-22-32-8/h2,5,10,14H,3-4H2,1H3,(H2,17,19)(H,20,24)(H,26,27)/b21-9-/t10-,14-/m1/s1	CXHKZHZLDMQGFF-ZSDSSEDPSA-N

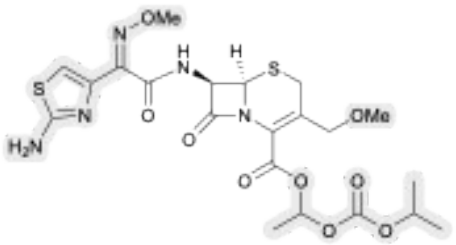
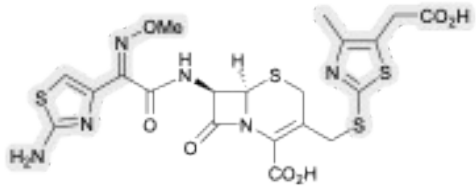
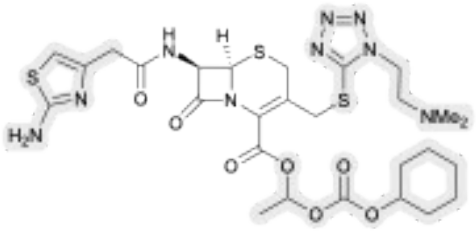
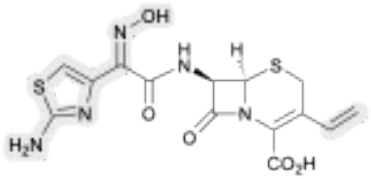
Name	#	Chemdraw	SMILES	InChI	InChIKey
cefuroxime axetil	**2.62**		O=C(C1=C(COC(N)=O)CS[C@@]([C@@H]2NC(/C(C3=CC=CO3)=N\OC)=O)([H])N1C2=O)OC(OC(C)=O)C	InChI=1S/C20H22N4O10S/c1-9(25)33-10(2)34-19(28)15-11(7-32-20(21)29)8-35-18-14(17(27)24(15)18)22-16(26)13(23-30-3)12-5-4-6-31-12/h4-6,10,14,18H,7-8H2,1-3H3,(H2,21,29)(H,22,26)/b23-13-/t10?,14-,18-/m1/s1	KEJCWVGMRLCZQQ-YJBYXUATSA-N
cefprozil Z isomer	**2.63a**		N[C@H](C1=CC=C(C=C1)O)C(N[C@H](C2=O)[C@]3([H])N2C(C(O)=O)=C(/C=C\C)CS3)=O	InChI=1S/C18H19N3O5S/c1-2-3-10-8-27-17-13(16(24)21(17)14(10)18(25)26)20-15(23)12(19)9-4-6-11(22)7-5-9/h2-7,12-13,17,22H,8,19H2,1H3,(H,20,23)(H,25,26)/b3-2-/t12-,13-,17-/m1/s1	WDLWHQDACQUCJR-AGGBKSKLSA-N
cefprozil E isomer	**2.63b**		N[C@H](C1=CC=C(C=C1)O)C(N[C@H](C2=O)[C@]3([H])N2C(C(O)=O)=C(/C=C/C)CS3)=O	InChI=1S/C18H19N3O5S/c1-2-3-10-8-27-17-13(16(24)21(17)14(10)18(25)26)20-15(23)12(19)9-4-6-11(22)7-5-9/h2-7,12-13,17,22H,8,19H2,1H3,(H,20,23)(H,25,26)/b3-2+/t12-,13-,17-/m1/s1	WDLWHQDACQUCJR-ZAMMOSSLSA-N
cefsulodin	**2.64**		O=C([C@H](S(=O)(O)=O)C1=CC=CC=C1)N[C@H](C2=O)[C@]3([H])N2C(C(O)=O)=C(C[N+]4=CC=C(C(N)=O)C=C4)CS3	InChI=1S/C22H20N4O8S2/c23-18(27)13-6-8-25(9-7-13)10-14-11-35-21-15(20(29)26(21)16(14)22(30)31)24-19(28)17(36(32,33)34)12-4-2-1-3-5-12/h1-9,15,17,21H,10-11H2,(H4-,23,24,27,28,30,31,32,33,34)/p+1/t15-,17-,21-/m1/s1	SYLKGLMBLAAGSC-QLVMHMETSA-O

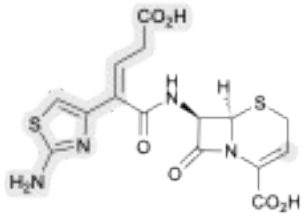
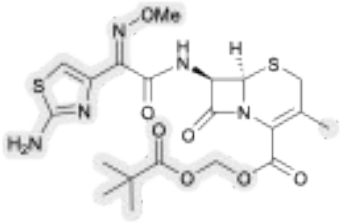
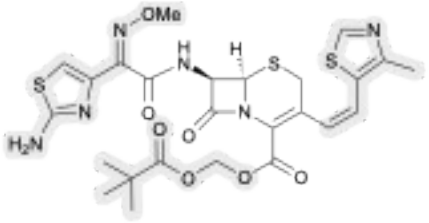
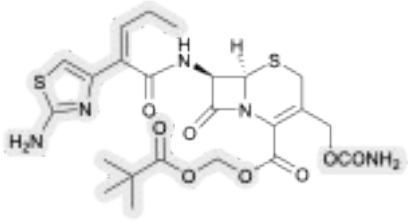
Name	#	Chemdraw	SMILES	InChI	InChIKey
cefotaxime	**2.65**		O=C1[C@@H](NC(/C(C2=CSC(N)=N2)=N\OC)=O)[C@@]3([H])SCC(COC(C)=O)=C(C(O)=O)N31	InChI=1S/C16H17N5O7S2/c1-6(22)28-3-7-4-29-14-10(13(24)21(14)11(7)15(25)26)19-12(23)9(20-27-2)8-5-30-16(17)18-8/h5,10,14H,3-4H2,1-2H3,(H2,17,18)(H,19,23)(H,25,26)/b20-9-/t10-,14-/m1/s1	GPRBEKHLDVQUJE-QSWIMTSFSA-N
cefoperazone	**2.66**		O=C([C@H](NC(N1CCN(C(C1=O)=O)CC)=O)C2=CC=C(O)C=C2)N[C@H](C3=O)[C@]4([H])N3C(C(O)=O)=C(CSC5=NN=NN5C)CS4	InChI=1S/C25H27N9O8S2/c1-3-32-8-9-33(21(39)20(32)38)24(42)27-15(12-4-6-14(35)7-5-12)18(36)26-16-19(37)34-17(23(40)41)13(10-43-22(16)34)11-44-25-28-29-30-31(25)2/h4-7,15-16,22,35H,3,8-11H2,1-2H3,(H,26,36)(H,27,42)(H,40,41)/t15-,16-,22-/m1/s1	GCFBRXLSHGKWDP-XCGNWRKASA-N
cefotiam	**2.67**		O=C(CC1=CSC(N)=N1)N[C@H](C2=O)[C@]3([H])N2C(C(O)=O)=C(CSC4=NN=NN4CCN(C)C)CS3	InChI=1S/C18H23N9O4S3/c1-25(2)3-4-26-18(22-23-24-26)34-7-9-6-32-15-12(14(29)27(15)13(9)16(30)31)21-11(28)5-10-8-33-17(19)20-10/h8,12,15H,3-7H2,1-2H3,(H2,19,20)(H,21,28)(H,30,31)/t12-,15-/m1/s1	QYQDKDWGWDOFFU-IUODEOHRSA-N
ceftizoxime	**2.68**		O=C1[C@@H](NC(/C(C2=CSC(N)=N2)=N\OC)=O)[C@]3([H])N1C(C(O)=O)=CCS3	InChI=1S/C13H13N5O5S2/c1-23-17-7(5-4-25-13(14)15-5)9(19)16-8-10(20)18-6(12(21)22)2-3-24-11(8)18/h2,4,8,11H,3H2,1H3,(H2,14,15)(H,16,19)(H,21,22)/b17-7-/t8-,11-/m1/s1	NNULBSISHYWZJU-LLKWHZGFSA-N

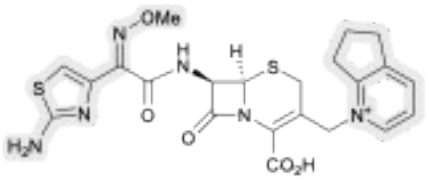
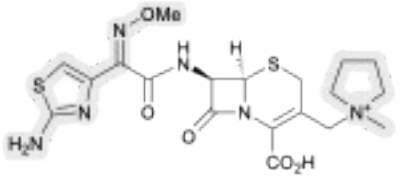
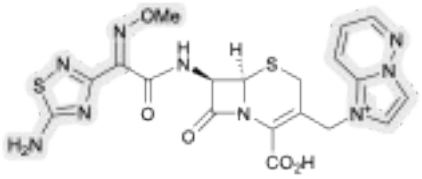
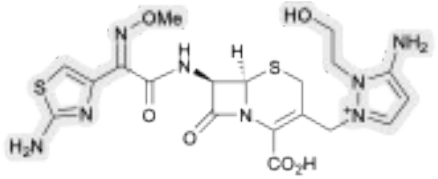
Name	#	Chemdraw	SMILES	InChI	InChIKey
ceftriaxone	**2.69**		O=C1[C@@H](NC(/C(C2=CSC(N)=N2)=N\OC)=O)[C@]3([H])N1C(C(O)=O)=C(CSC4=NC(C(NN4C)=O)=O)CS3	InChI=1S/C18H18N8O7S3/c1-25-18(22-12(28)13(29)23-25)36-4-6-3-34-15-9(14(30)26(15)10(6)16(31)32)21-11(27)8(24-33-2)7-5-35-17(19)20-7/h5,9,15H,3-4H2,1-2H3,(H2,19,20)(H,21,27)(H,23,29)(H,31,32)/b24-8-/t9-,15-/m1/s1	VAAUVRVFOQPIGI-SPQHTLEESA-N
cefmenoxime	**2.70**		O=C1[C@@H](NC(/C(C2=CSC(N)=N2)=N\OC)=O)[C@@]3([H])SCC(CSC4=NN=NN4C)=C(C(O)=O)N31	InChI=1S/C16H17N9O5S3/c1-24-16(20-22-23-24)33-4-6-3-31-13-9(12(27)25(13)10(6)14(28)29)19-11(26)8(21-30-2)7-5-32-15(17)18-7/h5,9,13H,3-4H2,1-2H3,(H2,17,18)(H,19,26)(H,28,29)/b21-8-/t9-,13-/m1/s1	HJJDBAOLQAWBMH-YCRCPZNHSA-N
ceftazidime	**2.71a**		O=C1[C@@H](NC(/C(C2=CSC(N)=N2)=N\OC(C)C(O)=O)=O)[C@@]3([H])SCC(C[N+]4=CC=CC=C4)=C(C(O)=O)N31	InChI=1S/C21H20N6O7S2/c1-10(19(30)31)34-25-13(12-9-36-21(22)23-12)16(28)24-14-17(29)27-15(20(32)33)11(8-35-18(14)27)7-26-5-3-2-4-6-26/h2-6,9-10,14,18H,7-8H2,1H3,(H4-,22,23,24,28,30,31,32,33)/p+1/b25-13-/t10?,14-,18-/m1/s1	GDYSLJXJSQEUHA-FBXRGJNPSA-O
avibactam	**2.71b**		O=C(N1OS(=O)(O)=O)[N@@]2C[C@H]1CC[C@H]2C(N)=O	InChI=1S/C7H11N3O6S/c8-6(11)5-2-1-4-3-9(5)7(12)10(4)16-17(13,14)15/h4-5H,1-3H2,(H2,8,11)(H,13,14,15)/t4-,5+/m1/s1	NDCUAPJVLWFHHB-UHNVWZDZSA-N

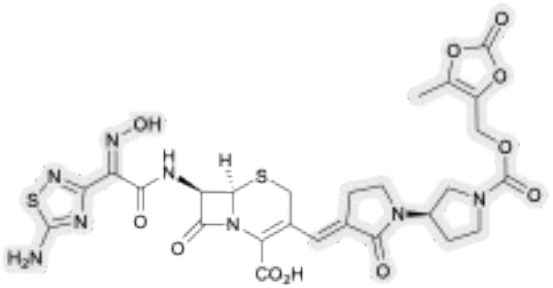
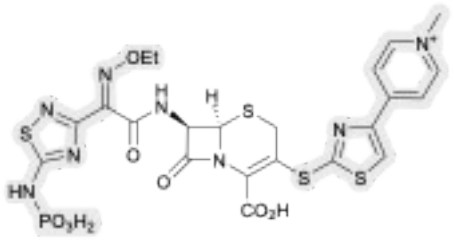
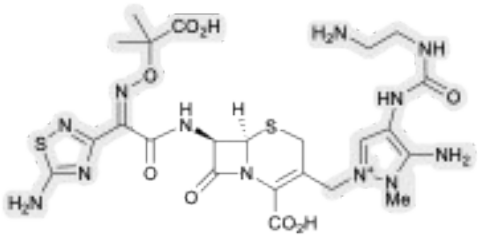
Name	#	Chemdraw	SMILES	InChI	InChIKey
metronidazole	**2.71c**		CC1=NC=C([N+]([O-])=O)N1CCO	InChI=1S/C6H9N3O3/c1-5-7-4-6(9(11)12)8(5)2-3-10/h4,10H,2-3H2,1H3	VAOCPAMSLUNLGC-UHFFFAOYSA-N
cefonicid	**2.72**		O[C@H](C1=CC=CC=C1)C(N[C@H](C2=O)[C@]3([H])N2C(C(O)=O)=C(CSC4=NN=NN4CS(=O)(O)=O)CS3)=O	InChI=1S/C18H18N6O8S3/c25-13(9-4-2-1-3-5-9)14(26)19-11-15(27)24-12(17(28)29)10(6-33-16(11)24)7-34-18-20-21-22-23(18)8-35(30,31)32/h1-5,11,13,16,25H,6-8H2,(H,19,26)(H,28,29)(H,30,31,32)/t11-,13-,16-/m1/s1	DYAIAHUQIPBDIP-AXAPSJFSSA-N
ceforanide	**2.73**		O=C(CC1=C(CN)C=CC=C1)N[C@H](C2=O)[C@]3([H])N2C(C(O)=O)=C(CSC4=NN=NN4CC(O)=O)CS3	InChI=1S/C20H21N7O6S2/c21-6-11-4-2-1-3-10(11)5-13(28)22-15-17(31)27-16(19(32)33)12(8-34-18(15)27)9-35-20-23-24-25-26(20)7-14(29)30/h1-4,15,18H,5-9,21H2,(H,22,28)(H,29,30)(H,32,33)/t15-,18-/m1/s1	SLAYUXIURFNXPG-CRAIPNDOSA-N
cefpiramide	**2.74**		OC(C=C1)=CC=C1[C@@H](NC(C2=CN=C(C=C2O)C)=O)C(N[C@H](C3=O)[C@]4([H])N3C(C(O)=O)=C(CSC5=NN=NN5C)CS4)=O	InChI=1S/C25H24N8O7S2/c1-11-7-16(35)15(8-26-11)20(36)27-17(12-3-5-14(34)6-4-12)21(37)28-18-22(38)33-19(24(39)40)13(9-41-23(18)33)10-42-25-29-30-31-32(25)2/h3-8,17-18,23,34H,9-10H2,1-2H3,(H,26,35)(H,27,36)(H,28,37)(H,39,40)/t17-,18-,23-/m1/s1	PWAUCHMQEXVFJR-PMAPCBKXSA-N

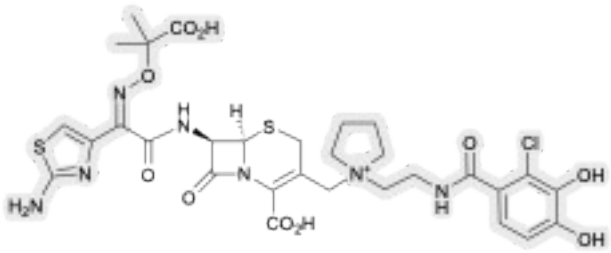
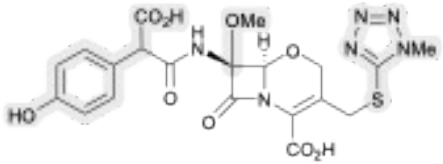
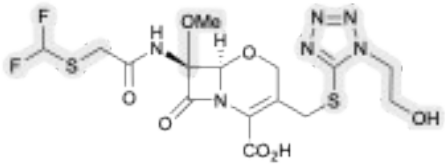
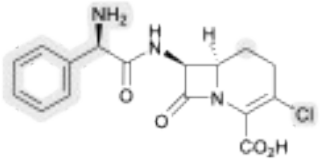
Name	#	Chemdraw	SMILES	InChI	InChIKey
cefixime	**2.75**		O=C1[C@@H](NC(/C(C2=CSC(N)=N2)=N\OCC(O)=O)=O)[C@@]3([H])SCC(C=C)=C(C(O)=O)N31	InChI=1S/C16H15N5O7S2/c1-2-6-4-29-14-10(13(25)21(14)11(6)15(26)27)19-12(24)9(20-28-3-8(22)23)7-5-30-16(17)18-7/h2,5,10,14H,1,3-4H2,(H2,17,18)(H,19,24)(H,22,23)(H,26,27)/b20-9-/t10-,14-/m1/s1	OKBVVJOGVLARMR-QSWIMTSFSA-N
cefpimizole	**2.76**		O=C(C1=C(N=CN1)C(O)=O)N[C@H](C2=CC=CC=C2)C(N[C@H](C3=O)[C@]4([H])N3C(C(O)=O)=C(C[N+]5=CC=C(CCS(=O)(O)=O)C=C5)CS4)=O	InChI=1S/C28H26N6O10S2/c35-23(18(16-4-2-1-3-5-16)31-24(36)19-20(27(38)39)30-14-29-19)32-21-25(37)34-22(28(40)41)17(13-45-26(21)34)12-33-9-6-15(7-10-33)8-11-46(42,43)44/h1-7,9-10,14,18,21,26H,8,11-13H2,(H5-,29,30,31,32,35,36,38,39,40,41,42,43,44)/p+1/t18-,21-,26-/m1/s1	LNZMRLHZGOBKAN-KAWPREARSA-O
cefteram pivoxil	**2.77**		O=C(OCOC(C1=C(CN2N=C(N=N2)C)CS[C@@]([C@@H]3NC(/C(C4=CSC(N)=N4)=N\OC)=O)([H])N1C3=O)=O)C(C)(C)C	InChI=1S/C22H27N9O7S2/c1-10-26-29-30(27-10)6-11-7-39-18-14(25-16(32)13(28-36-5)12-8-40-21(23)24-12)17(33)31(18)15(11)19(34)37-9-38-20(35)22(2,3)4/h8,14,18H,6-7,9H2,1-5H3,(H2,23,24)(H,25,32)/b28-13-/t14-,18-/m1/s1	UIYAXIPXULMHAI-JLGRZTKVSA-N

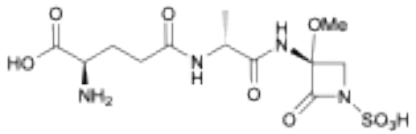
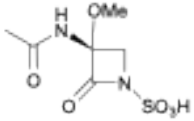
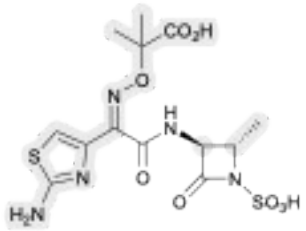
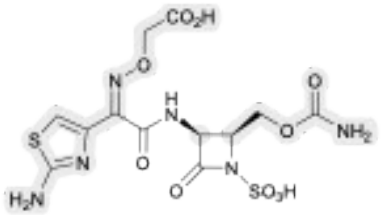
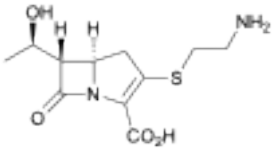
Name	#	Chemdraw	SMILES	InChI	InChIKey
cefpodoxime proxetil	**2.78**		O=C1[C@@H](NC(/C(C2=CSC(N)=N2)=N\OC)=O)[C@@]3([H])SCC(COC)=C(C(OC(OC(OC(C)C)=O)C)=O)N31	InChI=1S/C21H27N5O9S2/c1-9(2)33-21(30)35-10(3)34-19(29)15-11(6-31-4)7-36-18-14(17(28)26(15)18)24-16(27)13(25-32-5)12-8-37-20(22)23-12/h8-10,14,18H,6-7H2,1-5H3,(H2,22,23)(H,24,27)/b25-13-/t10?,14-,18-/m1/s1	LTINZAODLRIQIX-FBXRGJNPSA-N
cefodizime	**2.79**		O=C1[C@@H](NC(/C(C2=CSC(N)=N2)=N\OC)=O)[C@@]3([H])SCC(CSC4=NC(C)=C(CC(O)=O)S4)=C(C(O)=O)N31	InChI=1S/C20H20N6O7S4/c1-7-10(3-11(27)28)37-20(22-7)36-5-8-4-34-17-13(16(30)26(17)14(8)18(31)32)24-15(29)12(25-33-2)9-6-35-19(21)23-9/h6,13,17H,3-5H2,1-2H3,(H2,21,23)(H,24,29)(H,27,28)(H,31,32)/b25-12-/t13-,17-/m1/s1	XDZKBRJLTGRPSS-BGZQYGJUSA-N
cefotiam hexetil	**2.80**		O=C(CC1=CSC(N)=N1)N[C@H](C2=O)[C@]3([H])N2C(C(OC(OC(OC4CCCCC4)=O)C)=O)=C(CSC5=NN=NN5CCN(C)C)CS3	InChI=1S/C27H37N9O7S3/c1-15(42-27(40)43-18-7-5-4-6-8-18)41-24(39)21-16(13-46-26-31-32-33-35(26)10-9-34(2)3)12-44-23-20(22(38)36(21)23)30-19(37)11-17-14-45-25(28)29-17/h14-15,18,20,23H,4-13H2,1-3H3,(H2,28,29)(H,30,37)/t15?,20-,23-/m1/s1	VVFDMWZLBPUKTD-ZKRNHDOASA-N
cefdinir	**2.81**		O=C1[C@@H](NC(/C(C2=CSC(N)=N2)=N\O)=O)[C@@]3([H])SCC(C=C)=C(C(O)=O)N31	InChI=1S/C14H13N5O5S2/c1-2-5-3-25-12-8(11(21)19(12)9(5)13(22)23)17-10(20)7(18-24)6-4-26-14(15)16-6/h2,4,8,12,24H,1,3H2,(H2,15,16)(H,17,20)(H,22,23)/b18-7-/t8-,12-/m1/s1	RTXOFQZKPXMALH-GHXIOONMSA-N

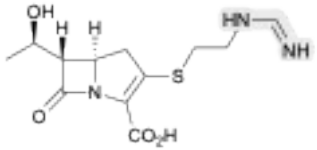
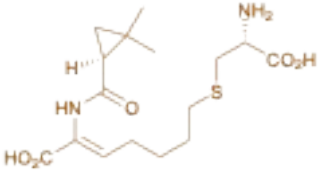
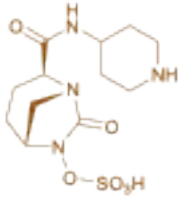
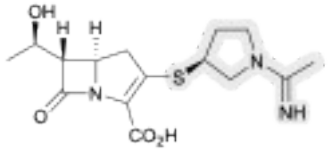
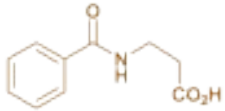
Name	#	Chemdraw	SMILES	InChI	InChIKey
ceftibuten	**2.82**		O=C1N2[C@@](SCC=C2C(O)=O)([H])[C@@H]1NC(/C(C3=CSC(N)=N3)=C\CC(O)=O)=O	InChI=1S/C15H14N4O6S2/c16-15-17-7(5-27-15)6(1-2-9(20)21)11(22)18-10-12(23)19-8(14(24)25)3-4-26-13(10)19/h1,3,5,10,13H,2,4H2,(H2,16,17)(H,18,22)(H,20,21)(H,24,25)/b6-1-/t10-,13-/m1/s1	UNJFKXSSGBWRBZ-BJCIPQKHSA-N
cefetamet pivoxil	**2.83**		O=C(OCOC(C1=C(C)CS[C@@]([C@@H]2NC(/C(C3=CSC(N)=N3)=N\OC)=O)([H])N1C2=O)=O)C(C)(C)C	InChI=1S/C20H25N5O7S2/c1-9-6-33-16-12(23-14(26)11(24-30-5)10-7-34-19(21)22-10)15(27)25(16)13(9)17(28)31-8-32-18(29)20(2,3)4/h7,12,16H,6,8H2,1-5H3,(H2,21,22)(H,23,26)/b24-11-/t12-,16-/m1/s1	DASYMCLQENWCJG-XUKDPADISA-N
cefditoren pivoxil	**2.84**		O=C(OCOC(C1=C(/C=C\C2=C(N=CS2)C)CS[C@@]([C@@H]3NC(/C(C4=CSC(N)=N4)=N\OC)=O)([H])N1C3=O)=O)C(C)(C)C	InChI=1S/C25H28N6O7S3/c1-12-15(41-10-27-12)7-6-13-8-39-21-17(29-19(32)16(30-36-5)14-9-40-24(26)28-14)20(33)31(21)18(13)22(34)37-11-38-23(35)25(2,3)4/h6-7,9-10,17,21H,8,11H2,1-5H3,(H2,26,28)(H,29,32)/b7-6-,30-16-/t17-,21-/m1/s1	AFZFFLVORLEPPO-UVYJNCLZSA-N
cefcapene pivoxil	**2.85**		O=C1[C@@H](NC(/C(C2=CSC(N)=N2)=C\CC)=O)[C@@]3([H])SCC(COC(N)=O)=C(C(OOC(C(C)(C)C)=O)=O)N31	InChI=1S/C23H29N5O8S2/c1-5-6-12(13-9-38-21(24)26-13)16(29)27-14-17(30)28-15(11(7-34-22(25)33)8-37-18(14)28)19(31)35-10-36-20(32)23(2,3)4/h6,9,14,18H,5,7-8,10H2,1-4H3,(H2,24,26)(H2,25,33)(H,27,29)/b12-6-/t14-,18-/m1/s1	WVPAABNYMHNFJG-QDVBXLKVSA-N

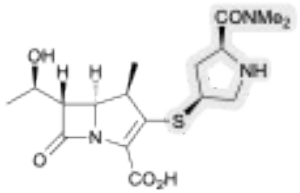
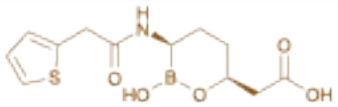
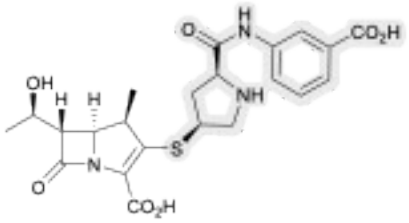
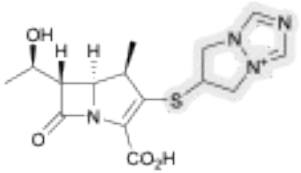
Name	#	Chemdraw	SMILES	InChI	InChIKey
cefpirome	**2.86**		O=C1[C@@H](NC(/C(C2=CSC(N)=N2)=N\OC)=O)[C@@]3([H])SCC(C[N+]4=C5C(CCC5)=CC=C4)=C(C(O)=O)N31	InChI=1S/C22H22N6O5S2/c1-33-26-15(13-10-35-22(23)24-13)18(29)25-16-19(30)28-17(21(31)32)12(9-34-20(16)28)8-27-7-3-5-11-4-2-6-14(11)27/h3,5,7,10,16,20H,2,4,6,8-9H2,1H3,(H3-,23,24,25,29,31,32)/p+1/b26-15-/t16-,20-/m1/s1	DKOQGJHPHLTOJR-WHRDSVKCSA-O
cefepime	**2.87**		O=C1[C@@H](NC(/C(C2=CSC(N)=N2)=N\OC)=O)[C@@]3([H])SCC(C[N+]4(CCCC4)C)=C(C(O)=O)N31	InChI=1S/C19H24N6O5S2/c1-25(5-3-4-6-25)7-10-8-31-17-13(16(27)24(17)14(10)18(28)29)22-15(26)12(23-30-2)11-9-32-19(20)21-11/h9,13,17H,3-8H2,1-2H3,(H3-,20,21,22,26,28,29)/p+1/b23-12-/t13-,17-/m1/s1	HVFLCNVBZFFHBT-ZKDACBOMSA-O
cefozopran	**2.88**		O=C1[C@@H](NC(/C(C2=NSC(N)=N2)=N\OC)=O)[C@@]3([H])SCC(C[N+]4=C5N(N=CC=C5)C=C4)=C(C(O)=O)N31	InChI=1S/C19H17N9O5S2/c1-33-24-11(14-23-19(20)35-25-14)15(29)22-12-16(30)28-13(18(31)32)9(8-34-17(12)28)7-26-5-6-27-10(26)3-2-4-21-27/h2-6,12,17H,7-8H2,1H3,(H3-,20,22,23,25,29,31,32)/p+1/b24-11-/t12-,17-/m1/s1	QDUIJCOKQCCXQY-WHJQOFBOSA-O
cefoselis	**2.89**		O=C1[C@@H](NC(/C(C2=CSC(N)=N2)=N\OC)=O)[C@@]3([H])SCC(C[N+]4=CC=C(N)N4CCO)=C(C(O)=O)N31	InChI=1S/C19H22N8O6S2/c1-33-24-12(10-8-35-19(21)22-10)15(29)23-13-16(30)27-14(18(31)32)9(7-34-17(13)27)6-25-3-2-11(20)26(25)4-5-28/h2-3,8,13,17,20,28H,4-7H2,1H3,(H4,21,22,23,29,31,32)/p+1/b24-12-/t13-,17-/m1/s1	BHXLLRXDAYEMPP-SBGRAJFYSA-O

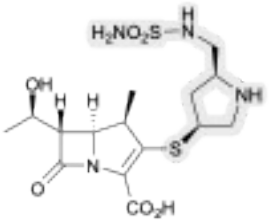
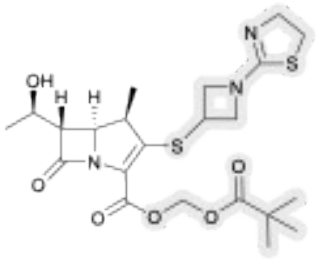
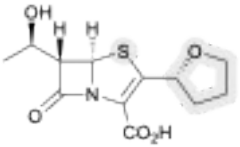
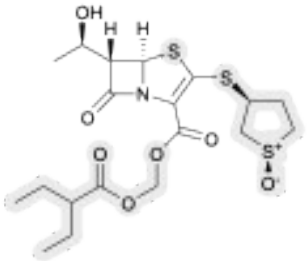
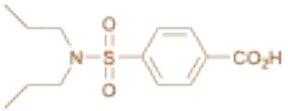
Name	#	Chemdraw	SMILES	InChI	InChIKey
ceftobiprole medocaril	**2.90**		O/N=C(C1=NSC(N)=N1)\C(N[C@H](C2=O)[C@]3([H])N2C(C(O)=O)=C(/C=C4C(N([C@H]5CN(CC5)C(OCC6=C(OC(O6)=O)C)=O)CC/4)=O)CS3)=O	InChI=1S/C26H26N8O11S2/c1-10-14(45-26(41)44-10)8-43-25(40)32-4-3-13(7-32)33-5-2-11(20(33)36)6-12-9-46-22-16(21(37)34(22)17(12)23(38)39)28-19(35)15(30-42)18-29-24(27)47-31-18/h6,13,16,22,42H,2-5,7-9H2,1H3,(H,28,35)(H,38,39)(H2,27,29,31)/b11-6+,30-15-/t13-,16-,22-/m1/s1	HFTSMHTWUFCYMJ-YIOMYIDASA-N
ceftaroline fosamil	**2.91**		O=C1[C@@H](NC(/C(C2=NSC(NP(O)(O)=O)=N2)=N\OCC)=O)[C@]3([H])N1C(C(O)=O)=C(SC4=NC(C5=CC=[N+](C=C5)C)=CS4)CS3	InChI=1S/C22H21N8O8PS4/c1-3-38-26-13(16-25-21(43-28-16)27-39(35,36)37)17(31)24-14-18(32)30-15(20(33)34)12(9-40-19(14)30)42-22-23-11(8-41-22)10-4-6-29(2)7-5-10/h4-8,14,19H,3,9H2,1-2H3,(H4-,24,25,27,28,31,33,34,35,36,37)/p+1/b26-13-/t14-,19-/m1/s1	ZCCUWMICIWSJIX-NQJJCJBVSA-O
ceftolozane	**2.92**		O=C1[C@@H](NC(/C(C2=NSC(N)=N2)=N\OC(C)(C)C(O)=O)=O)[C@@]3([H])SCC(C[N+]4=CC(NC(NCCN)=O)=C(N)N4C)=C(C(O)=O)N31	InChI=1S/C23H30N12O8S2/c1-23(2,20(40)41)43-31-11(15-30-21(26)45-32-15)16(36)29-12-17(37)35-13(19(38)39)9(8-44-18(12)35)6-34-7-10(14(25)33(34)3)28-22(42)27-5-4-24/h7,12,18,25H,4-6,8,24H2,1-3H3,(H7,26,27,28,29,30,32,36,38,39,40,41,42)/p+1/b31-11-/t12-,18-/m1/s1	JHFNIHVVXRKLEF-DCZLAGFPSA-O

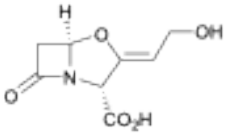
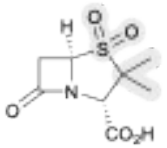
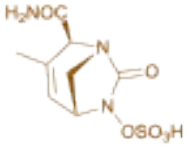
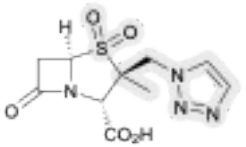
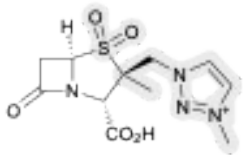
Name	#	Chemdraw	SMILES	InChI	InChIKey
cefiderocol	**2.93**		O=C1[C@@H](NC(/C(C2=CSC(N)=N2)=N\OC(C)(C)C(O)=O)=O)[C@@]3([H])SCC(C[N+]4(CCCC4)CCNC(C5=CC=C(O)C(O)=C5Cl)=O)=C(C(O)=O)N31	InChI=1S/C30H34ClN7O10S2/c1-30(2,28(46)47)48-36-19(16-13-50-29(32)34-16)24(42)35-20-25(43)37-21(27(44)45)14(12-49-26(20)37)11-38(8-3-4-9-38)10-7-33-23(41)15-5-6-17(39)22(40)18(15)31/h5-6,13,20,26H,3-4,7-12H2,1-2H3,(H7-,32,33,34,35,36,39,40,41,42,44,45,46,47)/p+1/t20-,26-/m1/s1	DBPPRLRVDVJOCL-FQRUVTKNSA-O
latamoxef	**2.94**		O=C(C(C(O)=O)C1=CC=C(O)C=C1)N[C@]2([C@]3([H])N(C(C(O)=O)=C(CO3)CSC4=NN=NN4C)C2=O)OC	InChI=1S/C20H20N6O9S/c1-25-19(22-23-24-25)36-8-10-7-35-18-20(34-2,17(33)26(18)13(10)16(31)32)21-14(28)12(15(29)30)9-3-5-11(27)6-4-9/h3-6,12,18,27H,7-8H2,1-2H3,(H,21,28)(H,29,30)(H,31,32)/t12?,18-,20+/m1/s1	JWCSIUVGFCSJCK-CAVRMKNVSA-N
flomoxef	**2.95**		FC(F)SCC(N[C@]1([C@]2([H])N(C(C(O)=O)=C(CO2)CSC3=NN=NN3CCO)C1=O)OC)=O	InChI=1S/C15H18F2N6O7S2/c1-29-15(18-8(25)6-31-13(16)17)11(28)23-9(10(26)27)7(4-30-12(15)23)5-32-14-19-20-21-22(14)2-3-24/h12-13,24H,2-6H2,1H3,(H,18,25)(H,26,27)/t12-,15+/m1/s1	UHRBTBZOWWGKMK-DOMZBBRYSA-N
loracarbef	**2.96**		O=C1N2[C@@](CCC(Cl)=C2C(O)=O)([H])[C@@H]1NC([C@@H](C3=CC=CC=C3)N)=O	InChI=1S/C16H16ClN3O4/c17-9-6-7-10-12(15(22)20(10)13(9)16(23)24)19-14(21)11(18)8-4-2-1-3-5-8/h1-5,10-12H,6-7,18H2,(H,19,21)(H,23,24)/t10-,11-,12+/m1/s1	JAPHQRWPEGVNBT-UTUOFQBUSA-N

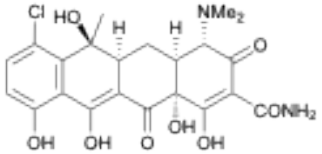
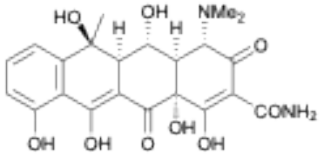
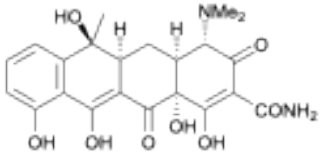
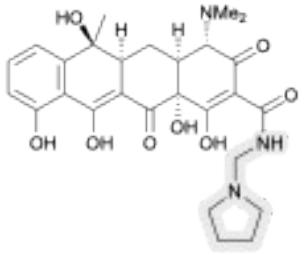
Name	#	Chemdraw	SMILES	InChI	InChIKey
sulfazecin	**2.97**		O=C([C@@](C1)(OC)NC([C@@H](C)NC(CC[C@@H](N)C(O)=O)=O)=O)N1S(=O)(O)=O	InChI=1S/C12H20N4O9S/c1-6(14-8(17)4-3-7(13)10(19)20)9(18)15-12(25-2)5-16(11(12)21)26(22,23)24/h6-7H,3-5,13H2,1-2H3,(H,14,17)(H,15,18)(H,19,20)(H,22,23,24)/t6-,7-,12-/m1/s1	MOBOUQJWGBVNCR-NQYJQULFSA-N
SQ 26,180	**2.98**		O=C([C@@](C1)(OC)NC(C)=O)N1S(=O)(O)=O	InChI=1S/C6H10N2O6S/c1-4(9)7-6(14-2)3-8(5(6)10)15(11,12)13/h3H2,1-2H3,(H,7,9)(H,11,12,13)/t6-/m1/s1	RFAUYXHDQGJQSD-ZCFIWIBFSA-N
aztreonam	**2.99**		O=C([C@H]([C@@H]1C)NC(/C(C2=CSC(N)=N2)=N\OC(C)(C)C(O)=O)=O)N1S(=O)(O)=O	InChI=1S/C13H17N5O8S2/c1-5-7(10(20)18(5)28(23,24)25)16-9(19)8(6-4-27-12(14)15-6)17-26-13(2,3)11(21)22/h4-5,7H,1-3H3,(H2,14,15)(H,16,19)(H,21,22)(H,23,24,25)/b17-8-/t5-,7-/m0/s1	WZPBZJONDBGPKJ-VEHQQRBSSA-N
carumonam	**2.100**		O=C(N[C@H]1[C@@H](COC(N)=O)N(S(=O)(O)=O)C1=O)/C(C2=CSC(N)=N2)=N\OCC(O)=O	InChI=1S/C12H14N6O10S2/c13-11-15-4(3-29-11)7(17-28-2-6(19)20)9(21)16-8-5(1-27-12(14)23)18(10(8)22)30(24,25)26/h3,5,8H,1-2H2,(H2,13,15)(H2,14,23)(H,16,21)(H,19,20)(H,24,25,26)/b17-7-/t5-,8+/m1/s1	UIMOJFJSJSIGLV-JNHMLNOCSA-N
thienamycin	**2.101**		O=C1N(C(C(O)=O)=C(SCCN)C2)[C@@]2([H])[C@@]1([H])[C@H](O)C	InChI=1S/C11H16N2O4S/c1-5(14)8-6-4-7(18-3-2-12)9(11(16)17)13(6)10(8)15/h5-6,8,14H,2-4,12H2,1H3,(H,16,17)/t5-,6-,8-/m1/s1	WKDDRNSBRWANNC-ATRFCDNQSA-N

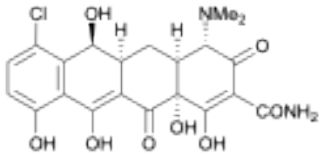
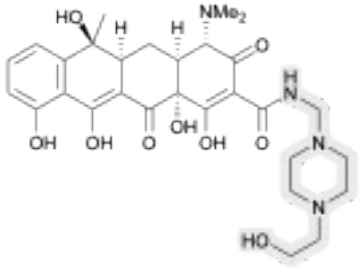
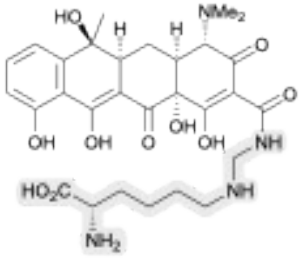
Name	#	Chemdraw	SMILES	InChI	InChIKey
imipenem	**2.102**		O=C1N(C(C(O)=O)=C(SCCNC=N)C2)[C@@]2([H])[C@@]1([H])[C@H](O)C	InChI=1S/C12H17N3O4S/c1-6(16)9-7-4-8(20-3-2-14-5-13)10(12(18)19)15(7)11(9)17/h5-7,9,16H,2-4H2,1H3,(H2,13,14)(H,18,19)/t6-,7-,9-/m1/s1	ZSKVGTPCRGIANV-ZXFLCMHBSA-N
cilastatin	**2.102a**		N[C@@H](CSCCCC/C=C(NC([C@]1([H])C(C)(C)C1)=O)/C(O)=O)C(O)=O	InChI=1S/C16H26N2O5S/c1-16(2)8-10(16)13(19)18-12(15(22)23)6-4-3-5-7-24-9-11(17)14(20)21/h6,10-11H,3-5,7-9,17H2,1-2H3,(H,18,19)(H,20,21)(H,22,23)/b12-6-/t10-,11+/m1/s1	DHSUYTOATWAVLW-WFVMDLQDSA-N
relebactam	**2.102b**		O=C(N1OS(=O)(O)=O)[N@@]2C[C@H]1CC[C@H]2C(NC3CCNCC3)=O	InChI=1S/C12H20N4O6S/c17-11(14-8-3-5-13-6-4-8)10-2-1-9-7-15(10)12(18)16(9)22-23(19,20)21/h8-10,13H,1-7H2,(H,14,17)(H,19,20,21)/t9-,10+/m1/s1	SMOBCLHAZXOKDQ-ZJUUUORDSA-N
panipenem	**2.103**		O=C1N(C(C(O)=O)=C(S[C@@H]2CN(C(C)=N)CC2)C3)[C@@]3([H])[C@@]1([H])[C@H](O)C	InChI=1S/C15H21N3O4S/c1-7(19)12-10-5-11(13(15(21)22)18(10)14(12)20)23-9-3-4-17(6-9)8(2)16/h7,9-10,12,16,19H,3-6H2,1-2H3,(H,21,22)/t7-,9+,10-,12-/m1/s1	TYMABNNERDVXID-DLYFRVTGSA-N
betamipron	**2.103a**		O=C(NCCC(O)=O)C1=CC=CC=C1	InChI=1S/C10H11NO3/c12-9(13)6-7-11-10(14)8-4-2-1-3-5-8/h1-5H,6-7H2,(H,11,14)(H,12,13)	CWXYHOHYCJXYFQ-UHFFFAOYSA-N

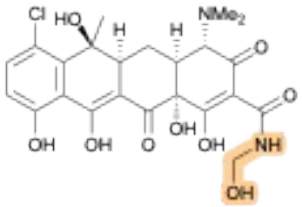
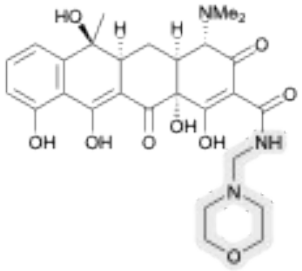
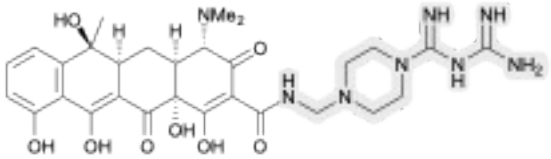
Name	#	Chemdraw	SMILES	InChI	InChIKey
meropenem	**2.104**		C[C@H]1C(S[C@@H]2CN[C@H](C(N(C)C)=O)C2)=C(C(O)=O)N([C@@]1([H])[C@@]3([H])[C@H](O)C)C3=O	InChI=1S/C17H25N3O5S/c1-7-12-11(8(2)21)16(23)20(12)13(17(24)25)14(7)26-9-5-10(18-6-9)15(22)19(3)4/h7-12,18,21H,5-6H2,1-4H3,(H,24,25)/t7-,8-,9+,10+,11-,12-/m1/s1	DMJNNHOOLUXYBV-PQTSNVLCSA-N
vaborbactam	**2.104a**		O=C(O)C[C@@H]1CC[C@H](NC(CC2=CC=CS2)=O)B(O)O1	InChI=1S/C12H16BNO5S/c15-11(7-9-2-1-5-20-9)14-10-4-3-8(6-12(16)17)19-13(10)18/h1-2,5,8,10,18H,3-4,6-7H2,(H,14,15)(H,16,17)/t8-,10-/m0/s1	IOOWNWLVCOUUEX-WPRPVWTQSA-N
ertapenem	**2.105**		O=C1N(C(C(O)=O)=C(S[C@@H]2CN[C@H](C(NC3=CC=CC(C(O)=O)=C3)=O)C2)[C@@H]4C)[C@@]4([H])[C@@]1([H])[C@H](O)C	InChI=1S/C22H25N3O7S/c1-9-16-15(10(2)26)20(28)25(16)17(22(31)32)18(9)33-13-7-14(23-8-13)19(27)24-12-5-3-4-11(6-12)21(29)30/h3-6,9-10,13-16,23,26H,7-8H2,1-2H3,(H,24,27)(H,29,30)(H,31,32)/t9-,10-,13+,14+,15-,16-/m1/s1	JUZNIMUFDBIJCM-ANEDZVCMSA-N
biapenem	**2.106**		O=C1N(C(C(O)=O)=C(SC2C[N+]3=CN=CN3C2)[C@@H]4C)[C@@]4([H])[C@@]1([H])[C@H](O)C	InChI=1S/C15H18N4O4S/c1-7-11-10(8(2)20)14(21)19(11)12(15(22)23)13(7)24-9-3-17-5-16-6-18(17)4-9/h5-11,20H,3-4H2,1-2H3/p+1/t7-,8-,10-,11-/m1/s1	MRMBZHPJVKCOMA-YJFSRANCSA-O

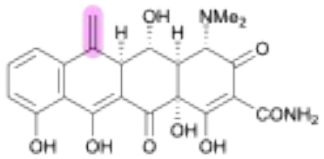
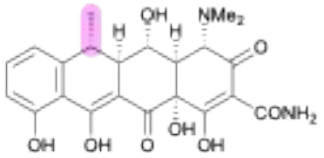
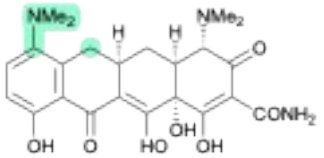
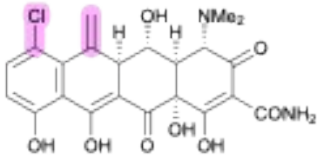
Name	#	Chemdraw	SMILES	InChI	InChIKey
doripenem	**2.107**		O=C1N(C(C(O)=O)=C(S[C@@H]2CN[C@H](CNS(=O)(N)=O)C2)[C@@H]3C)[C@@]3([H])[C@@]1([H])[C@H](O)C	InChI=1S/C15H24N4O6S2/c1-6-11-10(7(2)20)14(21)19(11)12(15(22)23)13(6)26-9-3-8(17-5-9)4-18-27(16,24)25/h6-11,17-18,20H,3-5H2,1-2H3,(H,22,23)(H2,16,24,25)/t6-,7-,8+,9+,10-,11-/m1/s1	AVAACINZEOAHHE-VFZPANTDSA-N
tebipenem pivoxil	**2.108**		O=C1N(C(C(OCOC(C(C)(C)C)=O)=O)=C(SC(C2)CN2C3=NCCS3)[C@@H]4C)[C@@]4([H])[C@@]1([H])[C@@H](C)O	InChI=1S/C22H31N3O6S2/c1-11-15-14(12(2)26)18(27)25(15)16(19(28)30-10-31-20(29)22(3,4)5)17(11)33-13-8-24(9-13)21-23-6-7-32-21/h11-15,26H,6-10H2,1-5H3/t11-,12-,14-,15-/m1/s1	SNUDIPVBUUXCDG-QHSBEEBCSA-N
faropenem	**2.109**		O=C1N(C(C(O)=O)=C([C@H]2CCCO2)S3)[C@@]3([H])[C@@]1([H])[C@H](O)C	InChI=1S/C12H15NO5S/c1-5(14)7-10(15)13-8(12(16)17)9(19-11(7)13)6-3-2-4-18-6/h5-7,11,14H,2-4H2,1H3,(H,16,17)/t5-,6-,7+,11-/m1/s1	HGGAKXAHAYOLDJ-FHZUQPTBSA-N
sulopenem etzadroxil	**2.110**		O=C1N(C(C(OCOC(C(CC)CC)=O)=O)=C(S[C@@H]2C[S@+]([O-])CC2)S3)[C@@]3([H])[C@@]1([H])[C@H](O)C	InChI=1S/C19H27NO7S3/c1-4-11(5-2)17(23)26-9-27-18(24)14-19(28-12-6-7-30(25)8-12)29-16-13(10(3)21)15(22)20(14)16/h10-13,16,21H,4-9H2,1-3H3/t10-,12+,13+,16-,30-/m1/s1	NBPVNGWRLGHULH-CSOWVJSESA-N
probenecid	**2.110a**		O=S(C1=CC=C(C(O)=O)C=C1)(N(CCC)CCC)=O	InChI=1S/C13H19NO4S/c1-3-9-14(10-4-2)19(17,18)12-7-5-11(6-8-12)13(15)16/h5-8H,3-4,9-10H2,1-2H3,(H,15,16)	DBABZHXKTCFAPX-UHFFFAOYSA-N

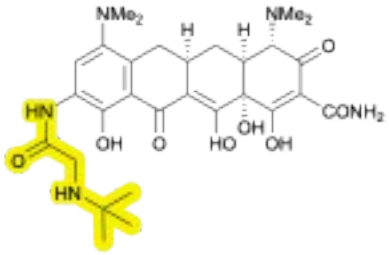
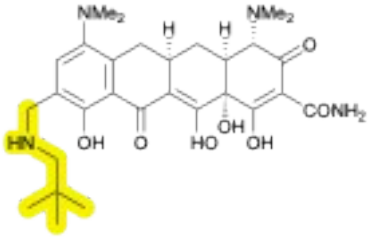
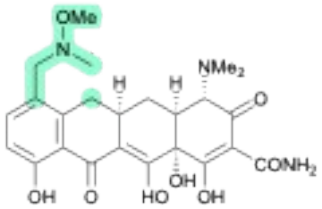
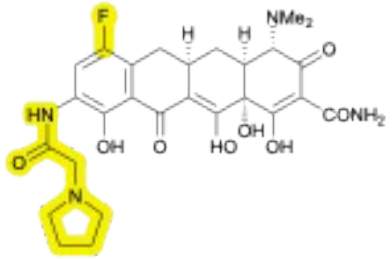
Name	#	Chemdraw	SMILES	InChI	InChIKey
clavulanic acid	**2.111**		O=C1C[C@]2([H])N1[C@@H](C(O)=O)/C(O2)=C/CO	InChI=1S/C8H9NO5/c10-2-1-4-7(8(12)13)9-5(11)3-6(9)14-4/h1,6-7,10H,2-3H2,(H,12,13)/b4-1-/t6-,7-/m1/s1	HZZVJAQRINQKSD-PBFISZAISA-N
sulbactam	**2.112**		O=C1C[C@]2([H])N1[C@@H](C(O)=O)C(C)(C)S2(=O)=O	InChI=1S/C8H11NO5S/c1-8(2)6(7(11)12)9-4(10)3-5(9)15(8,13)14/h5-6H,3H2,1-2H3,(H,11,12)/t5-,6+/m1/s1	FKENQMMABCRJMK-RITPCOANSA-N
durlobactam	**2.112a**		CC1=C[C@@H]2C[N@@](C(N2OS(=O)(O)=O)=O)[C@@H]1C(N)=O	InChI=1S/C8H11N3O6S/c1-4-2-5-3-10(6(4)7(9)12)8(13)11(5)17-18(14,15)16/h2,5-6H,3H2,1H3,(H2,9,12)(H,14,15,16)/t5-,6+/m1/s1	BISPBXFUKNXOQY-RITPCOANSA-N
tazobactam	**2.113**		O=C1C[C@]2([H])N1[C@@H](C(O)=O)[C@](C)(CN3C=CN=N3)S2(=O)=O	InChI=1S/C10H12N4O5S/c1-10(5-13-3-2-11-12-13)8(9(16)17)14-6(15)4-7(14)20(10,18)19/h2-3,7-8H,4-5H2,1H3,(H,16,17)/t7-,8+,10+/m1/s1	LPQZKKCYTLCDGQ-WEDXCCLWSA-N
enmetazobactam	**2.114**		O=C1C[C@]2([H])N1[C@@H](C(O)=O)[C@](C)(CN3C=C[N+](C)=N3)S2(=O)=O	InChI=1S/C11H14N4O5S/c1-11(6-14-4-3-13(2)12-14)9(10(17)18)15-7(16)5-8(15)21(11,19)20/h3-4,8-9H,5-6H2,1-2H3/p+1/t8-,9+,11+/m1/s1	HFZITXBUTWITPT-YWVKMMECSA-O

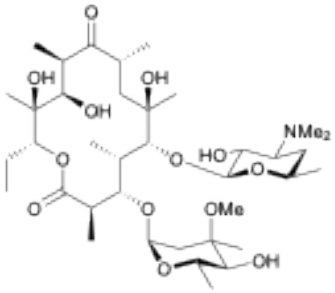
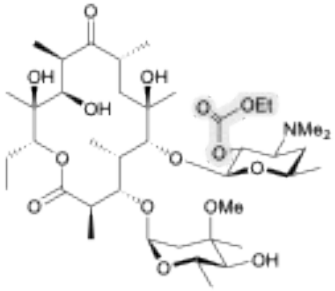
Name	#	Chemdraw	SMILES	InChI	InChIKey
chlortetracycline	**3.01**		O=C(C(C(N)=O)=C(O)[C@]12O)[C@@H](N(C)C)[C@]1([H])C[C@]3([H])[C@](C)(O)C(C(Cl)=CC=C4O)=C4C(O)=C3C2=O	InChI=1S/C22H23ClN2O8/c1-21(32)7-6-8-15(25(2)3)17(28)13(20(24)31)19(30)22(8,33)18(29)11(7)16(27)12-10(26)5-4-9(23)14(12)21/h4-5,7-8,15,26-27,30,32-33H,6H2,1-3H3,(H2,24,31)/t7-,8-,15-,21-,22-/m0/s1	DHPRQBPJLMKORJ-XRNKAMNCSA-N
oxytetracycline	**3.02**		O=C(C(C(N)=O)=C(O)[C@]12O)[C@@H](N(C)C)[C@]1([H])[C@@H](O)[C@]3([H])[C@](C)(O)C(C=CC=C4O)=C4C(O)=C3C2=O	InChI=1S/C22H24N2O9/c1-21(32)7-5-4-6-8(25)9(7)15(26)10-12(21)17(28)13-14(24(2)3)16(27)11(20(23)31)19(30)22(13,33)18(10)29/h4-6,12-14,17,25-26,28,30,32-33H,1-3H3,(H2,23,31)/t12-,13-,14+,17+,21-,22+/m1/s1	OWFJMIVZYSDULZ-PXOLEDIWSA-N
tetracycline	**3.03**		O=C(C(C(N)=O)=C(O)[C@]12O)[C@@H](N(C)C)[C@]1([H])C[C@]3([H])[C@](C)(O)C(C=CC=C4O)=C4C(O)=C3C2=O	InChI=1S/C22H24N2O8/c1-21(31)8-5-4-6-11(25)12(8)16(26)13-9(21)7-10-15(24(2)3)17(27)14(20(23)30)19(29)22(10,32)18(13)28/h4-6,9-10,15,25-26,29,31-32H,7H2,1-3H3,(H2,23,30)/t9-,10-,15-,21+,22-/m0/s1	NWXMGUDVXFXRIG-WESIUVDSSA-N
rolitetracycline	**3.04**		O=C(C(C(NCN1CCCC1)=O)=C(O)[C@]23O)[C@@H](N(C)C)[C@]2([H])C[C@]4([H])[C@](C)(O)C(C=CC=C5O)=C5C(O)=C4C3=O	InChI=1S/C27H33N3O8/c1-26(37)13-7-6-8-16(31)17(13)21(32)18-14(26)11-15-20(29(2)3)22(33)19(24(35)27(15,38)23(18)34)25(36)28-12-30-9-4-5-10-30/h6-8,14-15,20,31-32,35,37-38H,4-5,9-12H2,1-3H3,(H,28,36)/t14-,15-,20-,26+,27-/m0/s1	IKQRPFTXKQQLJF-IAHYZSEUSA-N

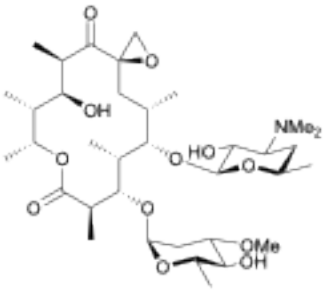
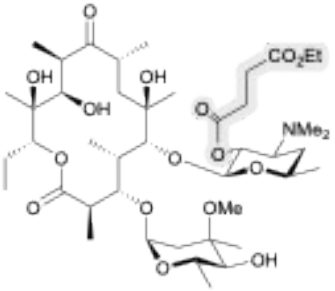
Name	#	Chemdraw	SMILES	InChI	InChIKey
demeclocycline	**3.05**		O=C(C(C(N)=O)=C(O)[C@]12O)[C@@H](N(C)C)[C@]1([H])C[C@]3([H])[C@H](O)C(C(Cl)=CC=C4O)=C4C(O)=C3C2=O	InChI=1S/C21H21ClN2O8/c1-24(2)14-7-5-6-10(16(27)12-9(25)4-3-8(22)11(12)15(6)26)18(29)21(7,32)19(30)13(17(14)28)20(23)31/h3-4,6-7,14-15,25-27,30,32H,5H2,1-2H3,(H2,23,31)/t6-,7-,14-,15-,21-/m0/s1	GUXHBMASAHGULD-SEYHBJAFSA-N
pipacycline	**3.06**		O=C(C(C(NCN1CCN(CC1)CCO)=O)=C(O)[C@]23O)[C@@H](N(C)C)[C@]2([H])C[C@]4([H])[C@](C)(O)C(C=CC=C5O)=C5C(O)=C4C3=O	InChI=1S/C29H38N4O9/c1-28(41)15-5-4-6-18(35)19(15)23(36)20-16(28)13-17-22(31(2)3)24(37)21(26(39)29(17,42)25(20)38)27(40)30-14-33-9-7-32(8-10-33)11-12-34/h4-6,16-17,22,34-36,39,41-42H,7-14H2,1-3H3,(H,30,40)/t16-,17-,22-,28+,29-/m0/s1	RAUQZDNDLCIQFJ-REHNUXHNSA-N
lymecycline	**3.07**		O=C(C(C(NCNCCCC[C@@H](C(O)=O)N)=O)=C(O)[C@]12O)[C@@H](N(C)C)[C@]1([H])C[C@]3([H])[C@](C)(O)C(C=CC=C4O)=C4C(O)=C3C2=O	InChI=1S/C29H38N4O10/c1-28(42)13-7-6-9-17(34)18(13)22(35)19-14(28)11-15-21(33(2)3)23(36)20(25(38)29(15,43)24(19)37)26(39)32-12-31-10-5-4-8-16(30)27(40)41/h6-7,9,14-16,21,31,34-35,38,42-43H,4-5,8,10-12,30H2,1-3H3,(H,32,39)(H,40,41)/t14-,15-,16-,21-,28+,29-/m0/s1	PZTCVADFMACKLU-UEPZRUIBSA-N

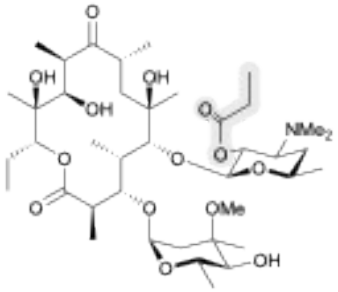
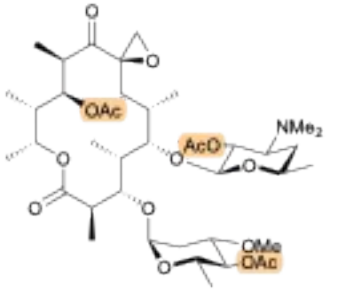
Name	#	Chemdraw	SMILES	InChI	InChIKey
clomocycline	**3.08**		O=C(C(C(NCO)=O)=C(O)[C@]12O)[C@@H](N(C)C)[C@]1([H])C[C@]3([H])[C@](C)(O)C(C(Cl)=CC=C4O)=C4C(O)=C3C2=O	InChI=1S/C23H25ClN2O9/c1-22(34)8-6-9-16(26(2)3)18(30)14(21(33)25-7-27)20(32)23(9,35)19(31)12(8)17(29)13-11(28)5-4-10(24)15(13)22/h4-5,8-9,16,27-29,32,34-35H,6-7H2,1-3H3,(H,25,33)/t8-,9-,16-,22-,23-/m0/s1	BXTHDFJCJQJHKD-KMVLDZISSA-N
morphocycline	**3.09**		O=C(C(C(NCN1CCOCC1)=O)=C(O)[C@]23O)[C@@H](N(C)C)[C@]2([H])C[C@]4([H])[C@](C)(O)C(C=CC=C5O)=C5C(O)=C4C3=O	InChI=1S/C27H33N3O9/c1-26(37)13-5-4-6-16(31)17(13)21(32)18-14(26)11-15-20(29(2)3)22(33)19(24(35)27(15,38)23(18)34)25(36)28-12-30-7-9-39-10-8-30/h4-6,14-15,20,31-32,35,37-38H,7-12H2,1-3H3,(H,28,36)/t14-,15-,20-,26+,27-/m0/s1	WUOOCVIWLSUJPF-IAHYZSEUSA-N
guamecycline	**3.10**		O=C(C(C(NCN1CCN(CC1)C(NC(N)=N)=N)=O)=C(O)[C@]23O)[C@@H](N(C)C)[C@]2([H])C[C@]4([H])[C@](C)(O)C(C=CC=C5O)=C5C(O)=C4C3=O	InChI=1S/C29H38N8O8/c1-28(44)13-5-4-6-16(38)17(13)21(39)18-14(28)11-15-20(35(2)3)22(40)19(24(42)29(15,45)23(18)41)25(43)33-12-36-7-9-37(10-8-36)27(32)34-26(30)31/h4-6,14-15,20,38-39,42,44-45H,7-12H2,1-3H3,(H,33,43)(H5,30,31,32,34)/t14-,15-,20-,28+,29-/m0/s1	FAMUIRDLAWWMCQ-AQFAATAFSA-N

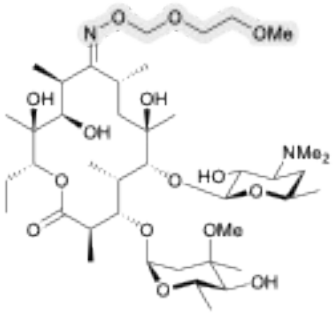
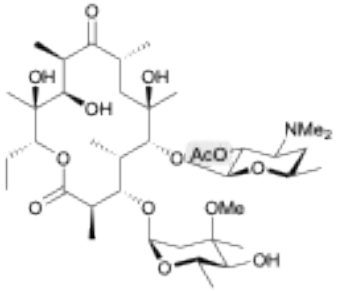
Name	#	Chemdraw	SMILES	InChI	InChIKey
methacycline	**3.11**		O=C(C(C(N)=O)=C(O)[C@@]1(O)C(C2=C(O)C3=C4C=CC=C3O)=O)[C@@H](N(C)C)[C@]1([H])[C@@H](O)[C@]2([H])C4=C	InChI=1S/C22H22N2O8/c1-7-8-5-4-6-9(25)11(8)16(26)12-10(7)17(27)14-15(24(2)3)18(28)13(21(23)31)20(30)22(14,32)19(12)29/h4-6,10,14-15,17,25-27,30,32H,1H2,2-3H3,(H2,23,31)/t10-,14-,15+,17+,22+/m1/s1	XIYOPDCBBDCGOE-IWVLMIASSA-N
doxycycline	**3.12**		O=C(C(C(N)=O)=C(O)[C@]12O)[C@@H](N(C)C)[C@]1([H])[C@@H](O)[C@]3([H])[C@@H](C)C(C=CC=C4O)=C4C(O)=C3C2=O	InChI=1S/C22H24N2O8/c1-7-8-5-4-6-9(25)11(8)16(26)12-10(7)17(27)14-15(24(2)3)18(28)13(21(23)31)20(30)22(14,32)19(12)29/h4-7,10,14-15,17,25-27,30,32H,1-3H3,(H2,23,31)/t7-,10+,14+,15-,17-,22-/m0/s1	SGKRLCUYIXIAHR-AKNGSSGZSA-N
minocycline	**3.13**		[H][C@@]1(C2)C(C(C3=C2C(N(C)C)=CC=C3O)=O)=C(O)[C@@](C(O)=C(C(N)=O)C([C@H]4N(C)C)=O)(O)[C@]4(C1)[H]	InChI=1S/C23H27N3O7/c1-25(2)12-5-6-13(27)15-10(12)7-9-8-11-17(26(3)4)19(29)16(22(24)32)21(31)23(11,33)20(30)14(9)18(15)28/h5-6,9,11,17,27,30-31,33H,7-8H2,1-4H3,(H2,24,32)/t9-,11-,17-,23-/m0/s1	KXEYSKGUYBJHIZ-KVUCHLLUSA-N
meclocycline	**3.14**		O=C(C(C(N)=O)=C(O)[C@@]1(O)C(C2=C(O)C3=C4C(Cl)=CC=C3O)=O)[C@@H](N(C)C)[C@]1([H])[C@@H](O)[C@]2([H])C4=C	InChI=1S/C22H21ClN2O8/c1-6-9-7(23)4-5-8(26)11(9)16(27)12-10(6)17(28)14-15(25(2)3)18(29)13(21(24)31)20(30)22(14,32)19(12)29/h4-5,10,14-15,17,26-28,31,33H,1H2,2-3H3,(H2,24,32)/t10-,14-,15+,17+,22+/m1/s1	RNIADBXQDMCFEN-IWVLMIASSA-N

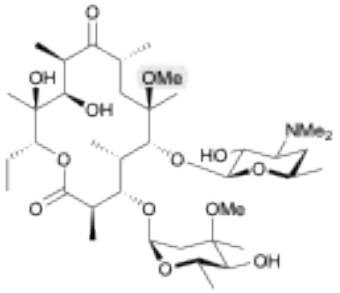
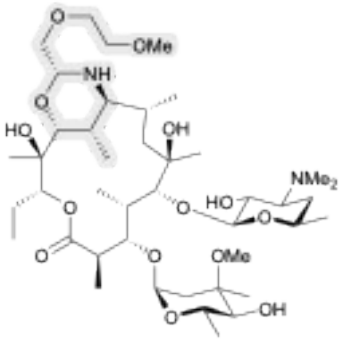
Name	#	Chemdraw	SMILES	InChI	InChIKey
tigecycline	**3.15**		[H][C@@]1(C2)C(C(C3=C2C(N(C)C)=CC(NC(CNC(C)(C)C)=O)=C3O)=O)=C(O)[C@@](C(O)=C(C(N)=O)C([C@H]4N(C)C)=O)(O)[C@]4(C1)[H]	InChI=1S/C29H39N5O8/c1-28(2,3)31-11-17(35)32-15-10-16(33(4)5)13-8-12-9-14-21(34(6)7)24(38)20(27(30)41)26(40)29(14,42)25(39)18(12)23(37)19(13)22(15)36/h10,12,14,21,31,36,39-40,42H,8-9,11H2,1-7H3,(H2,30,41)(H,32,35)/t12-,14-,21-,29-/m0/s1	ASQYYRVLGXHYQR-HJYUBDRYSA-N
omadacycline	**3.16**		[H][C@@]1(C2)C(C(C3=C2C(N(C)C)=CC(CNCC(C)(C)C)=C3O)=O)=C(O)[C@@](C(O)=C(C(N)=O)C([C@H]4N(C)C)=O)(O)[C@]4(C1)[H]	InChI=1S/C29H40N4O7/c1-28(2,3)12-31-11-14-10-17(32(4)5)15-8-13-9-16-21(33(6)7)24(36)20(27(30)39)26(38)29(16,40)25(37)18(13)23(35)19(15)22(14)34/h10,13,16,21,31,34,37-38,40H,8-9,11-12H2,1-7H3,(H2,30,39)/t13-,16-,21-,29-/m0/s1	YKVKHWYMBCFFSU-IQZGDKDPSA-N
sarecycline	**3.17**		[H][C@@]1(C2)C(C(C3=C2C(CN(C)OC)=CC=C3O)=O)=C(O)[C@@](C(O)=C(C(N)=O)C([C@H]4N(C)C)=O)(O)[C@]4(C1)[H]	InChI=1S/C24H29N3O8/c1-26(2)18-13-8-11-7-12-10(9-27(3)35-4)5-6-14(28)16(12)19(29)15(11)21(31)24(13,34)22(32)17(20(18)30)23(25)33/h5-6,11,13,18,28,31-32,34H,7-9H2,1-4H3,(H2,25,33)/t11-,13-,18-,24-/m0/s1	RNHLDTBWWMIPIL-SBAJWEJLSA-N
eravacycline	**3.18**		[H][C@@]1(C2)C(C(C3=C2C(F)=CC(NC(CN4CCCC4)=O)=C3O)=O)=C(O)[C@@](C(O)=C(C(N)=O)C([C@H]5N(C)C)=O)(O)[C@]5(C1)[H]	InChI=1S/C27H31FN4O8/c1-31(2)20-13-8-11-7-12-14(28)9-15(30-16(33)10-32-5-3-4-6-32)21(34)18(12)22(35)17(11)24(37)27(13,40)25(38)19(23(20)36)26(29)39/h9,11,13,20,34,37-38,40H,3-8,10H2,1-2H3,(H2,29,39)(H,30,33)/t11-,13-,20-,27-/m0/s1	NDRFSXNBDFIZPT-ISIOAQNYSA-N

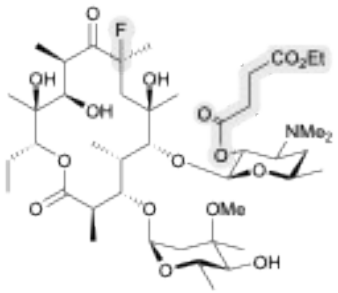
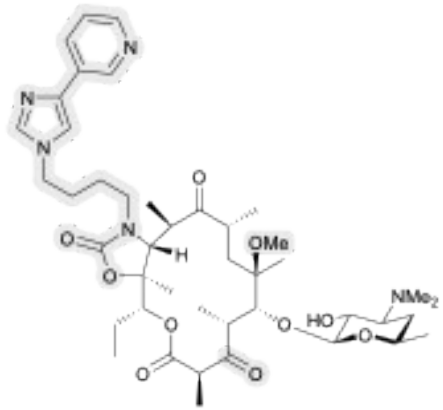
Name	#	Chemdraw	SMILES	InChI	InChIKey
erythromycin	**4.01**		O[C@@H]([C@@](O)(C)[C@@H](CC)O1)[C@@H](C)C([C@H](C)C[C@](O)(C)[C@H](O[C@H]2[C@H](O)[C@@H](N(C)C)C[C@@H](C)O2)[C@@H](C)[C@H](O[C@@H]3O[C@@H](C)[C@H](O)[C@](C)(OC)C3)[C@@H](C)C1=O)=O	InChI=1S/C37H67NO13/c1-14-25-37(10,45)30(41)20(4)27(39)18(2)16-35(8,44)32(51-34-28(40)24(38(11)12)15-19(3)47-34)21(5)29(22(6)33(43)49-25)50-26-17-36(9,46-13)31(42)23(7)48-26/h18-26,28-32,34,40-42,44-45H,14-17H2,1-13H3/t18-,19-,20+,21+,22-,23+,24+,25-,26+,28-,29+,30-,31+,32-,34+,35-,36-,37-/m1/s1	ULGZDMOVFRHVEP-RWJQBGPGSA-N
erythromycin ethylcarbonate	**4.02**		O[C@@H]([C@@](O)(C)[C@@H](CC)O1)[C@@H](C)C([C@H](C)C[C@](O)(C)[C@H](O[C@H]2[C@H](OC(OCC)=O)[C@@H](N(C)C)C[C@@H](C)O2)[C@@H](C)[C@H](O[C@@H]3O[C@@H](C)[C@H](O)[C@](C)(OC)C3)[C@@H](C)C1=O)=O	InChI=1S/C40H71NO15/c1-15-27-40(11,48)32(43)22(5)29(42)20(3)18-38(9,47)34(56-36-31(55-37(46)50-16-2)26(41(12)13)17-21(4)51-36)23(6)30(24(7)35(45)53-27)54-28-19-39(10,49-14)33(44)25(8)52-28/h20-28,30-34,36,43-44,47-48H,15-19H2,1-14H3/t20-,21-,22+,23+,24-,25+,26+,27-,28+,30+,31-,32-,33+,34-,36+,38-,39-,40-/m1/s1	BSUQCLSFQSUNED-PPPRQHODSA-N

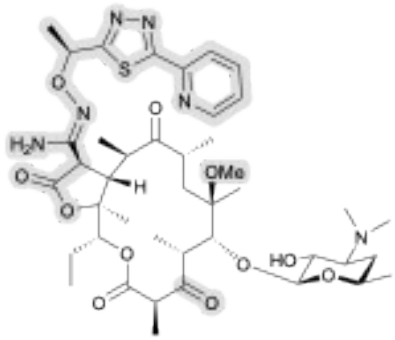
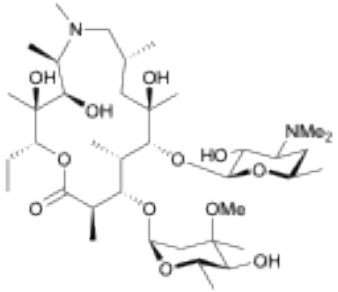
Name	#	Chemdraw	SMILES	InChI	InChIKey
oleandomycin	**4.03**		O=C1[C@@]2(C[C@@H]([C@@H]([C@H]([C@@H]([C@H](C(O[C@@H]([C@@H]([C@@H]([C@H]1C)O)C)C)=O)C)O[C@@H]3O[C@@H](C)[C@@H](O)[C@@H](OC)C3)C)O[C@H](O4)[C@H](O)[C@@H](N(C)C)C[C@H]4C)C)CO2	InChI=1S/C35H61NO12/c1-16-14-35(15-43-35)32(40)19(4)27(37)18(3)22(7)46-33(41)21(6)31(47-26-13-25(42-11)28(38)23(8)45-26)20(5)30(16)48-34-29(39)24(36(9)10)12-17(2)44-34/h16-31,34,37-39H,12-15H2,1-11H3/t16-,17+,18-,19+,20+,21+,22+,23-,24-,25-,26-,27-,28-,29+,30-,31-,34-,35+/m0/s1	RZPAKFUAFGMUPI-QESOVKLGSA-N
erythromycin ethylsuccinate	**4.04**		O[C@@H]([C@@](O)(C)[C@@H](CC)O1)[C@@H](C)C([C@H](C)C[C@](O)(C)[C@H](O[C@H]2[C@H](OC(CCC(OCC)=O)=O)[C@@H](N(C)C)C[C@@H](C)O2)[C@@H](C)[C@H](O[C@@H]3O[C@@H](C)[C@H](O)[C@](C)(OC)C3)[C@@H](C)C1=O)=O	InChI=1S/C43H75NO16/c1-15-29-43(11,52)36(48)24(5)33(47)22(3)20-41(9,51)38(25(6)34(26(7)39(50)57-29)59-32-21-42(10,53-14)37(49)27(8)56-32)60-40-35(28(44(12)13)19-23(4)55-40)58-31(46)18-17-30(45)54-16-2/h22-29,32,34-38,40,48-49,51-52H,15-21H2,1-14H3/t22-,23-,24+,25+,26-,27+,28+,29-,32+,34+,35-,36-,37+,38-,40+,41-,42-,43-/m1/s1	NSYZCCDSJNWWJL-YXOIYICCSA-N

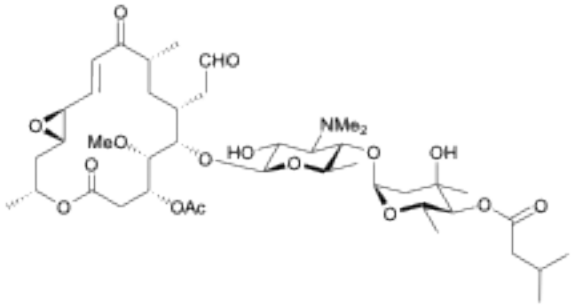
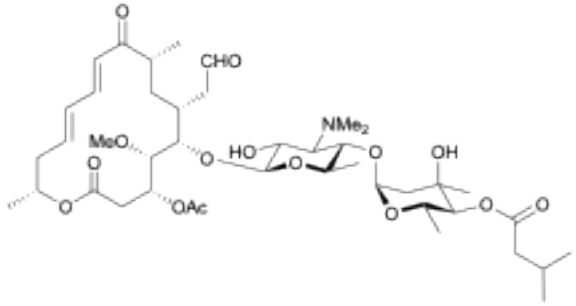
Name	#	Chemdraw	SMILES	InChI	InChIKey
erythromycin estolate	**4.05**		O[C@@H]([C@@](O)(C)[C@@H](CC)O1)[C@@H](C)C([C@H](C)C[C@](O)(C)[C@H](O[C@H]2[C@H](OC(CC)=O)[C@@H](N(C)C)C[C@@H](C)O2)[C@@H](C)[C@H](O[C@@H]3O[C@@H](C)[C@H](O)[C@](C)(OC)C3)[C@@H](C)C1=O)=O	InChI=1S/C40H71NO14/c1-15-27-40(11,48)33(44)22(5)30(43)20(3)18-38(9,47)35(55-37-32(53-28(42)16-2)26(41(12)13)17-21(4)50-37)23(6)31(24(7)36(46)52-27)54-29-19-39(10,49-14)34(45)25(8)51-29/h20-27,29,31-35,37,44-45,47-48H,15-19H2,1-14H3/t20-,21-,22+,23+,24-,25+,26+,27-,29+,31+,32-,33-,34+,35-,37+,38-,39-,40-/m1/s1	TYQXKHPOXXXCTP-CSLYCKPJSA-N
troleandomycin	**4.06**		O=C1[C@@]2(C[C@@H]([C@@H]([C@H]([C@@H]([C@H](C(O[C@@H]([C@@H]([C@@H]([C@H]1C)OC(C)=O)C)C)=O)C)O[C@@H]3O[C@@H](C)[C@H](OC(C)=O)[C@@H](OC)C3)C)O[C@H](O4)[C@H](OC(C)=O)[C@@H](N(C)C)C[C@H]4C)C)CO2	InChI=1S/C41H67NO15/c1-19-17-41(18-49-41)38(46)23(5)34(53-27(9)43)21(3)25(7)52-39(47)24(6)35(56-32-16-31(48-14)36(26(8)51-32)54-28(10)44)22(4)33(19)57-40-37(55-29(11)45)30(42(12)13)15-20(2)50-40/h19-26,30-37,40H,15-18H2,1-14H3/t19-,20+,21-,22+,23+,24+,25+,26-,30-,31-,32-,33-,34-,35-,36-,37+,40-,41+/m0/s1	LQCLVBQBTUVCEQ-QTFUVMRISA-N

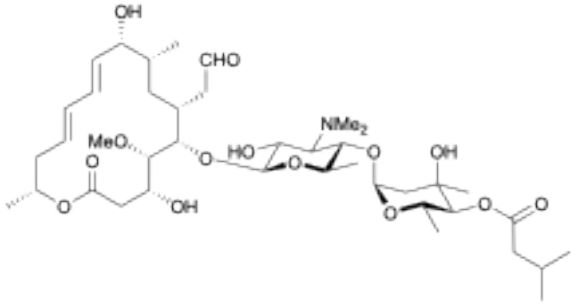
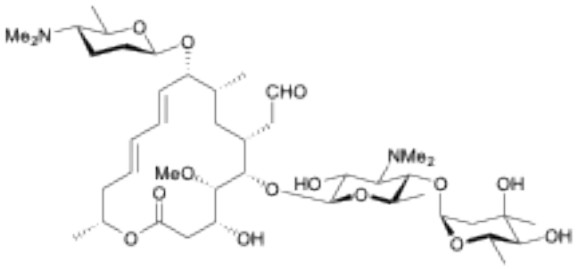
Name	#	Chemdraw	SMILES	InChI	InChIKey
roxithromycin	**4.07**		O[C@@H]([C@@](O)(C)[C@@H](CC)O1)[C@@H](C)/C([C@H](C)C[C@](O)(C)[C@H](O[C@H]2[C@H](O)[C@@H](N(C)C)C[C@@H](C)O2)[C@@H](C)[C@H](O[C@@H]3O[C@@H](C)[C@H](O)[C@](C)(OC)C3)[C@@H](C)C1=O)=N/OCOCCOC	InChI=1S/C41H76N2O15/c1-15-29-41(10,49)34(45)24(4)31(42-53-21-52-17-16-50-13)22(2)19-39(8,48)36(58-38-32(44)28(43(11)12)18-23(3)54-38)25(5)33(26(6)37(47)56-29)57-30-20-40(9,51-14)35(46)27(7)55-30/h22-30,32-36,38,44-46,48-49H,15-21H2,1-14H3/b42-31+/t22-,23-,24+,25+,26-,27+,28+,29-,30+,32-,33+,34-,35+,36-,38+,39-,40-,41-/m1/s1	RXZBMPWDPOLZGW-XMRMVWPWSA-N
erythromycin acistrate	**4.08**		O[C@@H]([C@@](O)(C)[C@@H](CC)O1)[C@@H](C)C([C@H](C)C[C@](O)(C)[C@H](O[C@H]2[C@H](OC(C)=O)[C@@H](N(C)C)C[C@@H](C)O2)[C@@H](C)[C@H](O[C@@H]3O[C@@H](C)[C@H](O)[C@](C)(OC)C3)[C@@H](C)C1=O)=O	InChI=1S/C39H69NO14/c1-15-27-39(11,47)32(43)21(4)29(42)19(2)17-37(9,46)34(54-36-31(51-25(8)41)26(40(12)13)16-20(3)49-36)22(5)30(23(6)35(45)52-27)53-28-18-38(10,48-14)33(44)24(7)50-28/h19-24,26-28,30-34,36,43-44,46-47H,15-18H2,1-14H3/t19-,20-,21+,22+,23-,24+,26+,27-,28+,30+,31-,32-,33+,34-,36+,37-,38-,39-/m1/s1	CVBHEIRZLPKMSH-SNWVVRALSA-N

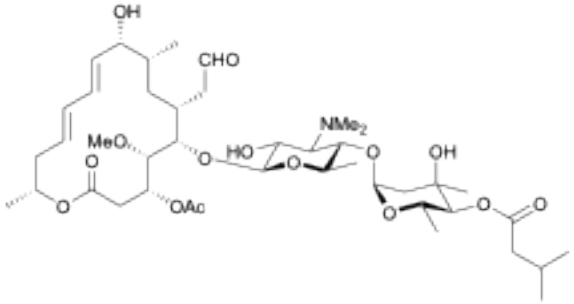
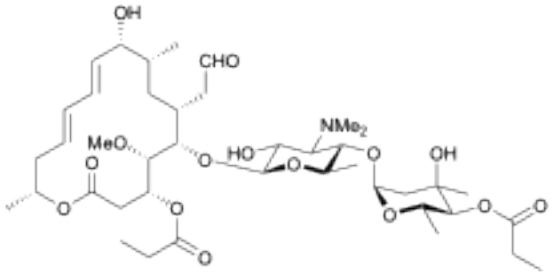
Name	#	Chemdraw	SMILES	InChI	InChIKey
clarithromycin	**4.09**		O[C@@H]([C@@](O)(C)[C@@H](CC)O1)[C@@H](C)C([C@H](C)C[C@@](C)(OC)[C@H](O[C@H]2[C@H](O)[C@@H](N(C)C)C[C@@H](C)O2)[C@@H](C)[C@H](O[C@@H]3O[C@@H](C)[C@H](O)[C@](C)(OC)C3)[C@@H](C)C1=O)=O	InChI=1S/C38H69NO13/c1-15-26-38(10,45)31(42)21(4)28(40)19(2)17-37(9,47-14)33(52-35-29(41)25(39(11)12)16-20(3)48-35)22(5)30(23(6)34(44)50-26)51-27-18-36(8,46-13)32(43)24(7)49-27/h19-27,29-33,35,41-43,45H,15-18H2,1-14H3/t19-,20-,21+,22+,23-,24+,25+,26-,27+,29-,30+,31-,32+,33-,35+,36-,37-,38-/m1/s1	AGOYDEPGAOXOCK-KCBOHYOISA-N
dirithromycin	**4.10**		O[C@@]([C@@H](CC)O1)(C)[C@H]2[C@@H](C)[C@H]([C@H](C)C[C@](O)(C)[C@H](O[C@H]3[C@H](O)[C@@H](N(C)C)C[C@@H](C)O3)[C@@H](C)[C@H](O[C@@H]4O[C@@H](C)[C@H](O)[C@](C)(OC)C4)[C@@H](C)C1=O)N[C@@H](COCCOC)O2	InChI=1S/C42H78N2O14/c1-15-29-42(10,49)37-24(4)32(43-30(56-37)21-52-17-16-50-13)22(2)19-40(8,48)36(58-39-33(45)28(44(11)12)18-23(3)53-39)25(5)34(26(6)38(47)55-29)57-31-20-41(9,51-14)35(46)27(7)54-31/h22-37,39,43,45-46,48-49H,15-21H2,1-14H3/t22-,23-,24+,25+,26-,27+,28+,29-,30-,31+,32+,33-,34+,35+,36-,37-,39+,40-,41-,42-/m1/s1	WLOHNSSYAXHWNR-DWIOZXRMSA-N

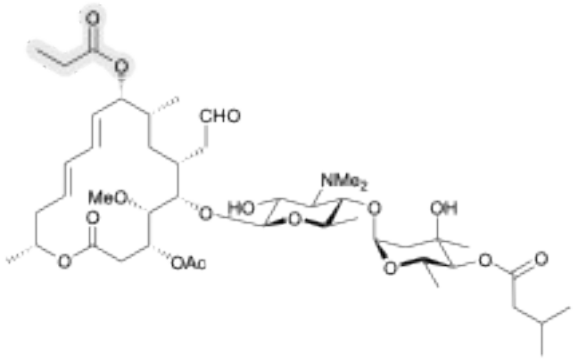
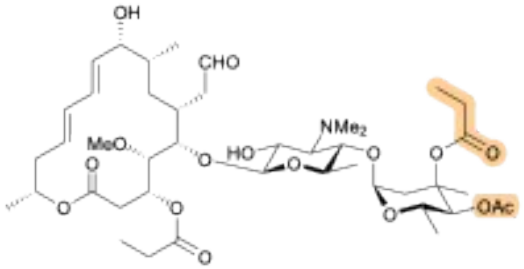
Name	#	Chemdraw	SMILES	InChI	InChIKey
flurithromycin ethylsuccinate	**4.11**		O[C@@H]([C@@](O)(C)[C@@H](CC)O1)[C@@H](C)C([C@@](C)(F)C[C@](O)(C)[C@H](O[C@H]2[C@H](OC(CCC(OCC)=O)=O)[C@@H](N(C)C)C[C@@H](C)O2)[C@@H](C)[C@H](O[C@@H]3O[C@@H](C)[C@H](O)[C@](C)(OC)C3)[C@@H](C)C1=O)=O	InChI=1S/C43H74FNO16/c1-15-28-43(11,53)35(49)25(6)34(48)40(8,44)21-41(9,52)37(23(4)32(24(5)38(51)58-28)60-31-20-42(10,54-14)36(50)26(7)57-31)61-39-33(27(45(12)13)19-22(3)56-39)59-30(47)18-17-29(46)55-16-2/h22-28,31-33,35-37,39,49-50,52-53H,15-21H2,1-14H3/t22-,23+,24-,25+,26+,27+,28-,31+,32+,33-,35-,36+,37-,39+,40+,41-,42-,43-/m1/s1	GFIQERTUSVTTRE-HCTDEEJFSA-N
telithromycin	**4.12**		O=C([C@H](C)[C@@]([C@@](O1)(C)[C@@H](CC)OC([C@@H]2C)=O)([H])N(CCCCN3C=NC(C4=CC=CN=C4)=C3)C1=O)[C@H](C)C[C@@](C)(OC)[C@H](O[C@H]5[C@H](O)[C@@H](N(C)C)C[C@@H](C)O5)[C@@H](C)C2=O	InChI=1S/C43H65N5O10/c1-12-33-43(8)37(48(41(53)58-43)19-14-13-18-47-23-31(45-24-47)30-16-15-17-44-22-30)27(4)34(49)25(2)21-42(7,54-11)38(28(5)35(50)29(6)39(52)56-33)57-40-36(51)32(46(9)10)20-26(3)55-40/h15-17,22-29,32-33,36-38,40,51H,12-14,18-21H2,1-11H3/t25-,26-,27+,28+,29-,32+,33-,36-,37-,38-,40+,42-,43-/m1/s1	LJVAJPDWBABPEJ-PNUFFHFMSA-N

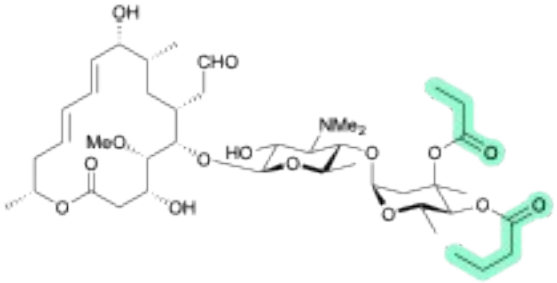
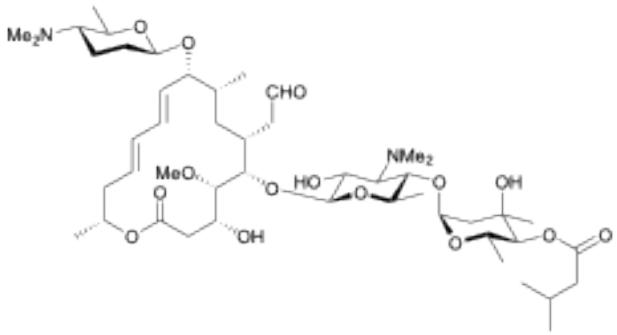
Name	#	Chemdraw	SMILES	InChI	InChIKey
nafithromycin	**4.13**		O=C1[C@@H]([C@]([C@@H]2/C(N)=N/O[C@@H](C)C3=NN=C(C4=NC=CC=C4)S3)([H])[C@](OC2=O)([C@H](OC([C@H](C)C([C@H](C)[C@@H](O[C@H](O[C@@H](C5)C)[C@H](O)[C@H]5N(C)C)[C@](C)(OC)C[C@H]1C)=O)=O)CC)C)C	InChI=1S/C42H62N6O11S/c1-13-28-42(9)30(29(39(53)58-42)35(43)47-59-25(7)36-45-46-37(60-36)26-16-14-15-17-44-26)22(4)31(49)20(2)19-41(8,54-12)34(23(5)32(50)24(6)38(52)56-28)57-40-33(51)27(48(10)11)18-21(3)55-40/h14-17,20-25,27-30,33-34,40,51H,13,18-19H2,1-12H3,(H2,43,47)/t20-,21-,22-,23+,24-,25+,27+,28-,29-,30+,33-,34-,40+,41-,42-/m1/s1	RLFCSBSRGRJFRO-QAOQTAGDSA-N
azithromycin	**4.14**		O[C@@H]([C@@](O)(C)[C@@H](CC)OC([C@H](C)[C@@H](O[C@@H]1O[C@@H](C)[C@H](O)[C@](C)(OC)C1)[C@H](C)[C@@H](O[C@H]2[C@H](O)[C@@H](N(C)C)C[C@@H](C)O2)[C@@](O)(C)C[C@H]3C)=O)[C@H](N(C)C3)C	InChI=1S/C38H72N2O12/c1-15-27-38(10,46)31(42)24(6)40(13)19-20(2)17-36(8,45)33(52-35-29(41)26(39(11)12)16-21(3)48-35)22(4)30(23(5)34(44)50-27)51-28-18-37(9,47-14)32(43)25(7)49-28/h20-33,35,41-43,45-46H,15-19H2,1-14H3/t20-,21-,22+,23-,24-,25+,26+,27-,28+,29-,30+,31-,32+,33-,35+,36-,37-,38-/m1/s1	MQTOSJVFKKJCRP-BICOPXKESA-N

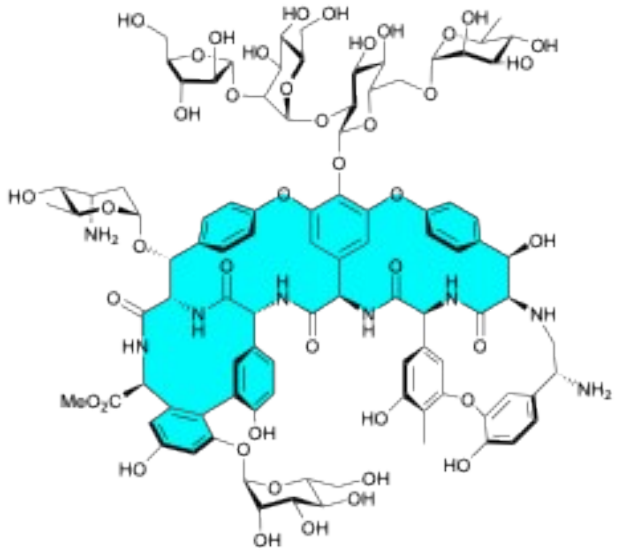
Name	#	Chemdraw	SMILES	InChI	InChIKey
carbomycin A	**4.15a**		C[C@@H]1C[C@H]2[C@@H](O2)/C=C/C([C@H](C)C[C@H](CC=O)[C@H](O[C@H]3[C@H](O)[C@@H](N(C)C)[C@H](O[C@@H]4O[C@@H](C)[C@H](OC(CC(C)C)=O)[C@@](O)(C)C4)[C@@H](C)O3)[C@@H](OC)[C@H](OC(C)=O)CC(O1)=O)=O	InChI=1S/C42H67NO16/c1-21(2)16-32(47)57-40-25(6)53-34(20-42(40,8)50)58-37-24(5)54-41(36(49)35(37)43(9)10)59-38-27(14-15-44)17-22(3)28(46)12-13-29-30(56-29)18-23(4)52-33(48)19-31(39(38)51-11)55-26(7)45/h12-13,15,21-25,27,29-31,34-41,49-50H,14,16-20H2,1-11H3/b13-12+/t22-,23-,24-,25+,27+,29+,30+,31-,34+,35-,36-,37-,38+,39+,40+,41+,42-/m1/s1	FQVHOULQCKDUCY-OGHXVOSASA-N
carbomycin B	**4.15b**		C[C@@H]1C/C=C/C=C/C([C@H](C)C[C@H](CC=O)[C@H](O[C@H]2[C@H](O)[C@@H](N(C)C)[C@H](O[C@@H]3O[C@@H](C)[C@H](OC(CC(C)C)=O)[C@@](O)(C)C3)[C@@H](C)O2)[C@@H](OC)[C@H](OC(C)=O)CC(O1)=O)=O	InChI=1S/C42H67NO15/c1-23(2)19-32(47)56-40-27(6)53-34(22-42(40,8)50)57-37-26(5)54-41(36(49)35(37)43(9)10)58-38-29(17-18-44)20-24(3)30(46)16-14-12-13-15-25(4)52-33(48)21-31(39(38)51-11)55-28(7)45/h12-14,16,18,23-27,29,31,34-41,49-50H,15,17,19-22H2,1-11H3/b13-12+,16-14+/t24-,25-,26-,27+,29+,31-,34+,35-,36-,37-,38+,39+,40+,41+,42-/m1/s1	ZRNXEMIDBIPJDC-HLPDZUSBSA-N

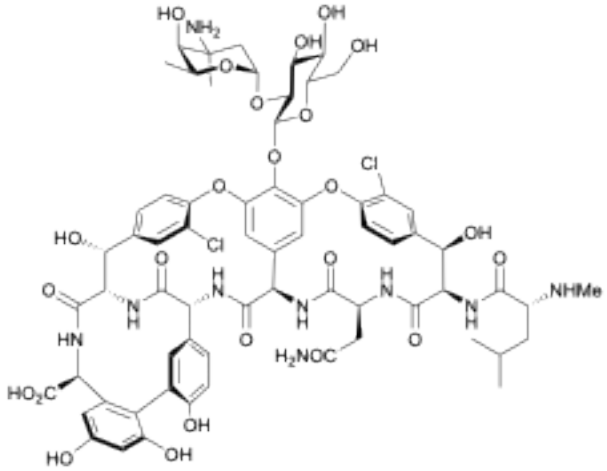
Name	#	Chemdraw	SMILES	InChI	InChIKey
leucomycin A_1	**4.16a**		C[C@@H]1C/C=C/C=C/[C@H](O)[C@H](C)C[C@H](CC=O)[C@H](O[C@H]2[C@H](O)[C@@H](N(C)C)[C@H](O[C@@H]3O[C@@H](C)[C@H](OC(CC(C)C)=O)[C@@](O)(C)C3)[C@@H](C)O2)[C@@H](OC)[C@H](O)CC(O1)=O	InChI=1S/C40H67NO14/c1-22(2)18-30(45)53-38-26(6)51-32(21-40(38,7)48)54-35-25(5)52-39(34(47)33(35)41(8)9)55-36-27(16-17-42)19-23(3)28(43)15-13-11-12-14-24(4)50-31(46)20-29(44)37(36)49-10/h11-13,15,17,22-29,32-39,43-44,47-48H,14,16,18-21H2,1-10H3/b12-11+,15-13+/t23-,24-,25-,26+,27+,28+,29-,32+,33-,34-,35-,36+,37+,38+,39+,40-/m1/s1	IEMDOFXTVAPVLX-YWQHLDGFSA-N
spiramycin I	**4.17**		C[C@@H]1C/C=C/C=C/[C@H](O[C@H]2CC[C@H](N(C)C)[C@@H](C)O2)[C@H](C)C[C@H](CC=O)[C@H](O[C@H]3[C@H](O)[C@@H](N(C)C)[C@H](O[C@@H]4O[C@@H](C)[C@H](O)[C@@](O)(C)C4)[C@@H](C)O3)[C@@H](OC)[C@H](O)CC(O1)=O	InChI=1S/C43H74N2O14/c1-24-21-29(19-20-46)39(59-42-37(49)36(45(9)10)38(27(4)56-42)58-35-23-43(6,51)41(50)28(5)55-35)40(52-11)31(47)22-33(48)53-25(2)15-13-12-14-16-32(24)57-34-18-17-30(44(7)8)26(3)54-34/h12-14,16,20,24-32,34-42,47,49-51H,15,17-19,21-23H2,1-11H3/b13-12+,16-14+/t24-,25-,26-,27-,28+,29+,30+,31-,32+,34+,35+,36-,37-,38-,39+,40+,41+,42+,43-/m1/s1	ACTOXUHEUCPTEW-CEUOBAOPSA-N

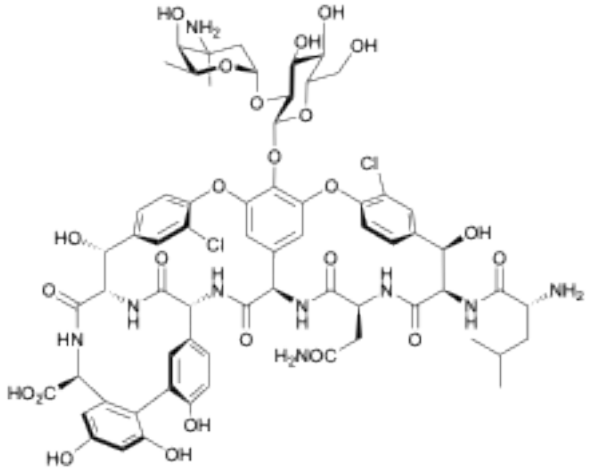
Name	#	Chemdraw	SMILES	InChI	InChIKey
josamycin	**4.18**		C[C@@H]1C/C=C/C=C/[C@H](O)[C@H](C)C[C@H](CC=O)[C@H](O[C@H]2[C@H](O)[C@@H](N(C)C)[C@H](O[C@@H]3O[C@@H](C)[C@H](OC(CC(C)C)=O)[C@@](O)(C)C3)[C@@H](C)O2)[C@@H](OC)[C@H](OC(C)=O)CC(O1)=O	InChI=1S/C42H69NO15/c1-23(2)19-32(47)56-40-27(6)53-34(22-42(40,8)50)57-37-26(5)54-41(36(49)35(37)43(9)10)58-38-29(17-18-44)20-24(3)30(46)16-14-12-13-15-25(4)52-33(48)21-31(39(38)51-11)55-28(7)45/h12-14,16,18,23-27,29-31,34-41,46,49-50H,15,17,19-22H2,1-11H3/b13-12+,16-14+/t24-,25-,26-,27+,29+,30+,31-,34+,35-,36-,37-,38+,39+,40+,41+,42-/m1/s1	XJSFLOJWULLJQS-NGVXBBESSA-N
midecamycin A1	**4.19**		C[C@@H]1C/C=C/C=C/[C@H](O)[C@H](C)C[C@H](CC=O)[C@H](O[C@H]2[C@H](O)[C@@H](N(C)C)[C@H](O[C@@H]3O[C@@H](C)[C@H](OC(CC=O)=O)[C@@](O)(C)C3)[C@@H](C)O2)[C@@H](OC)[C@H](OC(CC)=O)CC(O1)=O	InChI=1S/C41H67NO15/c1-11-30(45)54-29-21-32(47)51-24(4)16-14-13-15-17-28(44)23(3)20-27(18-19-43)37(38(29)50-10)57-40-35(48)34(42(8)9)36(25(5)53-40)56-33-22-41(7,49)39(26(6)52-33)55-31(46)12-2/h13-15,17,19,23-29,33-40,44,48-49H,11-12,16,18,20-22H2,1-10H3/b14-13+,17-15+/t23-,24-,25-,26+,27+,28+,29-,33+,34-,35-,36-,37+,38+,39+,40+,41-/m1/s1	DMUAPQTXSSNEDD-QALJCMCCSA-N

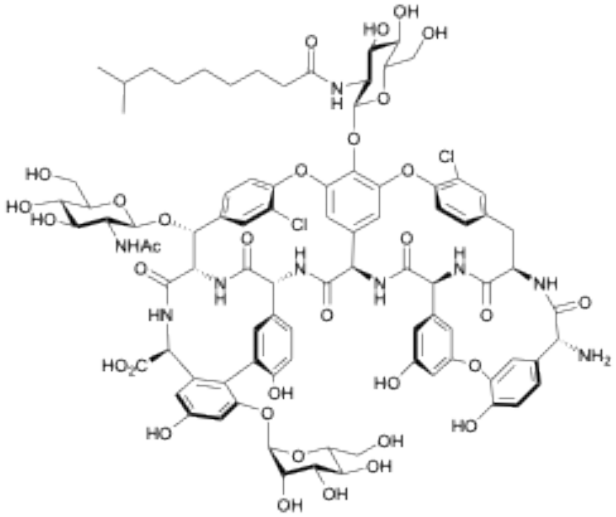
Name	#	Chemdraw	SMILES	InChI	InChIKey
josamycin propionate	**4.20**		C[C@@H]1C/C=C/C=C/[C@H](OC(CC)=O)[C@H](C)C[C@H](CC=O)[C@H](O[C@H]2[C@H](O)[C@@H](N(C)C)[C@H](O[C@@H]3O[C@@H](C)[C@H](OC(CC(C)C)=O)[C@@](O)(C)C3)[C@@H](C)O2)[C@@H](OC)[C@H](OC(C)=O)CC(O1)=O	InChI=1S/C45H73NO16/c1-13-34(49)59-32-18-16-14-15-17-27(5)55-36(51)23-33(58-30(8)48)42(54-12)41(31(19-20-47)22-26(32)4)62-44-39(52)38(46(10)11)40(28(6)57-44)61-37-24-45(9,53)43(29(7)56-37)60-35(50)21-25(2)3/h14-16,18,20,25-29,31-33,37-44,52-53H,13,17,19,21-24H2,1-12H3/b15-14+,18-16+/t26-,27-,28-,29+,31+,32+,33-,37+,38-,39-,40-,41+,42+,43+,44+,45-/m1/s1	NVBREHSOJSEKBQ-ZQMZUEOGSA-N
miokamycin	**4.21**		C[C@@H]1C/C=C/C=C/[C@H](O)[C@H](C)C[C@H](CC=O)[C@H](O[C@H]2[C@H](O)[C@@H](N(C)C)[C@H](O[C@@H]3O[C@@H](C)[C@H](OC(C)=O)[C@@](OC(CC)=O)(C)C3)[C@@H](C)O2)[C@@H](OC)[C@H](OC(CC)=O)CC(O1)=O	InChI=1S/C43H69NO16/c1-12-32(48)57-31-22-34(50)53-25(4)17-15-14-16-18-30(47)24(3)21-29(19-20-45)39(40(31)52-11)59-42-37(51)36(44(9)10)38(26(5)55-42)58-35-23-43(8,60-33(49)13-2)41(27(6)54-35)56-28(7)46/h14-16,18,20,24-27,29-31,35-42,47,51H,12-13,17,19,21-23H2,1-11H3/b15-14+,18-16+/t24-,25-,26-,27+,29+,30+,31-,35+,36-,37-,38-,39+,40+,41+,42+,43-/m1/s1	CJIQLZRLJUSNQX-CCGCOWOLSA-N

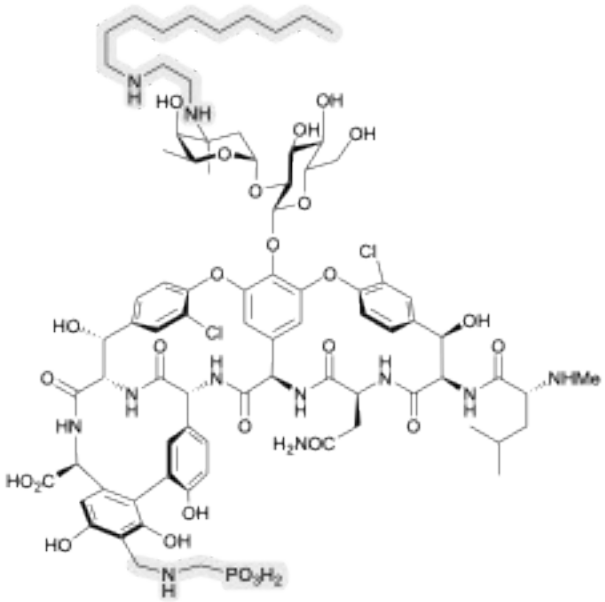
Name	#	Chemdraw	SMILES	InChI	InChIKey
rokitamycin	**4.22**		C[C@@H]1C/C=C/C=C/[C@H](O)[C@H](C)C[C@H](CC=O)[C@H](O[C@H]2[C@H](O)[C@@H](N(C)C)[C@H](O[C@@H]3O[C@@H](C)[C@H](OC(CCC)=O)[C@@](OC(CC)=O)(C)C3)[C@@H](C)O2)[C@@H](OC)[C@H](O)CC(O1)=O	InChI=1S/C42H69NO15/c1-11-16-32(48)55-40-27(6)53-34(23-42(40,7)58-31(47)12-2)56-37-26(5)54-41(36(50)35(37)43(8)9)57-38-28(19-20-44)21-24(3)29(45)18-15-13-14-17-25(4)52-33(49)22-30(46)39(38)51-10/h13-15,18,20,24-30,34-41,45-46,50H,11-12,16-17,19,21-23H2,1-10H3/b14-13+,18-15+/t24-,25-,26-,27+,28+,29+,30-,34+,35-,36-,37-,38+,39+,40+,41+,42-/m1/s1	VYWWNRMSAPEJLS-MDWYKHENSA-N
4"-O-isovaleryspiramycin I	**4.23**		C[C@@H]1C/C=C/C=C/[C@H](O[C@H]2CC[C@H](N(C)C)[C@@H](C)O2)[C@H](C)C[C@H](CC=O)[C@H](O[C@H]3[C@H](O)[C@@H](N(C)C)[C@H](O[C@@H]4O[C@@H](C)[C@H](OC(CC(C)C)=O)[C@@](O)(C)C4)[C@@H](C)O3)[C@@H](OC)[C@H](O)CC(O1)=O	InChI=1S/C48H82N2O15/c1-27(2)23-37(53)63-46-32(7)60-40(26-48(46,8)56)64-43-31(6)61-47(42(55)41(43)50(11)12)65-44-33(21-22-51)24-28(3)36(62-39-20-19-34(49(9)10)30(5)59-39)18-16-14-15-17-29(4)58-38(54)25-35(52)45(44)57-13/h14-16,18,22,27-36,39-47,52,55-56H,17,19-21,23-26H2,1-13H3/b15-14+,18-16+/t28-,29-,30-,31-,32+,33+,34+,35-,36+,39+,40+,41-,42-,43-,44+,45+,46+,47+,48-/m1/s1	GCIQAGXAZPUQNA-YDPAJNKASA-N

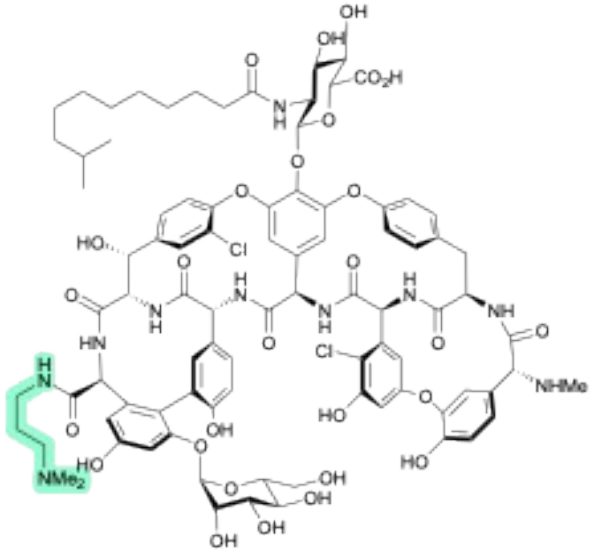
Name	#	Chemdraw	SMILES	InChI	InChIKey
ristocetin A	**5.01**		OC1=CC=C2C=C1C3=C([C@@H](C(OC)=O)NC([C@@H](NC([C@@H]2NC([C@@H]4NC5=O)=O)=O)[C@H](O[C@@H]6O[C@H]([C@@H]([C@@H](C6)N)O)C)C7=CC=C(OC8=CC4=CC(OC9=CC=C([C@@H](O)[C@@H](NC[C@H](N)C%10=CC=C(O)C%11=C%10)C(N[C@H]5C%12=CC(O%11)=C(C)C(O)=C%12)=O)C=C9)=C8O[C@@H]%13O[C@H](CO[C@@H]%14O[C@@H](C)[C@H](O)[C@@H](O)[C@H]%14O)[C@@H](O)[C@H](O)[C@H]%13O[C@@H]%15[C@@H](O[C@@H]%16[C@@H](O)[C@H](O)[C@@H](CO)O%16)[C@@H](O)[C@H](O)[C@@H](CO)O%15)C=C7)=O)C=C(O)C=C3O[C@@H]%17[C@@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O%17	InChI=1S/C95H112N8O43/c1-31-49(110)18-38-20-50(31)137-51-19-36(9-16-48(51)109)46(97)26-98-65-69(113)34-5-11-41(12-6-34)135-53-21-39-22-54(82(53)144-95-84(77(121)73(117)58(142-95)30-132-91-79(123)74(118)68(112)33(3)134-91)146-94-83(76(120)71(115)56(28-105)141-94)145-93-78(122)72(116)57(29-106)140-93)136-42-13-7-35(8-14-42)81(143-59-25-45(96)67(111)32(2)133-59)66-89(129)102-64(90(130)131-4)44-23-40(107)24-52(138-92-80(124)75(119)70(114)55(27-104)139-92)60(44)43-17-37(10-15-47(43)108)61(85(125)103-66)99-87(127)63(39)100-86(126)62(38)101-88(65)128/h5-24,32-33,45-46,55-59,61-81,83-84,91-95,98,104-124H,25-30,96-97H2,1-4H3,(H,99,127)(H,100,126)(H,101,128)(H,102,129)(H,103,125)/t32-,33-,45+,46-,55+,56+,57+,58+,59-,61+,62-,63+,64-,65+,66-,67-,68-,69+,70+,71+,72+,73+,74+,75-,76-,77-,78-,79+,80-,81+,83-,84+,91+,92-,93+,94+,95-/m0/s1	OXXGKPODRJZWDG-LBPNIUFLSA-N

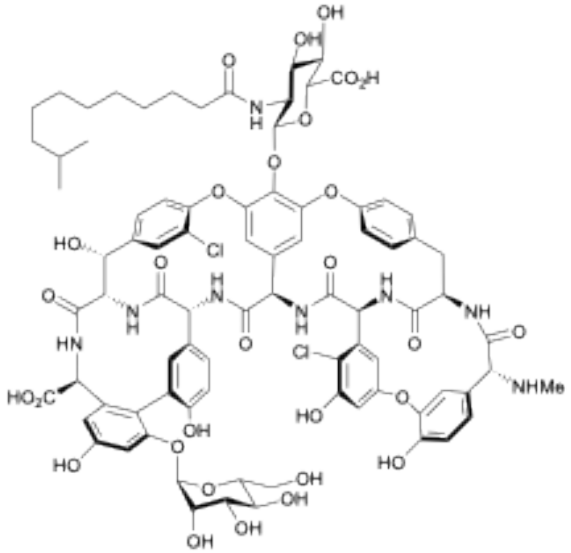
Name	#	Chemdraw	SMILES	InChI	InChIKey
vancomycin	**5.02**		OC1=CC(O)=CC([C@@H](C(O)=O)NC([C@@H](NC([C@@H]2NC([C@@H]3NC4=O)=O)=O)[C@H](O)C5=CC=C(OC6=CC3=CC(OC7=C(Cl)C=C([C@@H](O)[C@@H](NC([C@@H](CC(C)C)NC)=O)C(N[C@H]4CC(N)=O)=O)C=C7)=C6O[C@@H]8O[C@H](CO)[C@@H](O)[C@H](O)[C@H]8O[C@H](O9)C[C@](C)(N)[C@H](O)[C@@H]9C)C(Cl)=C5)=O)=C1C%10=CC2=CC=C%10O	InChI=1S/C66H75Cl2N9O24/c1-23(2)12-34(71-5)58(88)76-49-51(83)26-7-10-38(32(67)14-26)97-40-16-28-17-41(55(40)101-65-56(54(86)53(85)42(22-78)99-65)100-44-21-66(4,70)57(87)24(3)96-44)98-39-11-8-27(15-33(39)68)52(84)50-63(93)75-48(64(94)95)31-18-29(79)19-37(81)45(31)30-13-25(6-9-36(30)80)46(60(90)77-50)74-61(91)47(28)73-59(89)35(20-43(69)82)72-62(49)92/h6-11,13-19,23-24,34-35,42,44,46-54,56-57,65,71,78-81,83-87H,12,20-22,70H2,1-5H3,(H2,69,82)(H,72,92)(H,73,89)(H,74,91)(H,75,93)(H,76,88)(H,77,90)(H,94,95)/t24-,34+,35-,42+,44-,46+,47+,48-,49+,50-,51+,52+,53+,54-,56+,57+,65-,66-/m0/s1	MYPYJXKWCTUITO-LYRMYLQWSA-N

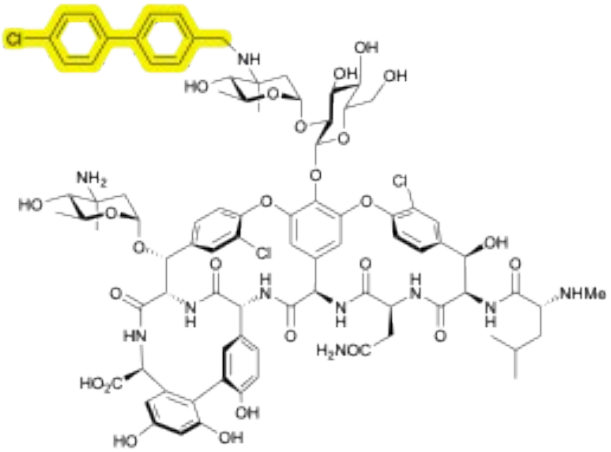
Name	#	Chemdraw	SMILES	InChI	InChIKey
norvancomycin	**5.03**		OC1=CC(O)=CC([C@@H](C(O)=O)NC([C@@H](NC([C@@H]2NC([C@@H]3NC4=O)=O)=O)[C@H](O)C5=CC=C(OC6=CC3=CC(OC7=C(Cl)C=C([C@@H](O)[C@@H](NC([C@@H](CC(C)C)N)=O)C(N[C@H]4CC(N)=O)=O)C=C7)=C6O[C@@H]8O[C@H](CO)[C@@H](O)[C@H](O)[C@H]8O[C@H](O9)C[C@](C)(N)[C@H](O)[C@@H]9C)C(Cl)=C5)=O)=C1C%10=CC2=CC=C%10O	InChI=1S/C65H73Cl2N9O24/c1-22(2)11-33(68)57(87)75-48-50(82)25-6-9-37(31(66)13-25)96-39-15-27-16-40(54(39)100-64-55(53(85)52(84)41(21-77)98-64)99-43-20-65(4,70)56(86)23(3)95-43)97-38-10-7-26(14-32(38)67)51(83)49-62(92)74-47(63(93)94)30-17-28(78)18-36(80)44(30)29-12-24(5-8-35(29)79)45(59(89)76-49)73-60(90)46(27)72-58(88)34(19-42(69)81)71-61(48)91/h5-10,12-18,22-23,33-34,41,43,45-53,55-56,64,77-80,82-86H,11,19-21,68,70H2,1-4H3,(H2,69,81)(H,71,91)(H,72,88)(H,73,90)(H,74,92)(H,75,87)(H,76,89)(H,93,94)/t23-,33+,34-,41+,43-,45+,46+,47-,48+,49-,50+,51+,52+,53-,55+,56+,64-,65-/m0/s1	NUAQIRUAZSJTAI-YRPZDAAMSA-N

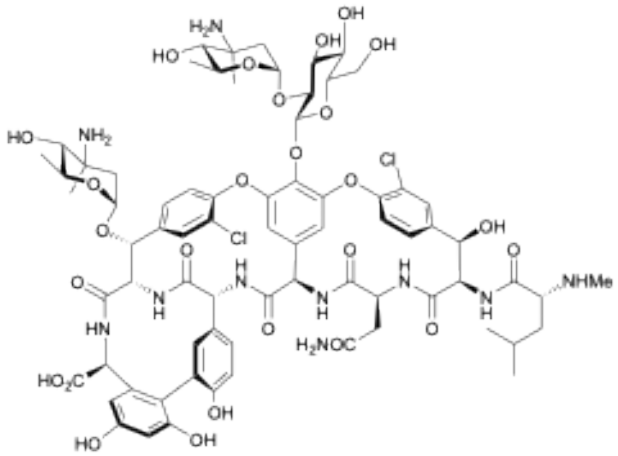
Name	#	Chemdraw	SMILES	InChI	InChIKey
teicoplanin A_2-2	**5.04**		OC1=CC=C2C=C1C3=C([C@@H](C(O)=O)NC([C@@H](NC([C@@H]2NC([C@@H]4NC5=O)=O)=O)[C@H](O[C@@H]6O[C@H](CO)[C@@H](O)[C@H](O)[C@H]6NC(C)=O)C7=CC=C(OC8=CC4=CC(OC(C=CC(C[C@@H](NC([C@H](N)C9=CC=C(O)C%10=C9)=O)C(N[C@H]5C%11=CC(O%10)=CC(O)=C%11)=O)=C%12)=C%12Cl)=C8O[C@@H]%13O[C@H](CO)[C@@H](O)[C@H](O)[C@H]%13NC(CCCCCCC(C)C)=O)C(Cl)=C7)=O)C=C(O)C=C3O[C@@H]%14[C@@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O%14	InChI=1S/C88H97Cl2N9O33/c1-33(2)8-6-4-5-7-9-60(108)94-68-74(113)71(110)58(31-101)129-87(68)132-78-55-25-40-26-56(78)126-52-17-13-38(23-47(52)90)77(131-86-67(92-34(3)103)73(112)70(109)57(30-100)128-86)69-84(121)98-66(85(122)123)45-28-42(105)29-54(127-88-76(115)75(114)72(111)59(32-102)130-88)61(45)44-22-37(12-14-49(44)106)63(81(118)99-69)96-83(120)65(40)97-82(119)64-39-20-41(104)27-43(21-39)124-53-24-36(11-15-50(53)107)62(91)80(117)93-48(79(116)95-64)19-35-10-16-51(125-55)46(89)18-35/h10-18,20-29,33,48,57-59,62-77,86-88,100-102,104-107,109-115H,4-9,19,30-32,91H2,1-3H3,(H,92,103)(H,93,117)(H,94,108)(H,95,116)(H,96,120)(H,97,119)(H,98,121)(H,99,118)(H,122,123)/t48-,57-,58-,59-,62-,63-,64+,65-,66+,67-,68-,69+,70-,71-,72-,73-,74-,75+,76+,77-,86+,87+,88+/m1/s1	GHOXVFYORXUCPY-PKMGYIMSSA-N

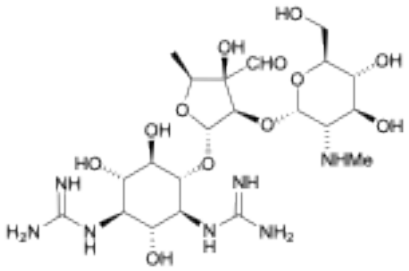
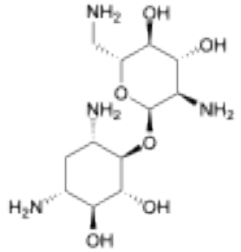
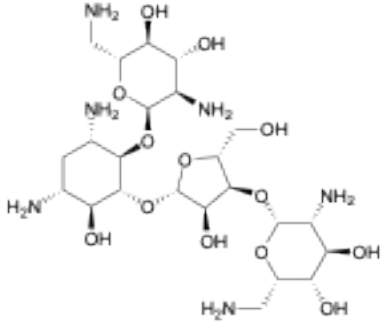
Name	#	Chemdraw	SMILES	InChI	InChIKey
telavancin	**5.05**		OC1=C(CNCP(O)(O)=O)C(O)=CC([C@@H](C(O)=O)NC([C@@H](NC([C@@H]2NC([C@@H]3NC4=O)=O)=O)[C@H](O)C5=CC=C(OC6=CC3=CC(OC7=C(Cl)C=C([C@@H](O)[C@@H](NC([C@@H](CC(C)C)NC)=O)C(N[C@H]4CC(N)=O)=O)C=C7)=C6O[C@@H]8O[C@H](CO)[C@@H](O)[C@H](O)[C@H]8O[C@H](O9)C[C@](C)(NCCNCCCCCCCCCC)[C@H](O)[C@@H]9C)C(Cl)=C5)=O)=C1C%10=CC2=CC=C%10O	InChI=1S/C80H106Cl2N11O27P/c1-7-8-9-10-11-12-13-14-21-85-22-23-87-80(5)32-57(115-37(4)71(80)103)119-70-68(102)67(101)55(34-94)118-79(70)120-69-53-28-41-29-54(69)117-52-20-17-40(27-46(52)82)65(99)63-77(109)91-61(78(110)111)43-30-50(96)44(33-86-35-121(112,113)114)66(100)58(43)42-25-38(15-18-49(42)95)59(74(106)93-63)90-75(107)60(41)89-73(105)48(31-56(83)97)88-76(108)62(92-72(104)47(84-6)24-36(2)3)64(98)39-16-19-51(116-53)45(81)26-39/h15-20,25-30,36-37,47-48,55,57,59-65,67-68,70-71,79,84-87,94-96,98-103H,7-14,21-24,31-35H2,1-6H3,(H2,83,97)(H,88,108)(H,89,105)(H,90,107)(H,91,109)(H,92,104)(H,93,106)(H,110,111)(H2,112,113,114)/t37-,47+,48-,55+,57-,59+,60+,61-,62+,63-,64+,65+,67+,68-,70+,71+,79-,80-/m0/s1	ONUMZHGUFYIKPM-MXNFEBESSA-N

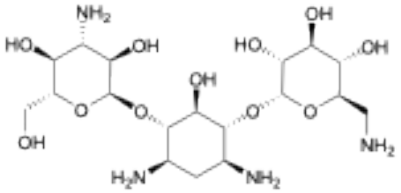
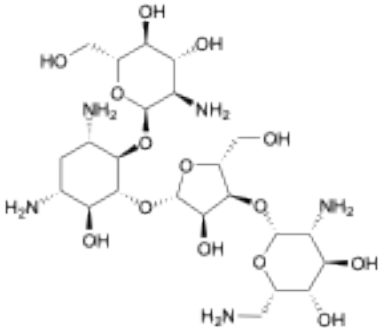
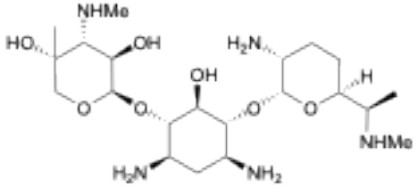
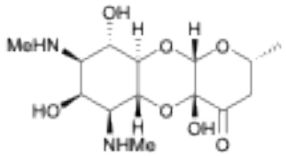
Name	#	Chemdraw	SMILES	InChI	InChIKey
dalbavancin	**5.06**		OC1=CC=C2C=C1C3=C([C@@H](C(NCCCN(C)C)=O)NC([C@@H](NC([C@@H]2NC([C@@H]4NC5=O)=O)=O)[C@H](O)C6=CC=C(OC7=CC4=CC(OC8=CC=C(C[C@@H](NC([C@H](NC)C9=CC=C(O)C%10=C9)=O)C(N[C@H]5C%11=CC(O%10)=CC(O)=C%11Cl)=O)C=C8)=C7O[C@@H]%12O[C@H](C(O)=O)[C@@H](O)[C@H](O)[C@H]%12NC(CCCCCCCCC(C)C)=O)C(Cl)=C6)=O)C=C(O)C=C3O[C@@H]%13[C@@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O%13	InChI=1S/C88H100Cl2N10O28/c1-38(2)13-10-8-6-7-9-11-14-61(106)94-70-73(109)75(111)78(86(120)121)128-87(70)127-77-58-31-43-32-59(77)124-55-24-19-42(29-50(55)89)71(107)69-85(119)98-67(80(114)92-25-12-26-100(4)5)48-33-44(102)34-57(125-88-76(112)74(110)72(108)60(37-101)126-88)62(48)47-28-40(17-22-52(47)103)65(82(116)99-69)95-83(117)66(43)96-84(118)68-49-35-46(36-54(105)63(49)90)123-56-30-41(18-23-53(56)104)64(91-3)81(115)93-51(79(113)97-68)27-39-15-20-45(122-58)21-16-39/h15-24,28-36,38,51,60,64-76,78,87-88,91,101-105,107-112H,6-14,25-27,37H2,1-5H3,(H,92,114)(H,93,115)(H,94,106)(H,95,117)(H,96,118)(H,97,113)(H,98,119)(H,99,116)(H,120,121)/t51-,60-,64-,65-,66-,67+,68+,69+,70-,71-,72-,73-,74+,75+,76+,78+,87-,88+/m1/s1	KGPGQDLTDHGEGT-SZUNQUCBSA-N

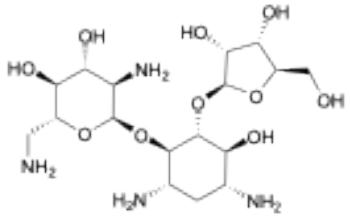
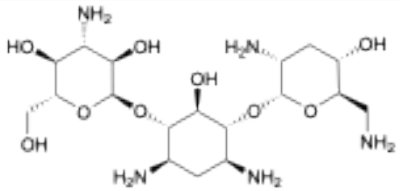
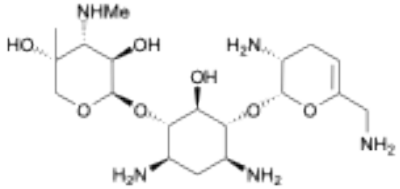
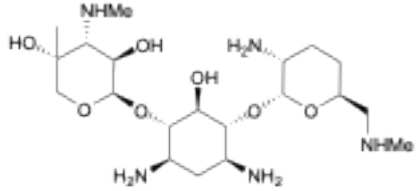
Name	#	Chemdraw	SMILES	InChI	InChIKey
A40926 Factor B_0	**5.06a**		OC1=CC=C2C=C1C3=C([C@@H](C(O)=O)NC([C@@H](NC([C@@H]2NC([C@@H]4NC5=O)=O)=O)[C@H](O)C6=CC=C(OC7=CC4=CC(OC8=CC=C(C[C@@H](NC([C@H](NC)C9=CC=C(O)C%10=C9)=O)C(N[C@H]5C%11=CC(O%10)=CC(O)=C%11Cl)=O)C=C8)=C7O[C@@H]%12O[C@H](C(O)=O)[C@@H](O)[C@H](O)[C@H]%12NC(CCCCCCCCC(C)C)=O)C(Cl)=C6)=O)C=C(O)C=C3O[C@@H]%13[C@@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O%13	InChI=1S/C83H88Cl2N8O29/c1-33(2)10-8-6-4-5-7-9-11-56(99)88-65-68(102)70(104)73(81(114)115)122-82(65)121-72-53-26-38-27-54(72)118-50-21-16-37(24-45(50)84)66(100)64-79(111)92-63(80(112)113)43-28-39(95)29-52(119-83-71(105)69(103)67(101)55(32-94)120-83)57(43)42-23-35(14-19-47(42)96)60(76(108)93-64)89-77(109)61(38)90-78(110)62-44-30-41(31-49(98)58(44)85)117-51-25-36(15-20-48(51)97)59(86-3)75(107)87-46(74(106)91-62)22-34-12-17-40(116-53)18-13-34/h12-21,23-31,33,46,55,59-71,73,82-83,86,94-98,100-105H,4-11,22,32H2,1-3H3,(H,87,107)(H,88,99)(H,89,109)(H,90,110)(H,91,106)(H,92,111)(H,93,108)(H,112,113)(H,114,115)/t46-,55-,59-,60-,61-,62+,63+,64+,65-,66-,67-,68-,69+,70+,71+,73+,82-,83+/m1/s1	PZMMGNLKWHJGSE-PSDJNXLUSA-N

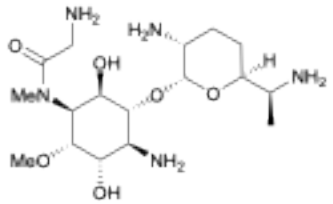
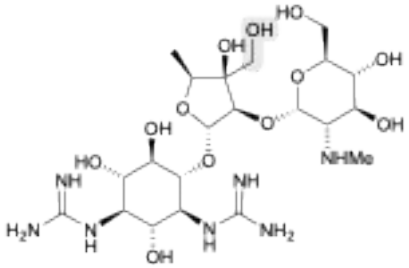
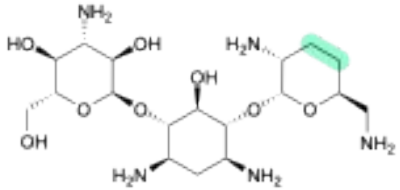
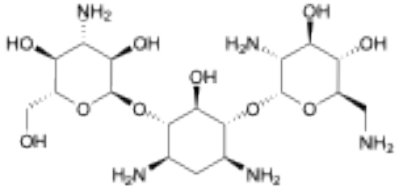
Name	#	Chemdraw	SMILES	InChI	InChIKey
oritavancin	**5.07**		OC1=CC(O)=CC([C@@H](C(O)=O)NC([C@@H](NC([C@@H]2NC([C@@H]3NC4=O)=O)=O)[C@H](O[C@H](O5)C[C@](C)(N)[C@@H](O)[C@@H]5C)C6=CC=C(OC7=CC3=CC(OC8=C(Cl)C=C([C@@H](O)[C@@H](NC([C@@H](CC(C)C)NC)=O)C(N[C@H]4CC(N)=O)=O)C=C8)=C7O[C@@H]9O[C@H](CO)[C@@H](O)[C@H](O)[C@H]9O[C@H](O%10)C[C@](C)(NCC%11=CC=C(C%12=CC=C(Cl)C=C%12)C=C%11)[C@@H](O)[C@@H]%10C)C(Cl)=C6)=O)=C1C%13=CC2=CC=C%13O	InChI=1S/C86H97Cl3N10O26/c1-35(2)22-51(92-7)77(110)98-67-69(105)42-15-20-55(49(88)24-42)120-57-26-44-27-58(73(57)125-84-74(71(107)70(106)59(34-100)122-84)124-62-32-86(6,76(109)37(4)119-62)93-33-38-8-10-39(11-9-38)40-12-17-45(87)18-13-40)121-56-21-16-43(25-50(56)89)72(123-61-31-85(5,91)75(108)36(3)118-61)68-82(115)97-66(83(116)117)48-28-46(101)29-54(103)63(48)47-23-41(14-19-53(47)102)64(79(112)99-68)96-80(113)65(44)95-78(111)52(30-60(90)104)94-81(67)114/h8-21,23-29,35-37,51-52,59,61-62,64-72,74-76,84,92-93,100-103,105-109H,22,30-34,91H2,1-7H3,(H2,90,104)(H,94,114)(H,95,111)(H,96,113)(H,97,115)(H,98,110)(H,99,112)(H,116,117)/t36-,37-,51+,52-,59+,61-,62-,64+,65+,66-,67+,68-,69+,70+,71-,72+,74+,75-,76-,84-,85-,86-/m0/s1	VHFGEBVPHAGQPI-LXKZPTCJSA-N

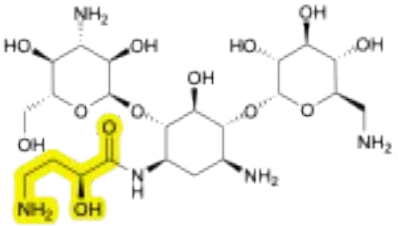
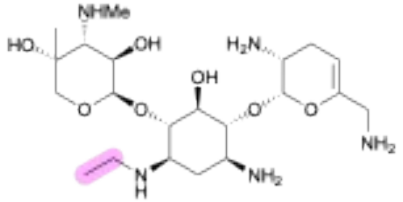
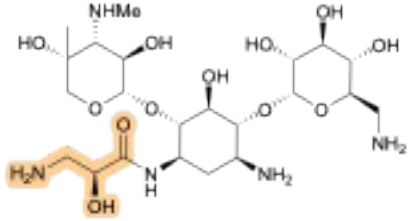
Name	#	Chemdraw	SMILES	InChI	InChIKey
chloroeremomycin	**5.07a**		OC1=CC(O)=CC([C@@H](C(O)=O)NC([C@@H](NC([C@@H]2NC([C@@H]3NC4=O)=O)=O)[C@H](O[C@H](O5)C[C@](C)(N)[C@@H](O)[C@@H]5C)C6=CC=C(OC7=CC3=CC(OC8=C(Cl)C=C([C@@H](O)[C@@H](NC([C@@H](CC(C)C)NC)=O)C(N[C@H]4CC(N)=O)=O)C=C8)=C7O[C@@H]9O[C@H](CO)[C@@H](O)[C@H](O)[C@H]9O[C@H](O%10)C[C@](C)(N)[C@@H](O)[C@@H]%10C)C(Cl)=C6)=O)=C1C%11=CC2=CC=C%11O	InChI=1S/C73H88Cl2N10O26/c1-26(2)14-38(79-7)64(96)84-54-56(91)30-9-12-42(36(74)16-30)106-44-18-32-19-45(60(44)111-71-61(58(93)57(92)46(25-86)108-71)110-49-24-73(6,78)63(95)28(4)105-49)107-43-13-10-31(17-37(43)75)59(109-48-23-72(5,77)62(94)27(3)104-48)55-69(101)83-53(70(102)103)35-20-33(87)21-41(89)50(35)34-15-29(8-11-40(34)88)51(66(98)85-55)82-67(99)52(32)81-65(97)39(22-47(76)90)80-68(54)100/h8-13,15-21,26-28,38-39,46,48-49,51-59,61-63,71,79,86-89,91-95H,14,22-25,77-78H2,1-7H3,(H2,76,90)(H,80,100)(H,81,97)(H,82,99)(H,83,101)(H,84,96)(H,85,98)(H,102,103)/t27-,28-,38+,39-,46+,48-,49-,51+,52+,53-,54+,55-,56+,57+,58-,59+,61+,62-,63-,71-,72-,73-/m0/s1	XJHXLMVKYIVZTE-LOALFDMRSA-N

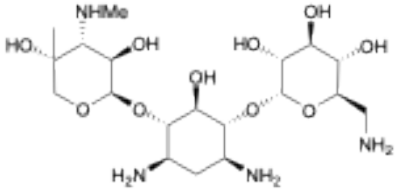
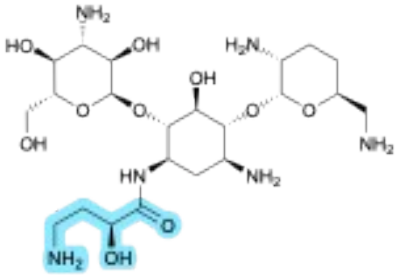
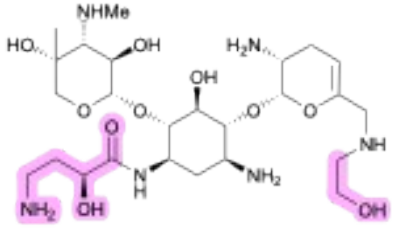
Name	#	Chemdraw	SMILES	InChI	InChIKey
streptomycin	**6.01**		O[C@@H]1[C@@H](NC(N)=N)[C@H](O)[C@@H](O)[C@H](O[C@H]2[C@H](O[C@H]3[C@@H](NC)[C@H](O)[C@@H](O)[C@H](CO)O3)[C@@](O)(C=O)[C@H](C)O2)[C@H]1NC(N)=N	InChI=1S/C21H39N7O12/c1-5-21(36,4-30)16(40-17-9(26-2)13(34)10(31)6(3-29)38-17)18(37-5)39-15-8(28-20(24)25)11(32)7(27-19(22)23)12(33)14(15)35/h4-18,26,29,31-36H,3H2,1-2H3,(H4,22,23,27)(H4,24,25,28)/t5-,6+,7+,8-,9-,10+,11+,12-,13+,14+,15+,16-,17+,18-,21+/m0/s1	UCSJYZPVAKXKNQ-IZICMZNXSA-N
neomycin A	**6.02**		O[C@H]([C@H]([C@@H](C[C@@H]1N)N)O)[C@@H]1O[C@H]2O[C@@H]([C@H]([C@@H]([C@H]2N)O)O)CN	InChI=1S/C12H26N4O6/c13-2-5-8(18)9(19)6(16)12(21-5)22-11-4(15)1-3(14)7(17)10(11)20/h3-12,17-20H,1-2,13-16H2/t3-,4+,5-,6-,7+,8-,9-,10-,11-,12-/m1/s1	SYJXFKPQNSDJLI-HKEUSBCWSA-N
framycetin	**6.03**		O[C@H]([C@@H]([C@H](O1)CO)O[C@H]2O[C@H]([C@H]([C@@H]([C@H]2N)O)O)CN)[C@@H]1O[C@H]([C@H]([C@@H](C[C@@H]3N)N)O)[C@@H]3O[C@H]4O[C@@H]([C@H]([C@@H]([C@H]4N)O)O)CN	InChI=1S/C23H46N6O13/c24-2-7-13(32)15(34)10(28)21(37-7)40-18-6(27)1-5(26)12(31)20(18)42-23-17(36)19(9(4-30)39-23)41-22-11(29)16(35)14(33)8(3-25)38-22/h5-23,30-36H,1-4,24-29H2/t5-,6+,7-,8+,9-,10-,11-,12+,13-,14-,15-,16-,17-,18-,19-,20-,21-,22-,23+/m1/s1	PGBHMTALBVVCIT-VCIWKGPPSA-N

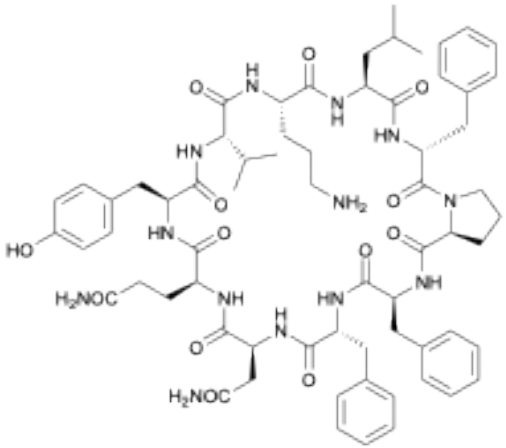
Name	#	Chemdraw	SMILES	InChI	InChIKey
kanamycin A	**6.04**		O[C@@H]([C@@H]([C@H](C[C@H]1N)N)O[C@H]2O[C@@H]([C@H]([C@@H]([C@H]2O)O)O)CN)[C@H]1O[C@H]3O[C@@H]([C@H]([C@@H]([C@H]3O)N)O)CO	InChI=1S/C18H36N4O11/c19-2-6-10(25)12(27)13(28)18(30-6)33-16-5(21)1-4(20)15(14(16)29)32-17-11(26)8(22)9(24)7(3-23)31-17/h4-18,23-29H,1-3,19-22H2/t4-,5+,6-,7-,8+,9-,10-,11-,12+,13-,14-,15+,16-,17-,18-/m1/s1	SBUJHOSQTJFQJX-NOAMYHISSA-N
paromomycin	**6.05**		O[C@H]([C@@H]([C@H](O1)CO)O[C@H]2O[C@H]([C@H]([C@@H]([C@H]2N)O)O)CN)[C@@H]1O[C@H]([C@H]([C@@H](C[C@@H]3N)N)O)[C@@H]3O[C@H]4O[C@@H]([C@H]([C@@H]([C@H]4N)O)O)CO	InChI=1S/C23H45N5O14/c24-2-7-13(32)15(34)10(27)21(37-7)41-19-9(4-30)39-23(17(19)36)42-20-12(31)5(25)1-6(26)18(20)40-22-11(28)16(35)14(33)8(3-29)38-22/h5-23,29-36H,1-4,24-28H2/t5-,6+,7+,8-,9-,10-,11-,12+,13-,14-,15-,16-,17-,18-,19-,20-,21-,22-,23+/m1/s1	UOZODPSAJZTQNH-LSWIJEOBSA-N
gentamicin C_1	**6.06**		O[C@@H]([C@@H]([C@H](C[C@H]1N)N)O[C@H]2O[C@](CC[C@H]2N)([H])[C@H](NC)C)[C@H]1O[C@@H]3[C@@H]([C@H]([C@@](O)(CO3)C)NC)O	InChI=1S/C21H43N5O7/c1-9(25-3)13-6-5-10(22)19(31-13)32-16-11(23)7-12(24)17(14(16)27)33-20-15(28)18(26-4)21(2,29)8-30-20/h9-20,25-29H,5-8,22-24H2,1-4H3/t9-,10-,11+,12-,13+,14+,15-,16-,17+,18-,19-,20-,21+/m1/s1	CEAZRRDELHUEMR-CAMVTXANSA-N
spectinomycin	**6.07**		O[C@](O1)(C(C[C@H](O2)C)=O)[C@]2([H])O[C@@]([C@H]([C@@H]([C@@H]3O)NC)O)([H])[C@@]1([H])[C@H]3NC	InChI=1S/C14H24N2O7/c1-5-4-6(17)14(20)13(21-5)22-12-10(19)7(15-2)9(18)8(16-3)11(12)23-14/h5,7-13,15-16,18-20H,4H2,1-3H3/t5-,7-,8+,9+,10+,11-,12-,13+,14+/m1/s1	UNFWWIHTNXNPBV-WXKVUWSESA-N

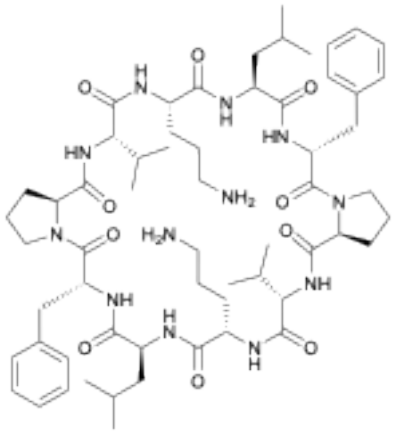
Name	#	Chemdraw	SMILES	InChI	InChIKey
ribostamycin	**6.08**		NC[C@H]([C@H]([C@@H]([C@H]1N)O)O)O[C@@H]1O[C@H]([C@H](C[C@H]([C@@H]2O)N)N)[C@@H]2O[C@@H]3O[C@@H]([C@H]([C@H]3O)O)CO	InChI=1S/C17H34N4O10/c18-2-6-10(24)12(26)8(21)16(28-6)30-14-5(20)1-4(19)9(23)15(14)31-17-13(27)11(25)7(3-22)29-17/h4-17,22-27H,1-3,18-21H2/t4-,5+,6-,7-,8-,9+,10-,11-,12-,13-,14-,15-,16-,17+/m1/s1	NSKGQURZWSPSBC-VVPCINPTSA-N
tobramycin	**6.09**		O[C@@H]([C@@H]([C@H](C[C@H]1N)N)O[C@H]2O[C@@H]([C@H](C[C@H]2N)O)CN)[C@H]1O[C@H]3O[C@@H]([C@H]([C@@H]([C@H]3O)N)O)CO	InChI=1S/C18H37N5O9/c19-3-9-8(25)2-7(22)17(29-9)31-15-5(20)1-6(21)16(14(15)28)32-18-13(27)11(23)12(26)10(4-24)30-18/h5-18,24-28H,1-4,19-23H2/t5-,6+,7+,8-,9+,10+,11-,12+,13+,14-,15+,16-,17+,18+/m0/s1	NLVFBUXFDBBNBW-PBSUHMDJSA-N
sisomicin	**6.10**		O[C@@H]([C@@H]([C@H](C[C@H]1N)N)O[C@H]2OC(CN)=CC[C@H]2N)[C@H]1O[C@@H]3[C@@H]([C@H]([C@@](O)(CO3)C)NC)O	InChI=1S/C19H37N5O7/c1-19(27)7-28-18(13(26)16(19)24-2)31-15-11(23)5-10(22)14(12(15)25)30-17-9(21)4-3-8(6-20)29-17/h3,9-18,24-27H,4-7,20-23H2,1-2H3/t9-,10+,11-,12+,13-,14-,15+,16-,17-,18-,19+/m1/s1	URWAJWIAIPFPJE-YFMIWBNJSA-N
micronomicin	**6.11**		O[C@@H]([C@@H]([C@H](C[C@H]1N)N)O[C@H]2O[C@@H](CC[C@H]2N)CNC)[C@H]1O[C@@H]3[C@@H]([C@H]([C@@](O)(CO3)C)NC)O	InChI=1S/C20H41N5O7/c1-20(28)8-29-19(14(27)17(20)25-3)32-16-12(23)6-11(22)15(13(16)26)31-18-10(21)5-4-9(30-18)7-24-2/h9-19,24-28H,4-8,21-23H2,1-3H3/t9-,10+,11-,12+,13-,14+,15+,16-,17+,18+,19+,20-/m0/s1	DNYGXMICFMACRA-XHEDQWPISA-N

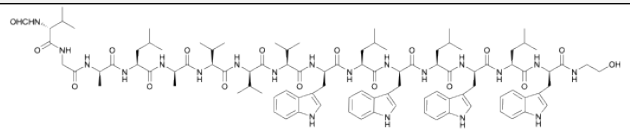
Name	#	Chemdraw	SMILES	InChI	InChIKey
astromicin	**6.12**		NCC(N([C@@H]1[C@H]([C@H]([C@@H]([C@H]([C@@H]1O)O[C@H]2O[C@](CC[C@H]2N)([H])[C@@H](N)C)N)O)OC)C)=O	InChI=1S/C17H35N5O6/c1-7(19)9-5-4-8(20)17(27-9)28-15-11(21)13(24)16(26-3)12(14(15)25)22(2)10(23)6-18/h7-9,11-17,24-25H,4-6,18-21H2,1-3H3/t7-,8+,9-,11-,12-,13-,14+,15+,16+,17+/m0/s1	BIDUPMYXGFNAEJ-APGVDKLISA-N
dihydrostreptomycin	**6.13**		O[C@@H]1[C@@H](NC(N)=N)[C@H](O)[C@@H](O)[C@H](O[C@H]2[C@H](O[C@H]3[C@@H](NC)[C@H](O)[C@@H](O)[C@H](CO)O3)[C@@](O)(CO)[C@H](C)O2)[C@H]1NC(N)=N	InChI=1S/C21H41N7O12/c1-5-21(36,4-30)16(40-17-9(26-2)13(34)10(31)6(3-29)38-17)18(37-5)39-15-8(28-20(24)25)11(32)7(27-19(22)23)12(33)14(15)35/h5-18,26,29-36H,3-4H2,1-2H3,(H4,22,23,27)(H4,24,25,28)/t5-,6-,7+,8-,9-,10-,11+,12-,13-,14+,15+,16-,17-,18-,21+/m0/s1	ASXBYYWOLISCLQ-HZYVHMACSA-N
dibekacin	**6.14**		O[C@@H]([C@@H]([C@H](C[C@H]1N)N)O[C@H]2O[C@@H](CC[C@H]2N)CN)[C@H]1O[C@H]3O[C@@H]([C@H]([C@@H]([C@H]3O)N)O)CO	InChI=1S/C18H37N5O8/c19-4-6-1-2-7(20)17(28-6)30-15-8(21)3-9(22)16(14(15)27)31-18-13(26)11(23)12(25)10(5-24)29-18/h6-18,24-27H,1-5,19-23H2/t6-,7+,8-,9+,10+,11-,12+,13+,14-,15+,16-,17+,18+/m0/s1	JJCQSGDBDPYCEO-XVZSLQNASA-N
kanamycin B	**6.14a**		O[C@@H]([C@@H]([C@H](C[C@H]1N)N)O[C@H]2O[C@@H]([C@@H](O)[C@H](O)[C@H]2N)CN)[C@H]1O[C@H]3O[C@@H]([C@H]([C@@H]([C@H]3O)N)O)CO	InChI=1S/C18H37N5O10/c19-2-6-11(26)12(27)9(23)17(30-6)32-15-4(20)1-5(21)16(14(15)29)33-18-13(28)8(22)10(25)7(3-24)31-18/h4-18,24-29H,1-3,19-23H2/t4-,5+,6+,7+,8-,9+,10+,11+,12+,13+,14-,15+,16-,17+,18+/m0/s1	SKKLOUVUUNMCJE-FQSMHNGLSA-N

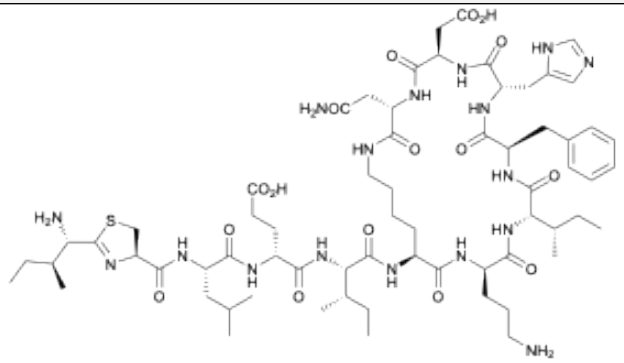
Name	#	Chemdraw	SMILES	InChI	InChIKey
amikacin	**6.15**		NCC[C@H](O)C(N[C@H](C[C@@H]([C@H]([C@@H]1O)O[C@H]2O[C@@H]([C@H]([C@@H]([C@H]2O)O)O)CN)N)[C@@H]1O[C@@H]3[C@@H]([C@H]([C@@H]([C@H](O3)CO)O)N)O)=O	InChI=1S/C22H43N5O13/c23-2-1-8(29)20(36)27-7-3-6(25)18(39-22-16(34)15(33)13(31)9(4-24)37-22)17(35)19(7)40-21-14(32)11(26)12(30)10(5-28)38-21/h6-19,21-22,28-35H,1-5,23-26H2,(H,27,36)/t6-,7+,8-,9+,10+,11-,12+,13+,14+,15-,16+,17-,18+,19-,21+,22+/m0/s1	LKCWBDHBTVXHDL-RMDFUYIESA-N
netilmicin	**6.16**		O[C@@H]([C@@H]([C@H](C[C@H]1NCC)N)O[C@H]2OC(CN)=CC[C@H]2N)[C@H]1O[C@@H]3[C@@H]([C@H]([C@@]([O)(CO3)C)NC)O	InChI=1S/C21H41N5O7/c1-4-26-13-7-12(24)16(32-19-11(23)6-5-10(8-22)31-19)14(27)17(13)33-20-15(28)18(25-3)21(2,29)9-30-20/h5,11-20,25-29H,4,6-9,22-24H2,1-3H3/t11-,12+,13-,14+,15-,16-,17+,18-,19-,20-,21+/m1/s1	CIDUJQMULVCIBT-MQDUPKMGSA-N
isepamicin	**6.17**		NC[C@H](O)C(N[C@H](C[C@@H]([C@H]([C@@H]1O)O[C@H]2O[C@@H]([C@H]([C@@H]([C@H]2O)O)O)CN)N)[C@@H]1O[C@@H]3OC[C@@](C)([C@@H]([C@H]3O)NC)O)=O	InChI=1S/C22H43N5O12/c1-22(35)6-36-20(15(33)18(22)26-2)39-17-8(27-19(34)9(28)4-23)3-7(25)16(14(17)32)38-21-13(31)12(30)11(29)10(5-24)37-21/h7-18,20-21,26,28-33,35H,3-6,23-25H2,1-2H3,(H,27,34)/t7-,8+,9-,10+,11+,12-,13+,14-,15+,16+,17-,18+,20-,21+,22-/m0/s1	UDIIBEDMEYAVNG-UTJMZDNOSA-N

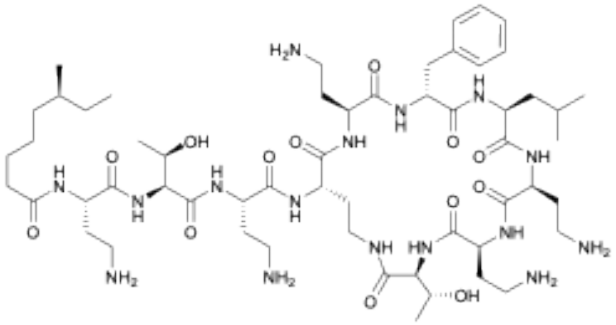
Name	#	Chemdraw	SMILES	InChI	InChIKey
gentamycin B	**6.17a**		O[C@@H]([C@@H]([C@H](C[C@H]1N)N)O[C@H]2O[C@@H]([C@@H](O)[C@H](O)[C@H]2O)CN)[C@H]1O[C@@H]3[C@@H]([C@H]([C@@](O)(CO3)C)NC)O	InChI=1S/C19H38N4O10/c1-19(29)5-30-17(13(28)16(19)23-2)32-14-6(21)3-7(22)15(12(14)27)33-18-11(26)10(25)9(24)8(4-20)31-18/h6-18,23-29H,3-5,20-22H2,1-2H3/t6-,7+,8-,9-,10+,11-,12-,13-,14+,15-,16-,17-,18-,19+/m1/s1	RHRAMPXHWHSKQB-GGEUKFTFSA-N
arbekacin	**6.18**		NCC[C@H](O)C(N[C@H](C[C@@H]([C@H]([C@@H]1O)O[C@H]2O[C@@H](CC[C@H]2N)CN)N)[C@@H]1O[C@@H]3[C@@H]([C@H]([C@@H]([C@H](O3)CO)O)N)O)=O	InChI=1S/C22H44N6O10/c23-4-3-12(30)20(34)28-11-5-10(26)18(37-21-9(25)2-1-8(6-24)35-21)17(33)19(11)38-22-16(32)14(27)15(31)13(7-29)36-22/h8-19,21-22,29-33H,1-7,23-27H2,(H,28,34)/t8-,9+,10-,11+,12-,13+,14-,15+,16+,17-,18+,19-,21+,22+/m0/s1	MKKYBZZTJQGVCD-XTCKQBCOSA-N
plazomicin	**6.19**		NCC[C@H](O)C(N[C@H](C[C@@H]([C@H]([C@@H]1O)O[C@H]2OC(CNCCO)=CC[C@H]2N)N)[C@@H]1O[C@@H]3OC[C@@](C)([C@@H]([C@H]3O)NC)O)=O	InChI=1S/C25H48N6O10/c1-25(37)11-38-24(18(35)21(25)29-2)41-20-15(31-22(36)16(33)5-6-26)9-14(28)19(17(20)34)40-23-13(27)4-3-12(39-23)10-30-7-8-32/h3,13-21,23-24,29-30,32-35,37H,4-11,26-28H2,1-2H3,(H,31,36)/t13-,14+,15-,16+,17+,18-,19-,20+,21-,23-,24+,25+/m1/s1	IYDYFVUFSPQPPV-JYUPHPNASA-N

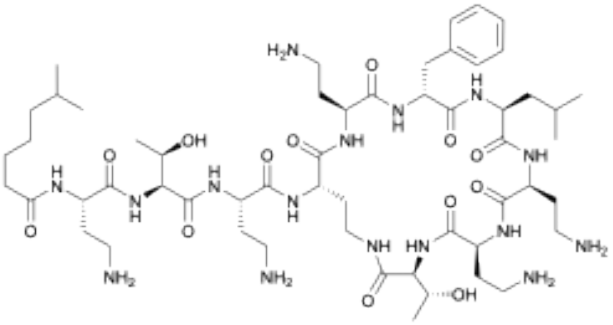
Name	#	Chemdraw	SMILES	InChI	InChIKey
tyrothricin A	**7.01**		O=C1N2[C@@H](CCC2)C(N[C@H](C(N[C@@H](C(N[C@H](C(N[C@H](C(N[C@H](C(N[C@H](C(N[C@H](C(N[C@@H]1CC3=CC=CC=C3)=O)CC(C)C)=O)CCCN)=O)C(C)C)=O)CC4=CC=C(C=C4O)=O)CCC(N)=O)=O)CC(N)=O)=O)CC5=CC=CC=C5)=O)CC6=CC=CC=C6)=O	InChI=1S/C66H87N13O13/c1-38(2)32-47-59(85)77-52(36-42-20-12-7-13-21-42)66(92)79-31-15-23-53(79)64(90)76-49(34-41-18-10-6-11-19-41)61(87)74-48(33-40-16-8-5-9-17-40)60(86)75-51(37-55(69)82)62(88)70-46(28-29-54(68)81)58(84)73-50(35-43-24-26-44(80)27-25-43)63(89)78-56(39(3)4)65(91)71-45(22-14-30-67)57(83)72-47/h5-13,16-21,24-27,38-39,45-53,56,80H,14-15,22-23,28-37,67H2,1-4H3,(H2,68,81)(H2,69,82)(H,70,88)(H,71,91)(H,72,83)(H,73,84)(H,74,87)(H,75,86)(H,76,90)(H,77,85)(H,78,89)/t45-,46-,47-,48+,49-,50-,51-,52+,53-,56-/m0/s1	GSXRBRIWJGAPDU-BBVRJQLQSA-N

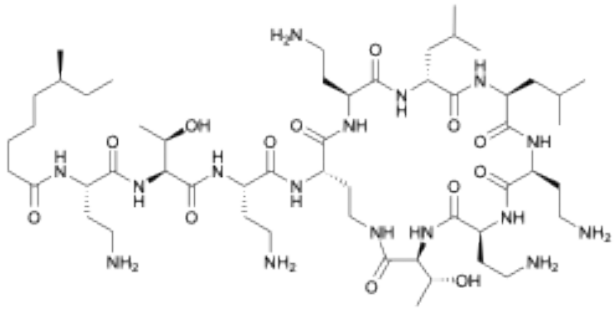
Name	#	Chemdraw	SMILES	InChI	InChIKey
gramicidin S	**7.02**		CC(C[C@H]1C(N[C@H](CC2=CC=CC=C2)C(N3CCC[C@H]3C(N[C@@H](C(C)C)C(N[C@@H](CCCN)C(N[C@@H](CC(C)C)C(N[C@H](CC4=CC=CC=C4)C(N5CCC[C@H]5C(N[C@@H](C(C)C)C(N[C@@H](CCCN)C(N1)=O)=O)=O)=O)=O)=O)=O)=O)=O)C	InChI=1S/C60H92N12O10/c1-35(2)31-43-53(75)67-45(33-39-19-11-9-12-20-39)59(81)71-29-17-25-47(71)55(77)70-50(38(7)8)58(80)64-42(24-16-28-62)52(74)66-44(32-36(3)4)54(76)68-46(34-40-21-13-10-14-22-40)60(82)72-30-18-26-48(72)56(78)69-49(37(5)6)57(79)63-41(23-15-27-61)51(73)65-43/h9-14,19-22,35-38,41-50H,15-18,23-34,61-62H2,1-8H3,(H,63,79)(H,64,80)(H,65,73)(H,66,74)(H,67,75)(H,68,76)(H,69,78)(H,70,77)/t41-,42-,43-,44-,45+,46+,47-,48-,49-,50-/m0/s1	IUAYMJGZBVDSGL-XNNAEKOYSA-N

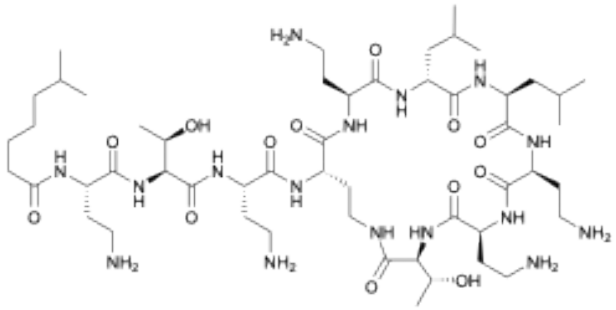
Name	#	Chemdraw	SMILES	InChI	InChIKey
valine-gramicidin A	**7.03**		C[C@@H](NC(CNC([C@H](NC=O)C(C)C)=O)=O)C(N[C@H](C(N[C@@H](C(N[C@H](C(N[C@@H](C(N[C@H](C(N[C@@H](C(N[C@H](C(N[C@@H](C(N[C@H](C(N[C@@H](C(NCCO)=O)CC1=CNC2=CC=CC=C21)=O)CC(C)C)=O)CC3=CNC4=CC=CC=C43)=O)CC(C)C)=O)CC5=CNC6=CC=CC=C65)=O)CC(C)C)=O)CC7=CNC8=CC=CC=C87)=O)C(C)C)=O)C(C)C)=O)C(C)C)=O)C(C)C)=O	InChI=1S/C99H140N20O17/c1-51(2)37-73(109-86(123)59(17)107-81(122)49-105-96(133)82(55(9)10)106-50-121)89(126)108-60(18)87(124)117-84(57(13)14)98(135)119-85(58(15)16)99(136)118-83(56(11)12)97(134)116-80(44-64-48-104-72-34-26-22-30-68(64)72)95(132)112-76(40-54(7)8)92(129)115-79(43-63-47-103-71-33-25-21-29-67(63)71)94(131)111-75(39-53(5)6)91(128)114-78(42-62-46-102-70-32-24-20-28-66(62)70)93(130)110-74(38-52(3)4)90(127)113-77(88(125)100-35-36-120)41-61-45-101-69-31-23-19-27-65(61)69/h19-34,45-48,50-60,73-80,82-85,101-104,120H,35-44,49H2,1-18H3,(H,100,125)(H,105,133)(H,106,121)(H,107,122)(H,108,126)(H,109,123)(H,110,130)(H,111,131)(H,112,132)(H,113,127)(H,114,128)(H,115,129)(H,116,134)(H,117,124)(H,118,136)(H,119,135)/t59-,60-,73-,74-,75+,76+,77-,78-,79-,80+,82+,83-,84+,85+/m0/s1	ZWCXYZRRTRDGQE-ASKBVUKBSA-N

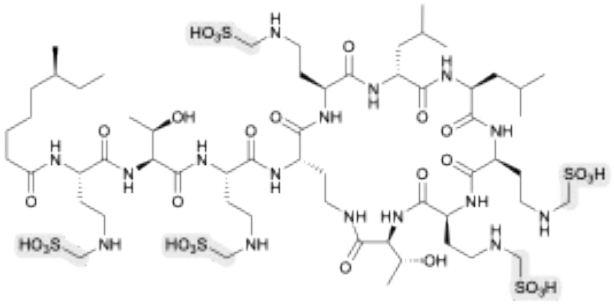
Name	#	Chemdraw	SMILES	InChI	InChIKey
bacitracin A	**7.04**		CC[C@@H]([C@@H](C1=N[C@@H](CS1)C(N[C@H](C(N[C@@H](C(N[C@H](C(N[C@H]2CCCCNC([C@@H](NC([C@H](NC([C@@H](NC([C@H](NC([C@@H](NC([C@H](NC2=O)CCCN)=O)[C@H](CC)C)=O)CC3=CC=CC=C3)=O)CC4=CN=CN4)=O)CC(O)=O)=O)CC(N)=O)=O)=O)[C@H](CC)C)=O)CCC(O)=O)=O)CC(C)C)=O)N)C	InChI=1S/C66H103N17O16S/c1-9-35(6)52(69)66-81-48(32-100-66)63(97)76-43(26-34(4)5)59(93)74-42(22-23-50(85)86)58(92)83-53(36(7)10-2)64(98)75-40-20-15-16-25-71-55(89)46(29-49(68)84)78-62(96)47(30-51(87)88)79-61(95)45(28-39-31-70-33-72-39)77-60(94)44(27-38-18-13-12-14-19-38)80-65(99)54(37(8)11-3)82-57(91)41(21-17-24-67)73-56(40)90/h12-14,18-19,31,33-37,40-48,52-54H,9-11,15-17,20-30,32,67,69H2,1-8H3,(H2,68,84)(H,70,72)(H,71,89)(H,73,90)(H,74,93)(H,75,98)(H,76,97)(H,77,94)(H,78,96)(H,79,95)(H,80,99)(H,82,91)(H,83,92)(H,85,86)(H,87,88)/t35-,36-,37-,40-,41+,42+,43-,44+,45-,46-,47+,48-,52-,53-,54-/m0/s1	CLKOFPXJLQSYAH-ABRJDSQDSA-N

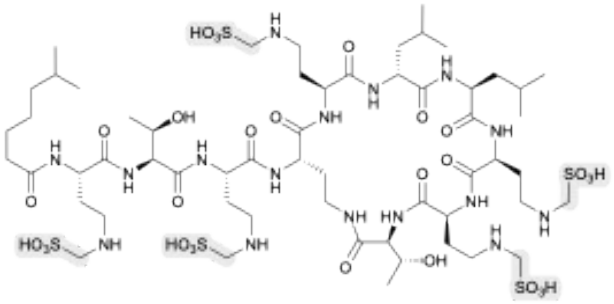
Name	#	Chemdraw	SMILES	InChI	InChIKey
polymyxin B_1	**7.05a**		CC[C@H](C)CCCCC(N[C@H](C(N[C@@H]([C@H](O)C)C(N[C@H](C(N[C@H]1CCNC([C@H]([C@H](O)C)NC([C@@H](NC([C@@H](NC([C@@H](NC([C@@H](NC([C@@H](NC1=O)CCN)=O)CC2=CC=CC=C2)=O)CC(C)C)=O)CCN)=O)CCN)=O)=O)=O)CCN)=O)=O)CCN)=O	InChI=1S/C56H98N16O13/c1-7-32(4)13-11-12-16-44(75)63-36(17-23-57)51(80)72-46(34(6)74)56(85)68-39(20-26-60)48(77)67-41-22-28-62-55(84)45(33(5)73)71-52(81)40(21-27-61)65-47(76)37(18-24-58)66-53(82)42(29-31(2)3)69-54(83)43(30-35-14-9-8-10-15-35)70-49(78)38(19-25-59)64-50(41)79/h8-10,14-15,31-34,36-43,45-46,73-74H,7,11-13,16-30,57-61H2,1-6H3,(H,62,84)(H,63,75)(H,64,79)(H,65,76)(H,66,82)(H,67,77)(H,68,85)(H,69,83)(H,70,78)(H,71,81)(H,72,80)/t32-,33+,34+,36-,37-,38-,39-,40-,41-,42-,43+,45-,46-/m0/s1	WQVJHHACXVLGBL-CTMZAJDNSA-N

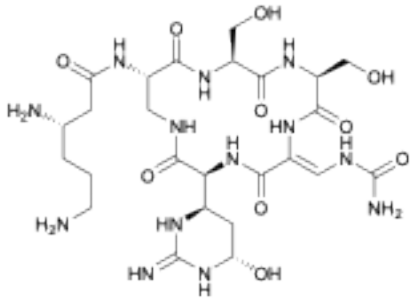
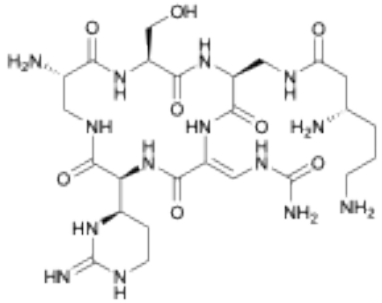
Name	#	Chemdraw	SMILES	InChI	InChIKey
polymyxin B_2	**7.05b**		NCC[C@@H](C(N[C@@H]([C@H](O)C)C(N[C@H](C(N[C@H]1CCNC([C@H]([C@H](O)C)NC([C@@H](NC([C@@H](NC([C@@H](NC([C@H](NC([C@@H](NC1=O)CCN)=O)CC2=CC=CC=C2)=O)CC(C)C)=O)CCN)=O)=O)=O)CCN)=O)=O)NC(CCCCC(C)C)=O	InChI=1S/C55H96N16O13/c1-30(2)12-10-11-15-43(74)62-35(16-22-56)50(79)71-45(33(6)73)55(84)67-38(19-25-59)47(76)66-40-21-27-61-54(83)44(32(5)72)70-51(80)39(20-26-60)64-46(75)36(17-23-57)65-52(81)41(28-31(3)4)68-53(82)42(29-34-13-8-7-9-14-34)69-48(77)37(18-24-58)63-49(40)78/h7-9,13-14,30-33,35-42,44-45,72-73H,10-12,15-29,56-60H2,1-6H3,(H,61,83)(H,62,74)(H,63,78)(H,64,75)(H,65,81)(H,66,76)(H,67,84)(H,68,82)(H,69,77)(H,70,80)(H,71,79)/t32-,33-,35+,36+,37+,38+,39+,40+,41+,42-,44+,45+/m1/s1	SGPYLFWAQBAXCZ-RUDZPDEXSA-N

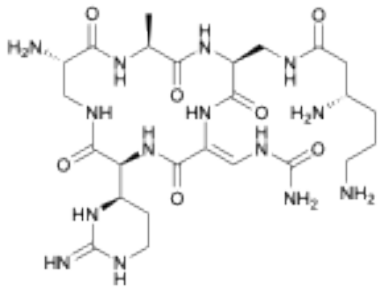
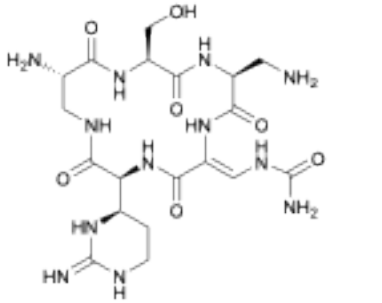
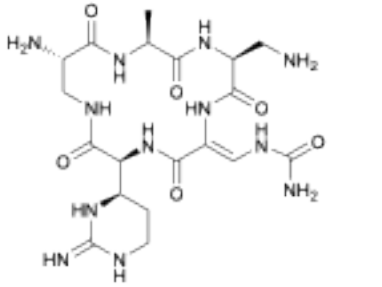
Name	#	Chemdraw	SMILES	InChI	InChIKey
polymyxin E_1	**7.06a**		CC[C@H](C)CCCCC(N[C@H](C(N[C@@H]([C@H](O)C)C(N[C@H](C(N[C@H]1CCNC([C@H]([C@H](O)C)NC([C@@H](NC([C@@H](NC([C@@H](NC([C@@H](NC([C@@H](NC1=O)CCN)=O)CC(C)C)=O)CC(C)C)=O)CCN)=O)CCN)=O)=O)=O)CCN)=O)=O)CCN)=O	InChI=1S/C53H100N16O13/c1-9-30(6)12-10-11-13-41(72)60-33(14-20-54)48(77)69-43(32(8)71)53(82)65-36(17-23-57)45(74)64-38-19-25-59-52(81)42(31(7)70)68-49(78)37(18-24-58)62-44(73)34(15-21-55)63-50(79)39(26-28(2)3)67-51(80)40(27-29(4)5)66-46(75)35(16-22-56)61-47(38)76/h28-40,42-43,70-71H,9-27,54-58H2,1-8H3,(H,59,81)(H,60,72)(H,61,76)(H,62,73)(H,63,79)(H,64,74)(H,65,82)(H,66,75)(H,67,80)(H,68,78)(H,69,77)/t30-,31+,32+,33-,34-,35-,36-,37-,38-,39-,40+,42-,43-/m0/s1	XDJYMJULXQKGMM-HHAJOKTESA-N

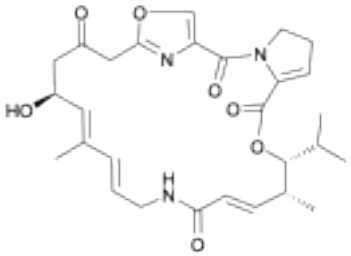
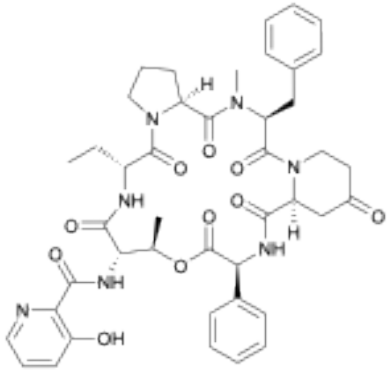
Name	#	Chemdraw	SMILES	InChI	InChIKey
polymyxin E_2	**7.06b**		NCC[C@@H](C(N[C@@H]([C@H](O)C)C(N[C@H](C(N[C@H]1CCNC([C@H]([C@H](O)C)NC([C@@H](NC([C@@H](NC([C@@H](NC([C@H](NC([C@@H](NC1=O)CCN)=O)CC(C)C)=O)CC(C)C)=O)CCN)=O)CCN)=O)=O)=O)CCN)=O)=O)NC(CCCCC(C)C)=O	InChI=1S/C52H98N16O13/c1-27(2)11-9-10-12-40(71)59-32(13-19-53)47(76)68-42(31(8)70)52(81)64-35(16-22-56)44(73)63-37-18-24-58-51(80)41(30(7)69)67-48(77)36(17-23-57)61-43(72)33(14-20-54)62-49(78)38(25-28(3)4)66-50(79)39(26-29(5)6)65-45(74)34(15-21-55)60-46(37)75/h27-39,41-42,69-70H,9-26,53-57H2,1-8H3,(H,58,80)(H,59,71)(H,60,75)(H,61,72)(H,62,78)(H,63,73)(H,64,81)(H,65,74)(H,66,79)(H,67,77)(H,68,76)/t30-,31-,32+,33+,34+,35+,36+,37+,38+,39-,41+,42+/m1/s1	KNIWPHSUTGNZST-SSWRVQTPSA-N

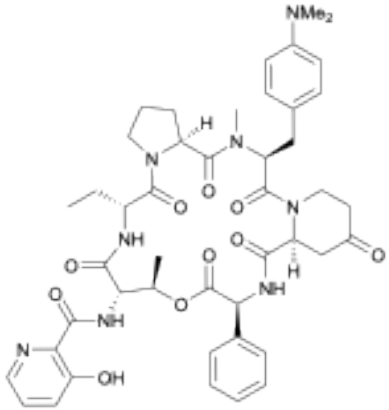
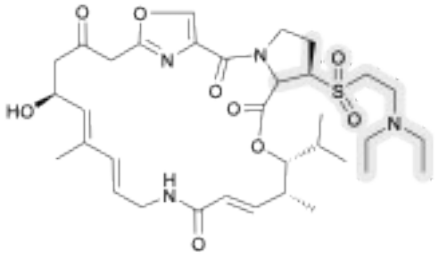
Name	#	Chemdraw	SMILES	InChI	InChIKey
colistin methanesulfonate E_1	**7.07a**		CC[C@H](C)CCCCC(N[C@H](C(N[C@@H]([C@H](O)C)C(N[C@H](C(N[C@H]1CCNC([C@H]([C@H](O)C)NC([C@@H](NC([C@@H](NC([C@@H](NC([C@@H](NC([C@@H](NC1=O)CCNCS(=O)(O)=O)=O)CC(C)C)=O)CC(C)C)=O)CCNCS(=O)(O)=O)=O)CCNCS(=O)(O)=O)=O)=O)CCNCS(=O)(O)=O)=O)=O)CCNCS(=O)(O)=O)=O	InChI=1S/C58H110N16O28S5/c1-9-35(6)12-10-11-13-46(77)65-38(14-20-59-28-103(88,89)90)53(82)74-48(37(8)76)58(87)70-41(17-23-62-31-106(97,98)99)50(79)68-43-19-25-64-57(86)47(36(7)75)73-54(83)42(18-24-63-32-107(100,101)102)67-49(78)39(15-21-60-29-104(91,92)93)69-55(84)44(26-33(2)3)72-56(85)45(27-34(4)5)71-52(81)40(66-51(43)80)16-22-61-30-105(94,95)96/h33-45,47-48,59-63,75-76H,9-32H2,1-8H3,(H,64,86)(H,65,77)(H,66,80)(H,67,78)(H,68,79)(H,69,84)(H,70,87)(H,71,81)(H,72,85)(H,73,83)(H,74,82)(H,88,89,90)(H,91,92,93)(H,94,95,96)(H,97,98,99)(H,100,101,102)/t35-,36+,37+,38-,39-,40-,41-,42-,43-,44-,45+,47-,48-/m0/s1	BSSIRFLGSWHWDE-LOFSPICBSA-N

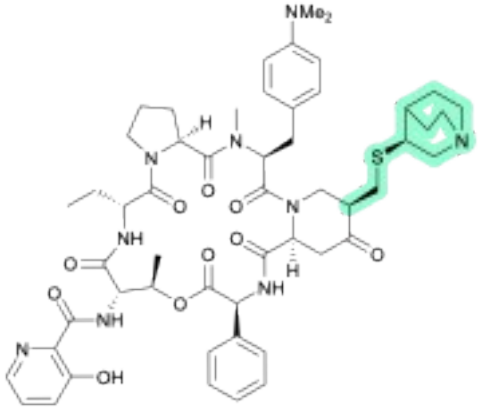
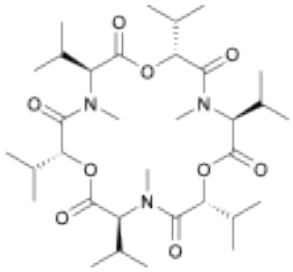
Name	#	Chemdraw	SMILES	InChI	InChIKey
colistin methanesulfonate E_2	**7.07b**		CC(C)C[C@H](NC([C@H](NC([C@@H](NC1=O)CCNCS(=O)(O)=O)=O)CC(C)C)=O)C(N[C@@H](CCNCS(=O)(O)=O)C(N[C@@H](CCNCS(=O)(O)=O)C(N[C@@H]([C@H](O)C)C(NCC[C@@H]1NC([C@H](CCNCS(=O)(O)=O)NC([C@H]([C@H](O)C)NC([C@H](CCNCS(=O)(O)=O)NC(CCCCC(C)C)=O)=O)=O)=O)=O)=O)=O	InChI=1S/C57H108N16O28S5/c1-32(2)11-9-10-12-45(76)64-37(13-19-58-27-102(87,88)89)52(81)73-47(36(8)75)57(86)69-40(16-22-61-30-105(96,97)98)49(78)67-42-18-24-63-56(85)46(35(7)74)72-53(82)41(17-23-62-31-106(99,100)101)66-48(77)38(14-20-59-28-103(90,91)92)68-54(83)43(25-33(3)4)71-55(84)44(26-34(5)6)70-51(80)39(65-50(42)79)15-21-60-29-104(93,94)95/h32-44,46-47,58-62,74-75H,9-31H2,1-8H3,(H,63,85)(H,64,76)(H,65,79)(H,66,77)(H,67,78)(H,68,83)(H,69,86)(H,70,80)(H,71,84)(H,72,82)(H,73,81)(H,87,88,89)(H,90,91,92)(H,93,94,95)(H,96,97,98)(H,99,100,101)/t35-,36-,37+,38+,39+,40+,41+,42+,43+,44-,46+,47+/m1/s1	DFSJNVZGJOIDRT-BJISPZADSA-N

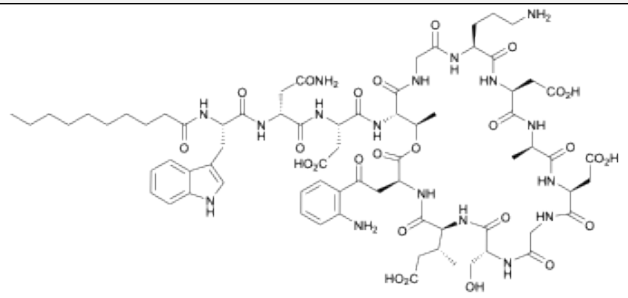
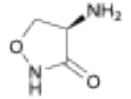
Name	#	Chemdraw	SMILES	InChI	InChIKey
viomycin	**7.08**		O[C@@H](C[C@H]([C@H]1C(NC[C@H](NC(C[C@@H](N)CCCN)=O)C(N[C@@H](CO)C(N[C@@H](CO)C(N/C(C(N1)=O)=C\NC(N)=O)=O)=O)=O)=O)N2)NC2=N	InChI=1S/C25H43N13O10/c26-3-1-2-10(27)4-16(41)32-12-6-30-23(47)18(11-5-17(42)37-24(28)36-11)38-20(44)13(7-31-25(29)48)33-21(45)14(8-39)35-22(46)15(9-40)34-19(12)43/h7,10-12,14-15,17-18,39-40,42H,1-6,8-9,26-27H2,(H,30,47)(H,32,41)(H,33,45)(H,34,43)(H,35,46)(H,38,44)(H3,28,36,37)(H3,29,31,48)/b13-7-/t10-,11+,12-,14-,15-,17-,18-/m0/s1	GXFAIFRPOKBQRV-GHXCTMGLSA-N
capreomycin IA	**7.09a**		N=C1N[C@@H]([C@H]2C(NC[C@H](N)C(N[C@@H](CO)C(N[C@@H](CNC(C[C@@H](N)CCCN)=O)C(N/C(C(N2)=O)=C\NC(N)=O)=O)=O)=O)=O)CCN1	InChI=1S/C25H44N14O8/c26-4-1-2-11(27)6-17(41)32-8-14-20(43)35-15(9-34-25(30)47)21(44)39-18(13-3-5-31-24(29)38-13)23(46)33-7-12(28)19(42)37-16(10-40)22(45)36-14/h9,11-14,16,18,40H,1-8,10,26-28H2,(H,32,41)(H,33,46)(H,35,43)(H,36,45)(H,37,42)(H,39,44)(H3,29,31,38)(H3,30,34,47)/b15-9-/t11-,12-,13+,14-,16-,18-/m0/s1	JNIIDKODPGHQSS-MPSMQSNBSA-N

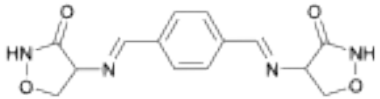
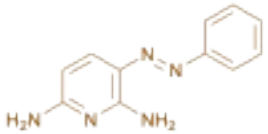
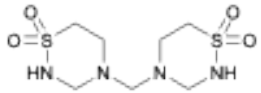
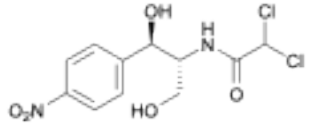
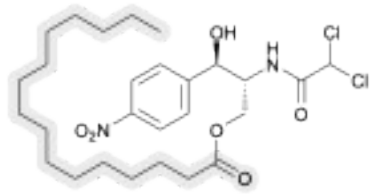
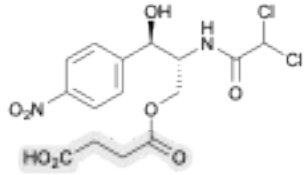
Name	#	Chemdraw	SMILES	InChI	InChIKey
capreomycin IB	**7.09b**		N=C1N[C@@H]([C@H]2C(NC[C@H](N)C(N[C@@H](C)C(N[C@@H](CNC(C[C@@H](N)CCCN)=O)C(N/C(C(N2)=O)=C\NC(N)=O)=O)=O)=O)=O)CCN1	InChI=1S/C25H44N14O7/c1-11-19(41)36-15(9-32-17(40)7-12(27)3-2-5-26)21(43)37-16(10-34-25(30)46)22(44)39-18(14-4-6-31-24(29)38-14)23(45)33-8-13(28)20(42)35-11/h10-15,18H,2-9,26-28H2,1H3,(H,32,40)(H,33,45)(H,35,42)(H,36,41)(H,37,43)(H,39,44)(H3,29,31,38)(H3,30,34,46)/b16-10-/t11-,12-,13-,14+,15-,18-/m0/s1	FRXNXDHFQYZYNA-GOTGUIIGSA-N
capreomycin IIA	**7.09c**		N=C1N[C@@H]([C@H]2C(NC[C@H](N)C(N[C@@H](CO)C(N[C@@H](CN)C(N/C(C(N2)=O)=C\NC(N)=O)=O)=O)=O)=O)CCN1	InChI=1S/C19H32N12O7/c20-3-9-14(34)28-10(5-26-19(23)38)15(35)31-12(8-1-2-24-18(22)30-8)17(37)25-4-7(21)13(33)29-11(6-32)16(36)27-9/h5,7-9,11-12,32H,1-4,6,20-21H2,(H,25,37)(H,27,36)(H,28,34)(H,29,33)(H,31,35)(H3,22,24,30)(H3,23,26,38)/b10-5-/t7-,8+,9-,11-,12-/m0/s1	XFGCTBYTRMLWCB-MRSVHRRQSA-N
capreomycin IIB	**7.09d**		N=C1N[C@@H]([C@H]2C(NC[C@H](N)C(N[C@@H](C)C(N[C@@H](CN)C(N/C(C(N2)=O)=C\NC(N)=O)=O)=O)=O)=O)CCN1	InChI=1S/C19H32N12O6/c1-7-13(32)28-10(4-20)15(34)29-11(6-26-19(23)37)16(35)31-12(9-2-3-24-18(22)30-9)17(36)25-5-8(21)14(33)27-7/h6-10,12H,2-5,20-21H2,1H3,(H,25,36)(H,27,33)(H,28,32)(H,29,34)(H,31,35)(H3,22,24,30)(H3,23,26,37)/b11-6-/t7-,8-,9+,10-,12-/m0/s1	MHBQQDNEPQYCOS-CBQPQWBASA-N

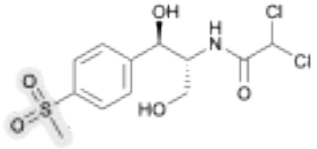
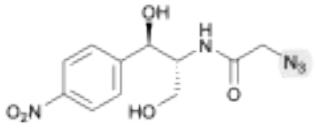
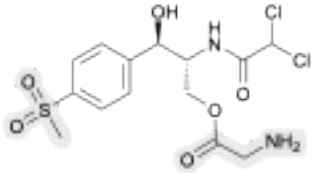
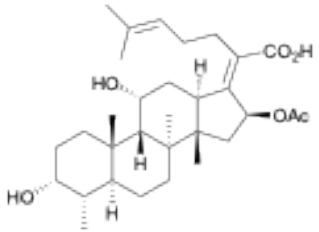
Name	#	Chemdraw	SMILES	InChI	InChIKey
virginiamycin M_1	**7.10a**		C[C@@H]1/C=C/C(NC/C=C/C(C)=C/[C@@H](O)CC(CC2=NC(C(N3CCC=C3C(O[C@@H]1C(C)C)=O)=O)=CO2)=O)=O	InChI=1S/C28H35N3O7/c1-17(2)26-19(4)9-10-24(34)29-11-5-7-18(3)13-20(32)14-21(33)15-25-30-22(16-37-25)27(35)31-12-6-8-23(31)28(36)38-26/h5,7-10,13,16-17,19-20,26,32H,6,11-12,14-15H2,1-4H3,(H,29,34)/b7-5+,10-9+,18-13+/t19-,20-,26-/m1/s1	DAIKHDNSXMZDCU-FQTGFAPKSA-N
virginiamycin S_1	**7.10b**		O=C1N2[C@](CC(CC2=O)([H])C(N[C@@H](C3=CC=CC=C3)C(O[C@@H]([C@@H](C(N[C@@H](C(N4[C@](CCC4)([H])C(N([C@H]1CC5=CC=CC=C5)C)=O)=O)CC)=O)NC(C6=C(O)C=CC=N6)=O)C)=O)=O	InChI=1S/C43H49N7O10/c1-4-29-40(56)49-21-12-17-30(49)41(57)48(3)32(23-26-13-7-5-8-14-26)42(58)50-22-19-28(51)24-31(50)37(53)47-35(27-15-9-6-10-16-27)43(59)60-25(2)34(38(54)45-29)46-39(55)36-33(52)18-11-20-44-36/h5-11,13-16,18,20,25,29-32,34-35,52H,4,12,17,19,21-24H2,1-3H3,(H,45,54)(H,46,55)(H,47,53)/t25-,29-,30+,31+,32+,34+,35+/m1/s1	FEPMHVLSLDOMQC-IYPFLVAKSA-N

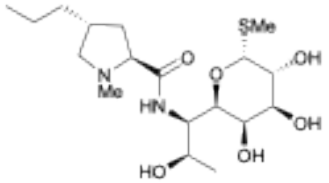
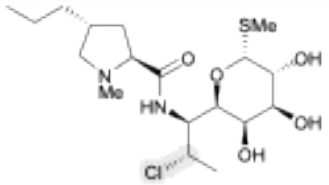
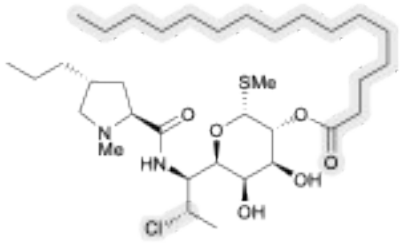
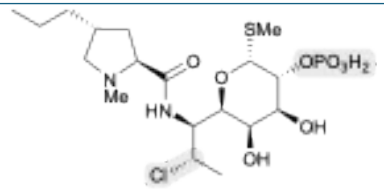
Name	#	Chemdraw	SMILES	InChI	InChIKey
pristinamycin I_A	**7.11**		O=C1N2[C@](CC(CC2)=O)([H])C(N[C@@H](C3=CC=CC=C3)C(O[C@@H]([C@@H](C(N[C@@H](C(N4[C@](CCC4)([H])C(N([C@H]1CC5=CC=C(C=C5)N(C)C)C)=O)=O)CC)=O)NC(C6=C(O)C=CC=N6)=O)C)=O)=O	InChI=1S/C45H54N8O10/c1-6-31-42(59)52-22-11-14-32(52)43(60)51(5)34(24-27-16-18-29(19-17-27)50(3)4)44(61)53-23-20-30(54)25-33(53)39(56)49-37(28-12-8-7-9-13-28)45(62)63-26(2)36(40(57)47-31)48-41(58)38-35(55)15-10-21-46-38/h7-10,12-13,15-19,21,26,31-34,36-37,55H,6,11,14,20,22-25H2,1-5H3,(H,47,57)(H,48,58)(H,49,56)/t26-,31-,32+,33+,34+,36+,37+/m1/s1	YGXCETJZBDTKRY-DZCVGBHJSA-N
dalfopristin	**7.12**		C[C@@H]1/C=C/C(NC/C=C/C(C)=C/[C@@H](O)CC(CC2=NC(C(N3CC[C@@H](S(CCN(CC)CC)(=O)=O)C3C(O[C@@H]1C(C)C)=O)=O)=CO2)=O)=O	InChI=1S/C34H50N4O9S/c1-7-37(8-2)16-17-48(44,45)28-13-15-38-31(28)34(43)47-32(22(3)4)24(6)11-12-29(41)35-14-9-10-23(5)18-25(39)19-26(40)20-30-36-27(21-46-30)33(38)42/h9-12,18,21-22,24-25,28,31-32,39H,7-8,13-17,19-20H2,1-6H3,(H,35,41)/b10-9+,12-11+,23-18+/t24-,25-,28-,31?,32-/m1/s1	SUYRLXYYZQTJHF-RJUFQJKESA-N

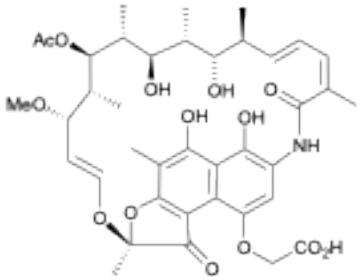
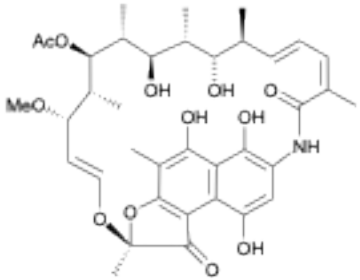
Name	#	Chemdraw	SMILES	InChI	InChIKey
quinupristin	**7.13**		O=C1N2[C@](CC([C@H](CS[C@@H]3CN4CCC3CC4)C2)=O)([H])C(N[C@@H](C5=CC=CC=C5)C(O[C@@H]([C@@H](C(N[C@@H](C(N6[C@](CCC6)([H])C(N([C@H]1CC7=CC=C(C=C7)N(C)C)C)=O)=O)CC)=O)NC(C8=C(O)C=CC=N8)=O)C)=O)=O	InChI=1S/C53H67N9O10S/c1-6-37-50(68)61-23-11-14-38(61)51(69)59(5)40(26-32-16-18-36(19-17-32)58(3)4)52(70)62-28-35(30-73-43-29-60-24-20-33(43)21-25-60)42(64)27-39(62)47(65)57-45(34-12-8-7-9-13-34)53(71)72-31(2)44(48(66)55-37)56-49(67)46-41(63)15-10-22-54-46/h7-10,12-13,15-19,22,31,33,35,37-40,43-45,63H,6,11,14,20-21,23-30H2,1-5H3,(H,55,66)(H,56,67)(H,57,65)/t31-,35+,37-,38+,39+,40+,43-,44+,45+/m1/s1	WTHRRGMBUAHGNI-LCYNINFDSA-N
enniatin B	**7.14**		CC([C@H]1C(O[C@H](C(C)C)C(N(C)[C@@H](C(C)C)C(O[C@H](C(C)C)C(N(C)[C@@H](C(C)C)C(O[C@H](C(C)C)C(N1C)=O)=O)=O)=O)=O)=O)C	InChI=1S/C33H57N3O9/c1-16(2)22-31(40)43-26(20(9)10)29(38)35(14)24(18(5)6)33(42)45-27(21(11)12)30(39)36(15)23(17(3)4)32(41)44-25(19(7)8)28(37)34(22)13/h16-27H,1-15H3/t22-,23-,24-,25+,26+,27+/m0/s1	MIZMDSVSLSIMSC-VYLWARHZSA-N

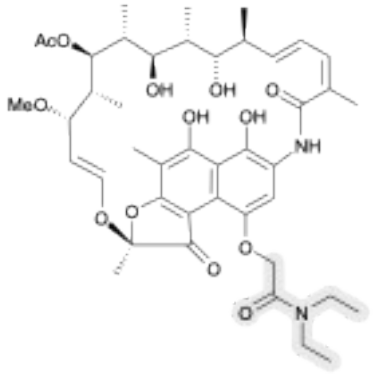
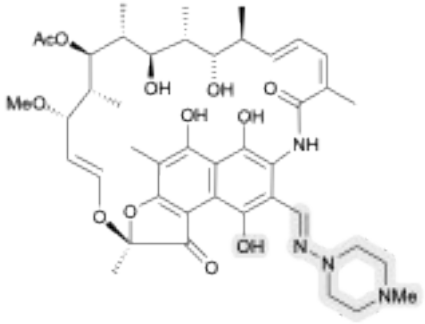
Name	#	Chemdraw	SMILES	InChI	InChIKey
daptomycin	**7.15**		C[C@@H](OC([C@@H](NC([C@@H](NC([C@H](NC(CNC([C@@H](NC([C@H](NC([C@@H](NC([C@@H](NC(CNC1=O)=O)CCCN)=O)CC(O)=O)=O)C)=O)CC(O)=O)=O)=O)CO)=O)[C@@H](CC(O)=O)C)=O)CC(C2=C(N)C=CC=C2)=O)=O)[C@@H]1NC([C@H](CC(O)=O)NC([C@@H](CC(N)=O)NC([C@@H](NC(CCCCCCCCC)=O)CC3=CNC4=CC=CC=C34)=O)=O)=O	InChI=1S/C72H101N17O26/c1-5-6-7-8-9-10-11-22-53(93)81-44(25-38-31-76-42-20-15-13-17-39(38)42)66(108)84-45(27-52(75)92)67(109)86-48(30-59(102)103)68(110)89-61-37(4)115-72(114)49(26-51(91)40-18-12-14-19-41(40)74)87-71(113)60(35(2)24-56(96)97)88-69(111)50(34-90)82-55(95)32-77-63(105)46(28-57(98)99)83-62(104)36(3)79-65(107)47(29-58(100)101)85-64(106)43(21-16-23-73)80-54(94)33-78-70(61)112/h12-15,17-20,31,35-37,43-50,60-61,76,90H,5-11,16,21-30,32-34,73-74H2,1-4H3,(H2,75,92)(H,77,105)(H,78,112)(H,79,107)(H,80,94)(H,81,93)(H,82,95)(H,83,104)(H,84,108)(H,85,106)(H,86,109)(H,87,113)(H,88,111)(H,89,110)(H,96,97)(H,98,99)(H,100,101)(H,102,103)/t35-,36-,37-,43+,44-,45+,46-,47-,48?,49+,50-,60+,61+/m0/s1	DOAKLVKFURWEDJ-FYKMPORGSA-N
D-cycloserine	**8.01**		N[C@H]1C(NOC1)=O	InChI=1S/C3H6N2O2/c4-2-1-7-5-3(2)6/h2H,1,4H2,(H,5,6)/t2-/m1/s1	DYDCUQKUCUHJBH-UWTATZPHSA-N

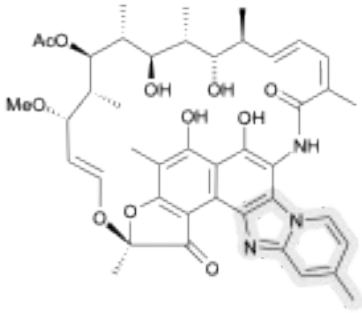
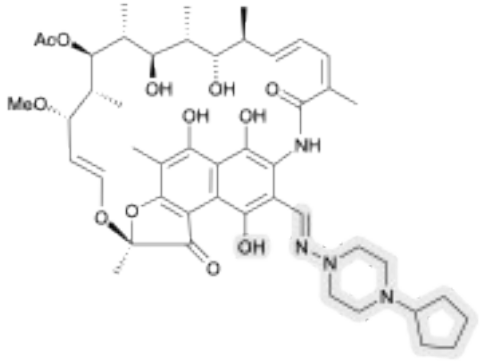
Name	#	Chemdraw	SMILES	InChI	InChIKey
terizidone	**8.02**		O=C1NOCC1/N=C/C2=CC=C(/C=N/C3CONC3=O)C=C2	InChI=1S/C14H14N4O4/c19-13-11(7-21-17-13)15-5-9-1-2-10(4-3-9)6-16-12-8-22-18-14(12)20/h1-6,11-12H,7-8H2,(H,17,19)(H,18,20)/b15-5+,16-6+	ODKYYBOHSVLGNU-IAGONARPSA-N
phenazopyridine	**8.02a**		NC(C=C1)=NC(N)=C1/N=N/C2=CC=CC=C2	InChI=1S/C11H11N5/c12-10-7-6-9(11(13)14-10)16-15-8-4-2-1-3-5-8/h1-7H,(H4,12,13,14)/b16-15+	QPFYXYFORQJZEC-FOCLMDBBSA-N
taurolidine	**8.03**		O=S1(CCN(CN2CNS(=O)(CC2)=O)CN1)=O	InChI=1S/C7H16N4O4S2/c12-16(13)3-1-10(5-8-16)7-11-2-4-17(14,15)9-6-11/h8-9H,1-7H2	AJKIRUJIDFJUKJ-UHFFFAOYSA-N
chloramphenicol	**9.01**		ClC(Cl)C(N[C@H](CO)[C@@H](C1=CC=C(C=C1)[N+]([O-])=O)O)=O	InChI=1S/C11H12Cl2N2O5/c12-10(13)11(18)14-8(5-16)9(17)6-1-3-7(4-2-6)15(19)20/h1-4,8-10,16-17H,5H2,(H,14,18)/t8-,9-/m1/s1	WIIZWVCIJKGZOK-RKDXNWHRSA-N
chloramphenicol palmitate	**9.02**		ClC(Cl)C(N[C@H](COC(CCCCCCCCCCCCCCC)=O)[C@@H](C1=CC=C(C=C1)[N+]([O-])=O)O)=O	InChI=1S/C27H42Cl2N2O6/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-24(32)37-20-23(30-27(34)26(28)29)25(33)21-16-18-22(19-17-21)31(35)36/h16-19,23,25-26,33H,2-15,20H2,1H3,(H,30,34)/t23-,25-/m1/s1	PXKHGMGELZGJQE-ILBGXUMGSA-N
chloramphenicol hemisuccinate	**9.03**		ClC(Cl)C(N[C@H](COC(CCC(O)=O)=O)[C@@H](C1=CC=C(C=C1)[N+]([O-])=O)O)=O	InChI=1S/C15H16Cl2N2O8/c16-14(17)15(24)18-10(7-27-12(22)6-5-11(20)21)13(23)8-1-3-9(4-2-8)19(25)26/h1-4,10,13-14,23H,5-7H2,(H,18,24)(H,20,21)/t10-,13+/m1/s1	LIRCDOVJWUGTMW-MFKMUULPSA-N

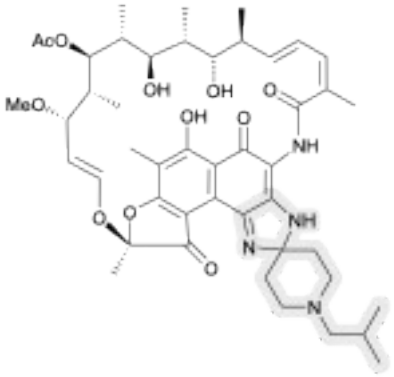
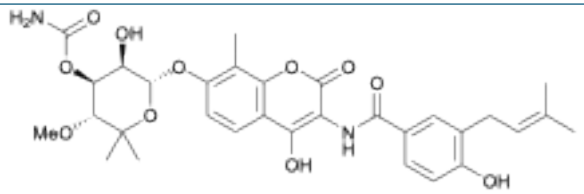
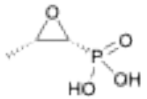
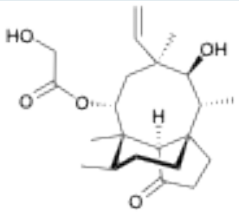
Name	#	Chemdraw	SMILES	InChI	InChIKey
thiamphenicol	**9.04**		ClC(Cl)C(N[C@H](CO)[C@@H](C1=CC=C(C=C1)S(C)(=O)=O)O)=O	InChI=1S/C12H15Cl2NO5S/c1-21(19,20)8-4-2-7(3-5-8)10(17)9(6-16)15-12(18)11(13)14/h2-5,9-11,16-17H,6H2,1H3,(H,15,18)/t9-,10-/m1/s1	OTVAEFIXJLOWRX-NXEZZACHSA-N
azidamfenicol	**9.05**		O=C(CN=[N+]=[N-])N[C@H](CO)[C@@H](C1=CC=C(C=C1)[N+]([O-])=O)O	InChI=1S/C11H13N5O5/c12-15-13-5-10(18)14-9(6-17)11(19)7-1-3-8(4-2-7)16(20)21/h1-4,9,11,17,19H,5-6H2,(H,14,18)/t9-,11-/m1/s1	SGRUZFCHLOFYHZ-MWLCHTKSSA-N
thiamphenicol glycinate	**9.06**		ClC(Cl)C(N[C@H](COC(CN)=O)[C@@H](C1=CC=C(C=C1)S(C)(=O)=O)O)=O	InChI=1S/C14H18Cl2N2O6S/c1-25(22,23)9-4-2-8(3-5-9)12(20)10(7-24-11(19)6-17)18-14(21)13(15)16/h2-5,10,12-13,20H,6-7,17H2,1H3,(H,18,21)/t10-,12-/m1/s1	AMGKHLVPQHMHGQ-ZYHUDNBSSA-N
fusidic acid	**10.01**		C[C@@]12[C@@]3([C@](C[C@H]([C@@]1([H])[C@@]4([C@@]([C@@H]([C@@H](CC4)O)C)([H])CC2)C)O)([H])/C([C@H](C3)OC(C)=O)=C(C(O)=O)\CC/C=C(C)\C)C	InChI=1S/C31H48O6/c1-17(2)9-8-10-20(28(35)36)26-22-15-24(34)27-29(5)13-12-23(33)18(3)21(29)11-14-30(27,6)31(22,7)16-25(26)37-19(4)32/h9,18,21-25,27,33-34H,8,10-16H2,1-7H3,(H,35,36)/b26-20-/t18-,21-,22-,23+,24+,25-,27-,29-,30-,31-/m0/s1	IECPWNUMDGFDKC-MZJAQBGESA-N

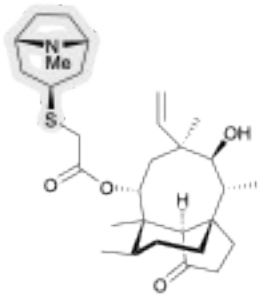
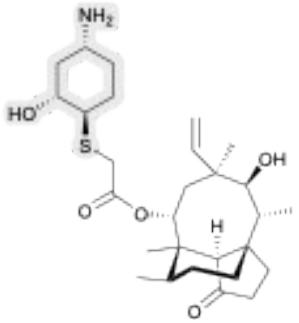
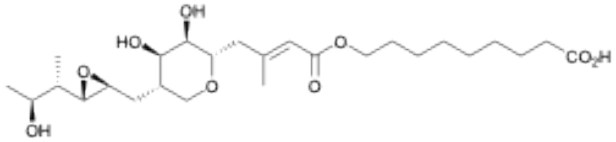
Name	#	Chemdraw	SMILES	InChI	InChIKey
lincomycin	**11.01**		O=C([C@H]1N(C[C@@H](C1)CCC)C)N[C@H]([C@@H](C)O)[C@H]2O[C@@H]([C@@H]([C@H]([C@H]2O)O)O)SC	InChI=1S/C18H34N2O6S/c1-5-6-10-7-11(20(3)8-10)17(25)19-12(9(2)21)16-14(23)13(22)15(24)18(26-16)27-4/h9-16,18,21-24H,5-8H2,1-4H3,(H,19,25)/t9-,10-,11+,12-,13+,14-,15-,16-,18-/m1/s1	OJMMVQQUTAEWLP-KIDUDLJLSA-N
clindamycin	**11.02**		O=C([C@H]1N(C[C@@H](C1)CCC)C)N[C@H]([C@H](C)Cl)[C@H]2O[C@@H]([C@@H]([C@H]([C@H]2O)O)O)SC	InChI=1S/C18H33ClN2O5S/c1-5-6-10-7-11(21(3)8-10)17(25)20-12(9(2)19)16-14(23)13(22)15(24)18(26-16)27-4/h9-16,18,22-24H,5-8H2,1-4H3,(H,20,25)/t9-,10+,11-,12+,13-,14+,15+,16+,18+/m0/s1	KDLRVYVGXIQJDK-AWPVFWJPSA-N
clindamycin palmitate	**11.03**		O=C([C@H]1N(C[C@@H](C1)CCC)C)N[C@H]([C@H](C)Cl)[C@H]2O[C@@H]([C@@H]([C@H]([C@H]2O)O)OC(CCCCCCCCCCCCCCC)=O)SC	InChI=1S/C34H63ClN2O6S/c1-6-8-9-10-11-12-13-14-15-16-17-18-19-21-27(38)42-32-30(40)29(39)31(43-34(32)44-5)28(24(3)35)36-33(41)26-22-25(20-7-2)23-37(26)4/h24-26,28-32,34,39-40H,6-23H2,1-5H3,(H,36,41)/t24-,25+,26-,28+,29+,30-,31+,32+,34+/m0/s1	OYSKUZDIHNKWLV-PRUAPSLNSA-N
clindamycin phosphate	**11.04**		O=C([C@H]1N(C[C@@H](C1)CCC)C)N[C@H]([C@H](C)Cl)[C@H]2O[C@@H]([C@@H]([C@H]([C@H]2O)O)OP(O)(O)=O)SC	InChI=1S/C18H34ClN2O8PS/c1-5-6-10-7-11(21(3)8-10)17(24)20-12(9(2)19)16-14(23)13(22)15(29-16)31-4)29-30(25,26)27/h9-16,18,22-23H,5-8H2,1-4H3,(H,20,24)(H2,25,26,27)/t9-,10+,11-,12+,13+,14-,15+,16+,18+/m0/s1	UFUVLHLTWXBHGZ-MGZQPHGTSA-N

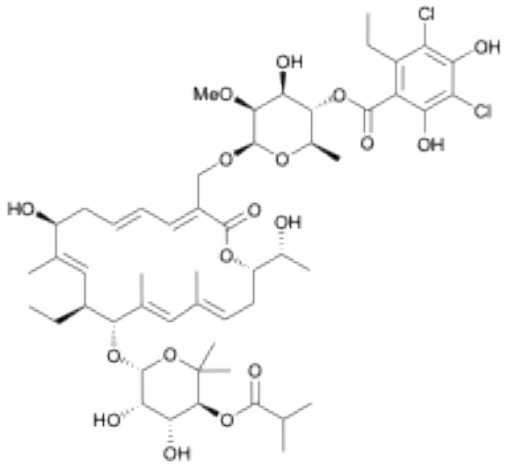
Name	#	Chemdraw	SMILES	InChI	InChIKey
rifamycin B	**12.01**		C/C(C(N1)=O)=C/C=C/[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(C)=O)[C@H](C)[C@@H](OC)/C=C/O[C@@]2(C)OC3=C(C(C(OCC(O)=O)=CC1=C4O)=C4C(O)=C3C)C2=O	InChI=1S/C39H49NO14/c1-17-11-10-12-18(2)38(49)40-24-15-26(51-16-27(42)43)28-29(34(24)47)33(46)22(6)36-30(28)37(48)39(8,54-36)52-14-13-25(50-9)19(3)35(53-23(7)41)21(5)32(45)20(4)31(17)44/h10-15,17,19-21,25,31-32,35,44-47H,16H2,1-9H3,(H,40,49)(H,42,43)/b11-10+,14-13+,18-12-/t17-,19+,20+,21+,25-,31-,32+,35+,39-/m0/s1	SQTCRTQCPJICLD-KTQDUKAHSA-N
rifamycin SV	**12.02**		C/C(C(N1)=O)=C/C=C/[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(C)=O)[C@H](C)[C@@H](OC)/C=C/O[C@@]2(C)OC3=C(C(C(O)=CC1=C4O)=C4C(O)=C3C)C2=O	InChI=1S/C37H47NO12/c1-16-11-10-12-17(2)36(46)38-23-15-24(40)26-27(32(23)44)31(43)21(6)34-28(26)35(45)37(8,50-34)48-14-13-25(47-9)18(3)33(49-22(7)39)20(5)30(42)19(4)29(16)41/h10-16,18-20,25,29-30,33,40-44H,1-9H3,(H,38,46)/b11-10+,14-13+,17-12-/t16-,18+,19+,20+,25-,29-,30+,33+,37-/m0/s1	HJYYPODYNSCCOU-ODRIEIDWSA-N

Name	#	Chemdraw	SMILES	InChI	InChIKey
rifamide	**12.03**		C/C(C(N1)=O)=C/C=C/[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(C)=O)[C@H](C)[C@@H](OC)/C=C/O[C@@]2(C)OC3=C(C(C(OCC(N(CC)CC)=O)=CC1=C4O)=C4C(O)=C3C)C2=O	InChI=1S/C43H58N2O13/c1-12-45(13-2)31(47)20-55-30-19-28-38(51)33-32(30)34-40(26(8)37(33)50)58-43(10,41(34)52)56-18-17-29(54-11)23(5)39(57-27(9)46)25(7)36(49)24(6)35(48)21(3)15-14-16-22(4)42(53)44-28/h14-19,21,23-25,29,35-36,39,48-51H,12-13,20H2,1-11H3,(H,44,53)/b15-14+,18-17+,22-16-/t21-,23+,24+,25+,29-,35-,36+,39+,43-/m0/s1	VFYNXKZVOUXHDX-VDPUEHCXSA-N
rifampicin	**12.04**		C/C(C(N1)=O)=C/C=C/[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(C)=O)[C@H](C)[C@@H](OC)/C=C/O[C@@]2(C)OC3=C(C(C(O)=C(/C=N/N4CCN(CC4)C)C1=C5O)=C5C(O)=C3C)C2=O	InChI=1S/C43H58N4O12/c1-21-12-11-13-22(2)42(55)45-33-28(20-44-47-17-15-46(9)16-18-47)37(52)30-31(38(33)53)36(51)26(6)40-32(30)41(54)43(8,59-40)57-19-14-29(56-10)23(3)39(58-27(7)48)25(5)35(50)24(4)34(21)49/h11-14,19-21,23-25,29,34-35,39,49-53H,15-18H2,1-10H3,(H,45,55)/b12-11+,19-14+,22-13-,44-20+/t21-,23+,24+,25+,29-,34-,35+,39+,43-/m0/s1	JQXXHWHPUNPDRT-WLSIYKJHSA-N

Name	#	Chemdraw	SMILES	InChI	InChIKey
rifaximin	**12.05**		C/C(C(N1)=O)=C/C=C/[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(C)=O)[C@H](C)[C@@H](OC)/C=C/O[C@@]2(C)OC3=C(C(C(N=C4N5C=CC(C)=C4)=C5C1=C6O)=C6C(O)=C3C)C2=O	InChI=1S/C43H51N3O11/c1-19-14-16-46-28(18-19)44-32-29-30-37(50)25(7)40-31(29)41(52)43(9,57-40)55-17-15-27(54-10)22(4)39(56-26(8)47)24(6)36(49)23(5)35(48)20(2)12-11-13-21(3)42(53)45-33(34(32)46)38(30)51/h11-18,20,22-24,27,35-36,39,48-51H,1-10H3,(H,45,53)/b12-11+,17-15+,21-13-/t20-,22+,23+,24+,27-,35-,36+,39+,43+/m0/s1	NZCRJKRKKOLAOJ-LUJLLCOKSA-N
rifapentine	**12.06**		C/C(C(N1)=O)=C/C=C/[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(C)=O)[C@H](C)[C@@H](OC)/C=C/O[C@@]2(C)OC3=C(C(C(O)=C(/C=N/N4CCN(CC4)C5CCCC5)C1=C6O)=C6C(O)=C3C)C2=O	InChI=1S/C47H64N4O12/c1-24-13-12-14-25(2)46(59)49-37-32(23-48-51-20-18-50(19-21-51)31-15-10-11-16-31)41(56)34-35(42(37)57)40(55)29(6)44-36(34)45(58)47(8,63-44)61-22-17-33(60-9)26(3)43(62-30(7)52)28(5)39(54)27(4)38(24)53/h12-14,17,22-24,26-28,31,33,38-39,43,53-57H,10-11,15-16,18-21H2,1-9H3,(H,49,59)/b13-12+,22-17+,25-14-,48-23+/t24-,26+,27+,28+,33-,38-,39+,43+,47-/m0/s1	WDZCUPBHRAEYDL-GZAUEHORSA-N

Name	#	Chemdraw	SMILES	InChI	InChIKey
rifabutin	**12.07**		C/C(C(N1)=O)=C/C=C/[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(C)=O)[C@H](C)[C@@H](OC)/C=C/O[C@@]2(C)OC3=C(C(C4=NC5(CCN(CC(C)C)CC5)NC4=C1C6=O)=C6C(O)=C3C)C2=O	InChI=1S/C46H62N4O11/c1-22(2)21-50-18-16-46(17-19-50)48-34-31-32-39(54)28(8)42-33(31)43(56)45(10,61-42)59-20-15-30(58-11)25(5)41(60-29(9)51)27(7)38(53)26(6)37(52)23(3)13-12-14-24(4)44(57)47-36(40(32)55)35(34)49-46/h12-15,20,22-23,25-27,30,37-38,41,49,52-54H,16-19,21H2,1-11H3,(H,47,57)/b13-12+,20-15+,24-14-/t23-,25+,26+,27+,30-,37-,38+,41+,45-/m0/s1	ATEBXHFBFRCZMA-VXTBVIBXSA-N
novobiocin	**13.01**		CC1=C(O[C@H]2[C@H](O)[C@H](OC(N)=O)[C@@H](OC)C(C)(C)O2)C=CC3=C1OC(C(NC(C4=CC(C/C=C(C)\C)=C(O)C=C4)=O)=C3O)=O	InChI=1S/C31H36N2O11/c1-14(2)7-8-16-13-17(9-11-19(16)34)27(37)33-21-22(35)18-10-12-20(15(3)24(18)42-28(21)38)41-29-23(36)25(43-30(32)39)26(40-6)31(4,5)44-29/h7,9-13,23,25-26,29,34-36H,8H2,1-6H3,(H2,32,39)(H,33,37)/t23-,25+,26-,29-/m1/s1	YJQPYGGHQPGBLI-KGSXXDOSSA-N
fosfomycin	**14.01**		C[C@H]1[C@@H](P(O)(O)=O)O1	InChI=1S/C3H7O4P/c1-2-3(7-2)8(4,5)6/h2-3H,1H3,(H2,4,5,6)/t2-,3+/m0/s1	YMDXZJFXQJVXBF-STHAYSLISA-N
pleuromutilin	**15.01**		[H][C@@]1([C@@]2(C)[C@H](C)CC[C@]13[C@@H](C)[C@H](O)[C@@](C=C)(C)C[C@H]2OC(CO)=O)C(CC3)=O	InChI=1S/C22H34O5/c1-6-20(4)11-16(27-17(25)12-23)21(5)13(2)7-9-22(14(3)19(20)26)10-8-15(24)18(21)22/h6,13-14,16,18-19,23,26H,1,7-12H2,2-5H3/t13-,14+,16-,18+,19+,20-,21+,22+/m1/s1	ZRZNJUXESFHSIO-BKUNHTPHSA-N

Name	#	Chemdraw	SMILES	InChI	InChIKey
retapamulin	**15.02**		[H][C@@]1([C@@]2(C)[C@H](C)CC[C@]13[C@@H](C)[C@H](O)[C@@](C=C)(C)C[C@H]2OC(CS[C@@H]4C[C@@H](CC[C@H]5C4)N5C)=O)C(CC3)=O	InChI=1S/C30H47NO4S/c1-7-28(4)16-24(35-25(33)17-36-22-14-20-8-9-21(15-22)31(20)6)29(5)18(2)10-12-30(19(3)27(28)34)13-11-23(32)26(29)30/h7,18-22,24,26-27,34H,1,8-17H2,2-6H3/t18-,19+,20+,21+,24-,26+,27+,28-,29+,30+/m1/s1	STZYTFJPGGDRJD-PFNMIMLKSA-N
lefamulin	**15.03**		[H][C@@]1([C@@]2(C)[C@H](C)CC[C@]13[C@@H](C)[C@H](O)[C@@](C=C)(C)C[C@H]2OC(CS[C@@H]4CC[C@H](C[C@H]4O)N)=O)C(CC3)=O	InChI=1S/C28H45NO5S/c1-6-26(4)14-22(34-23(32)15-35-21-8-7-18(29)13-20(21)31)27(5)16(2)9-11-28(17(3)25(26)33)12-10-19(30)24(27)28/h6,16-18,20-22,24-25,31,33H,1,7-15,29H2,2-5H3/t16-,17+,18-,20-,21-,22-,24+,25+,26-,27+,28+/m1/s1	KPVIXBKIJXZQJX-FCEONZPQSA-N
mupirocin	**16.01**		C/C(C[C@@H]1OC[C@H](C[C@H](O2)[C@@H]2[C@@H](C)[C@@H](O)C)[C@@H](O)[C@H]1O)=C\C(OCCCCCCCCC(O)=O)=O	InChI=1S/C26H44O9/c1-16(13-23(30)33-11-9-7-5-4-6-8-10-22(28)29)12-20-25(32)24(31)19(15-34-20)14-21-26(35-21)17(2)18(3)27/h13,17-21,24-27,31-32H,4-12,14-15H2,1-3H3,(H,28,29)/b16-13+/t17-,18-,19-,20-,21+,24+,25-,26-/m0/s1	MINDHVHHQZYEEK-HBBNESRFSA-N

Name	#	Chemdraw	SMILES	InChI	InChIKey
fidaxomicin	**17.01**		O=C1/C(CO[C@@H]2O[C@H](C)[C@@H](OC(C3=C(CC)C(Cl)=C(O)C(Cl)=C3O)=O)[C@H](O)[C@@H]2OC)=C/C=C/C[C@H](O)/C(C)=C/[C@H](CC)[C@@H](O[C@H]4[C@@H](O)[C@@H](O)[C@H](OC(C(C)C)=O)C(C)(C)O4)/C(C)=C/C(C)=C/[C@@H]([C@@H](C)O)O1	InChI=1S/C52H74Cl2O18/c1-13-30-22-26(6)33(56)18-16-15-17-31(23-66-51-45(65-12)42(61)44(29(9)67-51)69-49(64)35-32(14-2)36(53)39(58)37(54)38(35)57)48(63)68-34(28(8)55)20-19-25(5)21-27(7)43(30)70-50-41(60)40(59)46(52(10,11)72-50)71-47(62)24(3)4/h15-17,19,21-22,24,28-30,33-34,40-46,50-51,55-61H,13-14,18,20,23H2,1-12H3/b16-15+,25-19+,26-22+,27-21+,31-17+/t28-,29-,30+,33+,34+,40-,41+,42+,43+,44-,45+,46+,50-,51-/m1/s1	ZVGNESXIJDCBKN-UUEYKCAUSA-N