



# GD6 - Biotecnologie industriali: la produzione degli antibiotici - dal laboratorio allo scaffale

# LA CHEMOINFORMATICA NELLO SVILUPPO DI NUOVI FARMACI (UN APPROCCIO PRATICO)

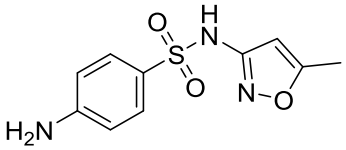
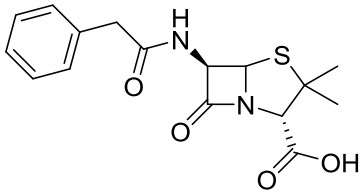
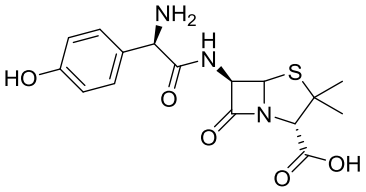
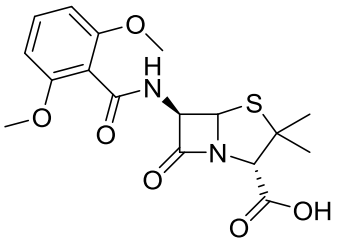
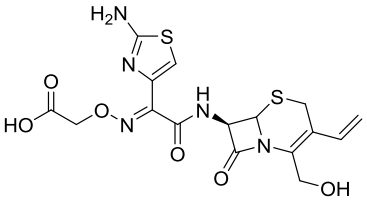
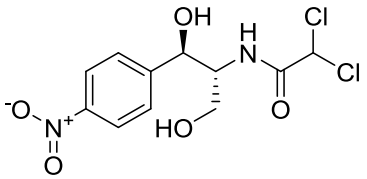
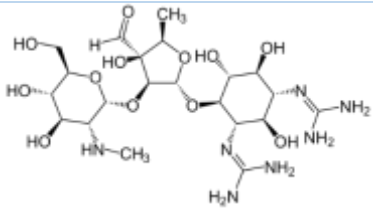
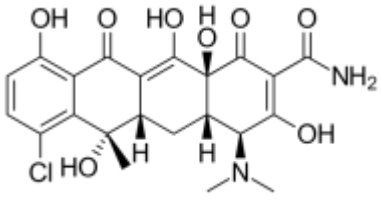
ITT «Buonarroti-Pozzo» Trento, 16 Aprile 2018

**A CURA DI ANDREA DEFANT PHD**

AZIONI A SUPPORTO DEL PIANO "TRENTINO TRILINGUE"
Potenziamento delle aree disciplinari di base per studenti del primo e del secondo ciclo di istruzione
Cod. 2015_3_1022_IP.01

Questa iniziativa è realizzata nell'ambito del Programma operativo FSE 2014-2020 della Provincia autonoma di Trento grazie al sostegno finanziario del Fondo sociale europeo, dello Stato italiano e della Provincia autonoma di Trento

# STRUTTURE DI ANTIBIOTICI E ANTIBATTERICI DI SINTESI

| N° | STRUTTURA | NOME (Classe) | SMILES |
|---|---|---|---|
| 1 |  | Sulfametossazolo (Sulfamidici) | CC1=CC(NS(=O)(C2=CC=C(N)C=C2)=O)=NO1 |
| 2 |  | Benzil-penicillina (β-lattamici) | CC1(C)[C@H](C(O)=O)N2C([C@H](NC(CC3=CC=CC=C3)=O)C2=O)S1 |
| 3 |  | Amoxicillina (β-lattamici) | CC1(C)[C@H](C(O)=O)N2C([C@H](NC([C@H](N)C3=CC=C(O)C=C3)=O)C2=O)S1 |
| 4 |  | Meticillina (β-lattamici) | CC1(C)[C@H](C(O)=O)N2C([C@H](NC(C3=C(OC)C=CC=C3OC)=O)C2=O)S1 |
| 5 |  | Cefiximina (β-lattamici) | C=CC1=C(CO)N2C(SC1)[C@H](NC(/C(C3=CSC(N)=N3)=N/OCC(O)=O)=O)C2=O |
| 6 |  | Cloramfenicolo | OC[C@@H](NC(C(Cl)Cl)=O)[C@H](O)C1=CC=C([N+]([O-])=O)C=C1 |
| 7 |  | Streptomicina (Aminoglicosidici) | C[C@H]1[C@@]([C@H]([C@@H](O1)O[C@@H]2[C@H]([C@@H]([C@H]([C@@H]([C@H]2O)O)N=C(N)N)O)N=C(N)N)O[C@H]3[C@H]([C@@H]([C@H]([C@@H](O3)CO)O)O)NC)(C=O)O |
| 8 |  | Aureomicina (Tetracicline) | CC1([C@H]2C[C@H]3[C@@H](C(=O)C(=C([C@]3(C(=O)C2=C(C4=C(C=CC(=C41)Cl)O)O)O)O)C(=O)N)N(C)C)O |

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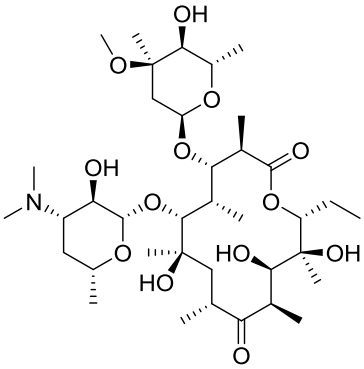
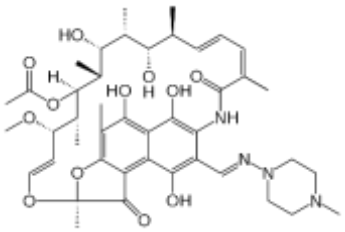
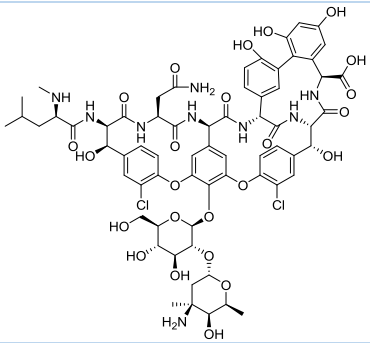
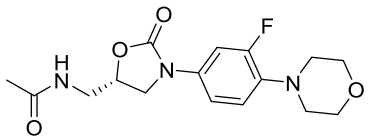
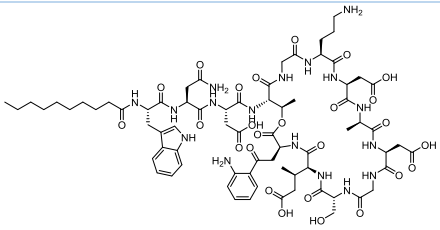
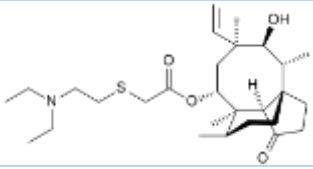
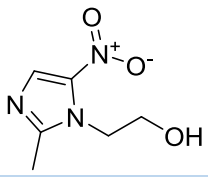
|---|---|---|---|
| **9** |  | Eritromicina (Macrolidi) | CC[C@@H]1[C@@]([C@@H]([C@H](C(=O)[C@@H](C[C@@]([C@@H]([C@H]([C@@H]([C@H](C(=O)O1)C)O[C@H]2C[C@@]([C@H]([C@@H](O2)C)O)(C)OC)C)O[C@H]3[C@@H]([C@H](C[C@H](O3)C)N(C)C)O)(C)O)C)C)O)(C)O |
| **10** |  | Rifampicina (Ansamicine) | C[C@H]1/C=C/C=C(\C(=O)NC\2=C(C3=C(C(=C4C(=C3C(=O)/C2=C/NN5CCN(CC5)C)C(=O)[C@](O4)(O/C=C/[C@@H]([C@H]([C@H]([C@@H]([C@@H]([C@@H]([C@H]1O)C)O)C)OC(=O)C)C)OC)C)C)O)O)/C |
| **11** |  | Vancomicina (Glicopeptidici) | C[C@H]1[C@H]([C@@](C[C@@H](O1)O[C@@H]2[C@H]([C@@H]([C@H](O[C@H]2OC3=C4C=C5C=C3OC6=C(C=C(C=C6)[C@H]([C@H](C(=O)N[C@H](C(=O)N[C@H]5C(=O)N[C@@H]7C8=CC(=C(C=C8)O)C9=C(C=C(C=C9[C@H](NC(=O)[C@H]([C@@H](C1=CC(=C(O4)C=C1)Cl)O)NC7=O)C(=O)O)O)O)CC(=O)N)NC(=O)[C@@H](CC(C)C)NC)O)Cl)CO)O)O)(C)N)O |
| **12** |  | Linezolid (Ossazolidinoni) | CC(=O)NC[C@H]1CN(C(=O)O1)C2=CC(=C(C=C2)N3CCOCC3)F |
| **13** |  | Daptomicina (Lipopeptidici) | CCCCCCCCCC(=O)N[C@@H](CC1=CNC2=CC=CC=C21)C(=O)N[C@@H](CC(=O)N)C(=O)N[C@@H](CC(=O)O)C(=O)N[C@H]3[C@H](OC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H](NC(=O)CNC(=O)[C@@H](NC(=O)[C@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)CNC3=O)CCCN)CC(=O)O)C)CC(=O)O)CO)[C@H](C)CC(=O)O)CC(=O)C4=CC=CC=C4N)C |
| **14** |  | Tiamulina (Diterpeni) | CCN(CC)CCSCC(=O)O[C@@H]1C[C@@]([C@H]([C@@H]([C@@]23CC[C@H]([C@@]1([C@@H]2C(=O)CC3)C)C)C)O)(C)C=C |
| **15** |  | Metronidazolo (Nitroimidazoli) | CC1=NC=C(N1CCO)[N+](=O)[O-] |

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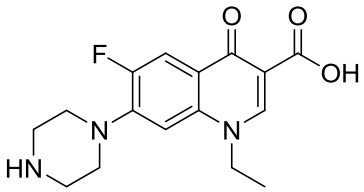
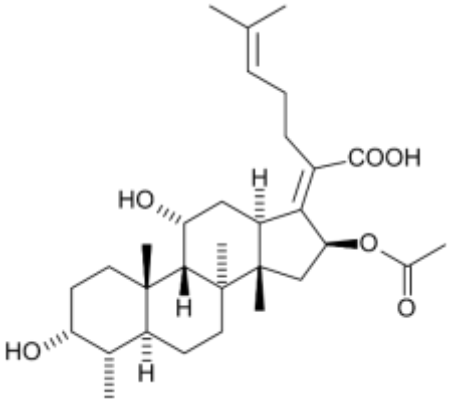
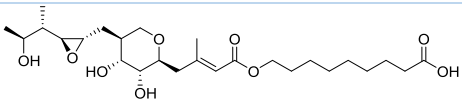
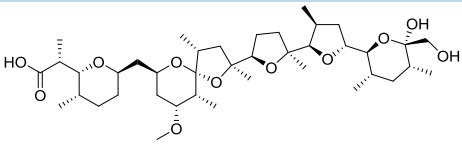
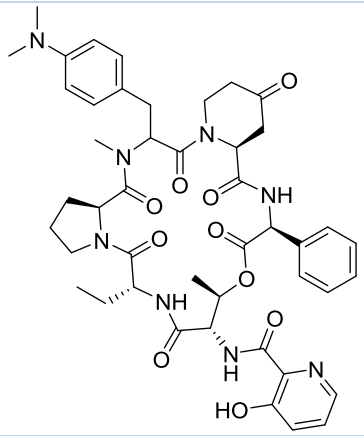
|---|---|---|---|
| 16 |  | Norfloxacina (Fluorochinolonici) | CCN1C=C(C(=O)C2=CC(=C(C=C21)N3CCNCC3)F)C(=O)O |
| 17 |  | Acido Fusidico | C[C@H]1[C@@H]2CC[C@]3([C@H]([C@]2(CC[C@H]1O)C)[C@@H](C[C@@H]\4[C@@]3(C[C@@H](/C4=C(/CCC=C(C)C)\C(=O)O)OC(=O)C)C)O)C |
| 18 |  | Mupirocina | C[C@H]([C@H]1[C@@H](O1)C[C@H]2CO[C@H]([C@@H]([C@@H]2O)O)C/C(=C/C(=O)OCCCCCCCCC(=O)O)/C)[C@H](C)O |
| 19 |  | Nigericina (polieteri ionofori) | C[C@H]1CC[C@@H](O[C@H]1[C@@H](C)C(=O)O)C[C@@H]2C[C@H]([C@H]([C@@]3(O2)[C@@H](C[C@@](O3)(C)[C@H]4CC[C@@](O4)(C)[C@H]5[C@H](C[C@@H](O5)[C@@H]6[C@H](C[C@H]([C@@](O6)(CO)O)C)C)C)C)OC |
| 20 |  | Mikamicina B (Ciclopeptide) | C1=C(C(=C(N=C1)C(=O)N[C@H]2[C@H](OC(=O)[C@@H](NC(=O)[C@@H]3CC(=O)CCN3C(=O)C(N(C(=O)[C@@H]4CCCN4C(=O)[C@H](NC2=O)CC)C)CC5=CC=C(C=C5)N(C)C)C6=CC=CC=C6)C)O) |

**Link per fare i calcoli:**

**Molinspiration:** http://www.molinspiration.com/

**Molsoft:** http://molsoft.com/mprop/

**Swiss Target Prediction:** http://www.swisstargetprediction.ch/

**Swiss ADME:** http://www.swissadme.ch/