2014

The Betulin Project Introduction 2014 - Accompanying Slide Show

The Betulin Project – Fall Semester CH 203, 2014 Boston University

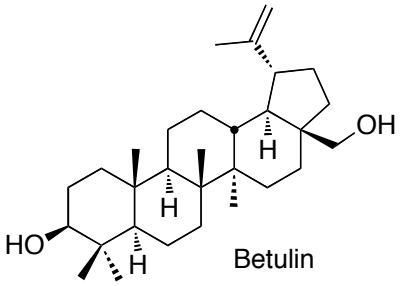
Instructor: Prof. John K. Snyder

Laboratory Fellow: Dr. Ya Zhou, PFF

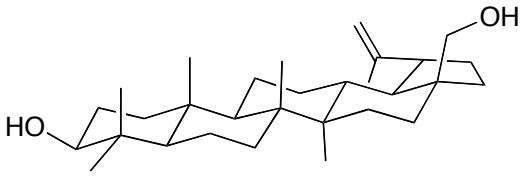
Betulin Group Meetings – Thursdays, 3 pm

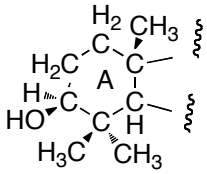
Betulin Laboratory: Alternate Fridays, 1 - ? pm

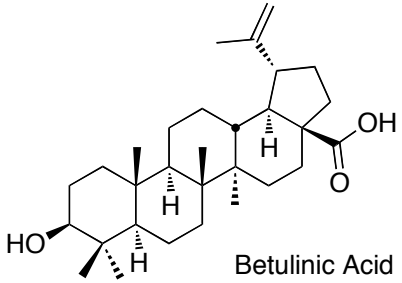
Betulin: Protective Compound from White and Paper Birch



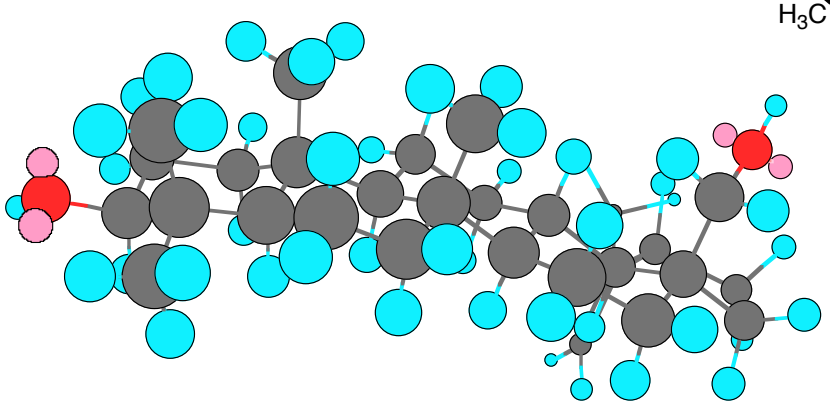
Betulin

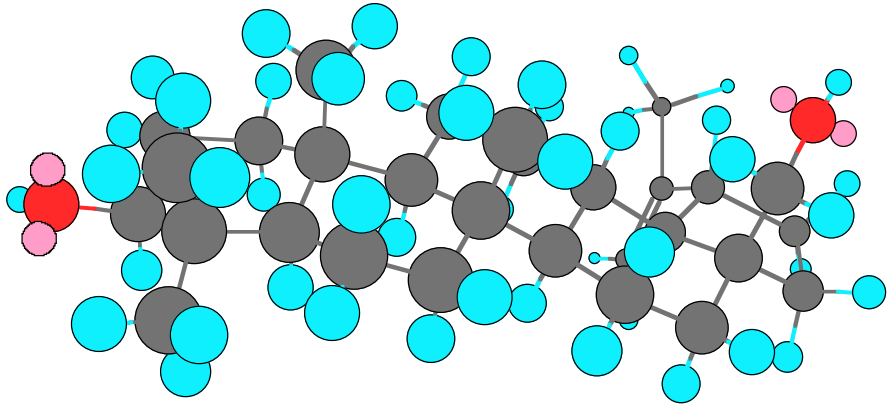




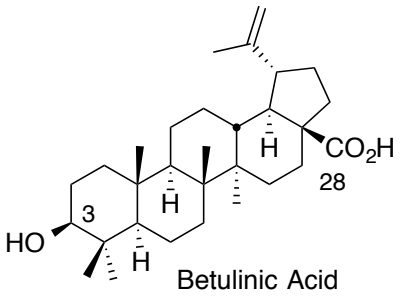


Betulinic Acid





Anti-Melanoma – Betulinic Acid

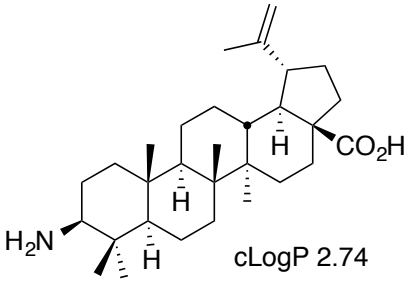


Betulinic Acid

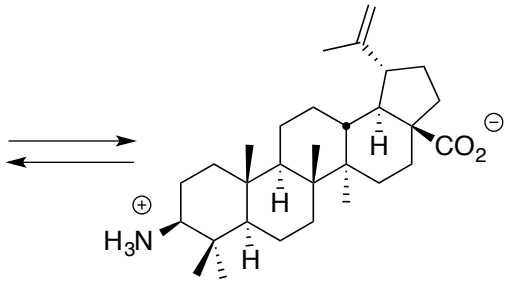
MW 456.36
cLogP 7.38

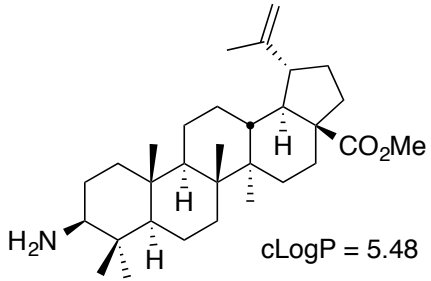
Lipinski's Rule of Five

1) No more than 5 Hydrogen Bond Donors (N-H and O-H)
2) No more than 10 Hydrogen Bond Acceptors (all N's and O's)
3) MW less than 500
4) cLogP = 5 or less



cLogP 2.74

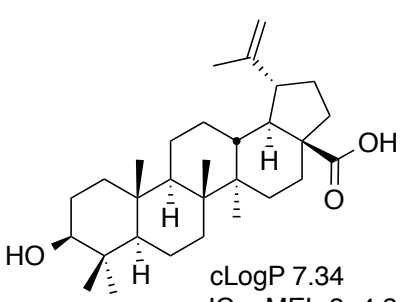




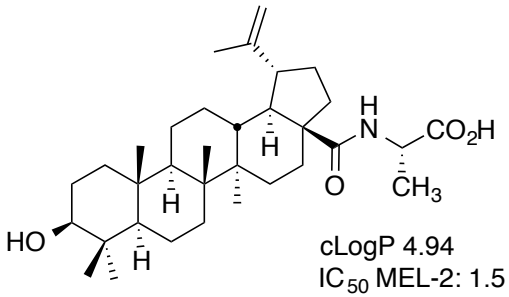
cLogP = 5.48

Betulinic Acid Derivatives

Anti-Melanoma

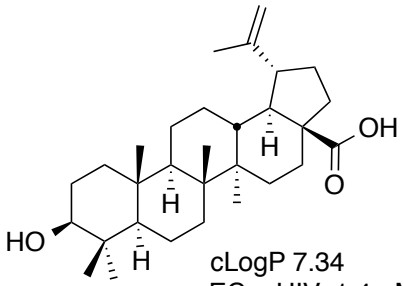


cLogP 7.34
IC_{50} MEL-2: 4.2 μM
IC_{50} KB: >20 μM



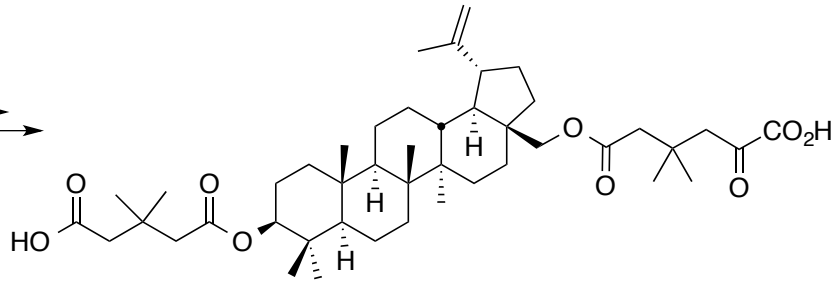
cLogP 4.94
IC_{50} MEL-2: 1.5 μM
IC_{50} KB: 4.6 μM

Anti-HIV



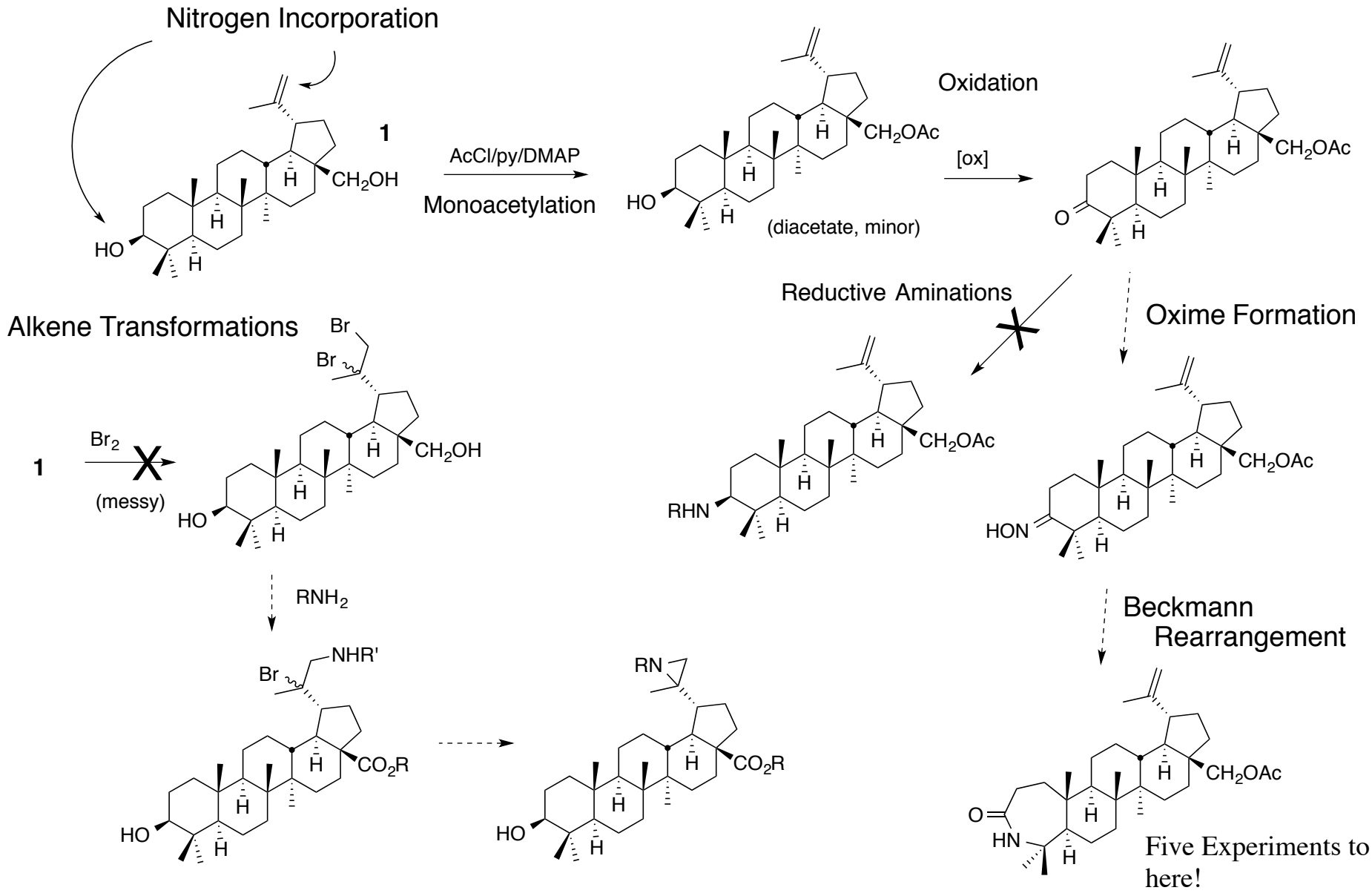
cLogP 7.34
EC_{50} HIV: 1.4 μM
IC_{50} cytotox.: 13.0 μM
Therapeutic Index: 9.0

Betulin

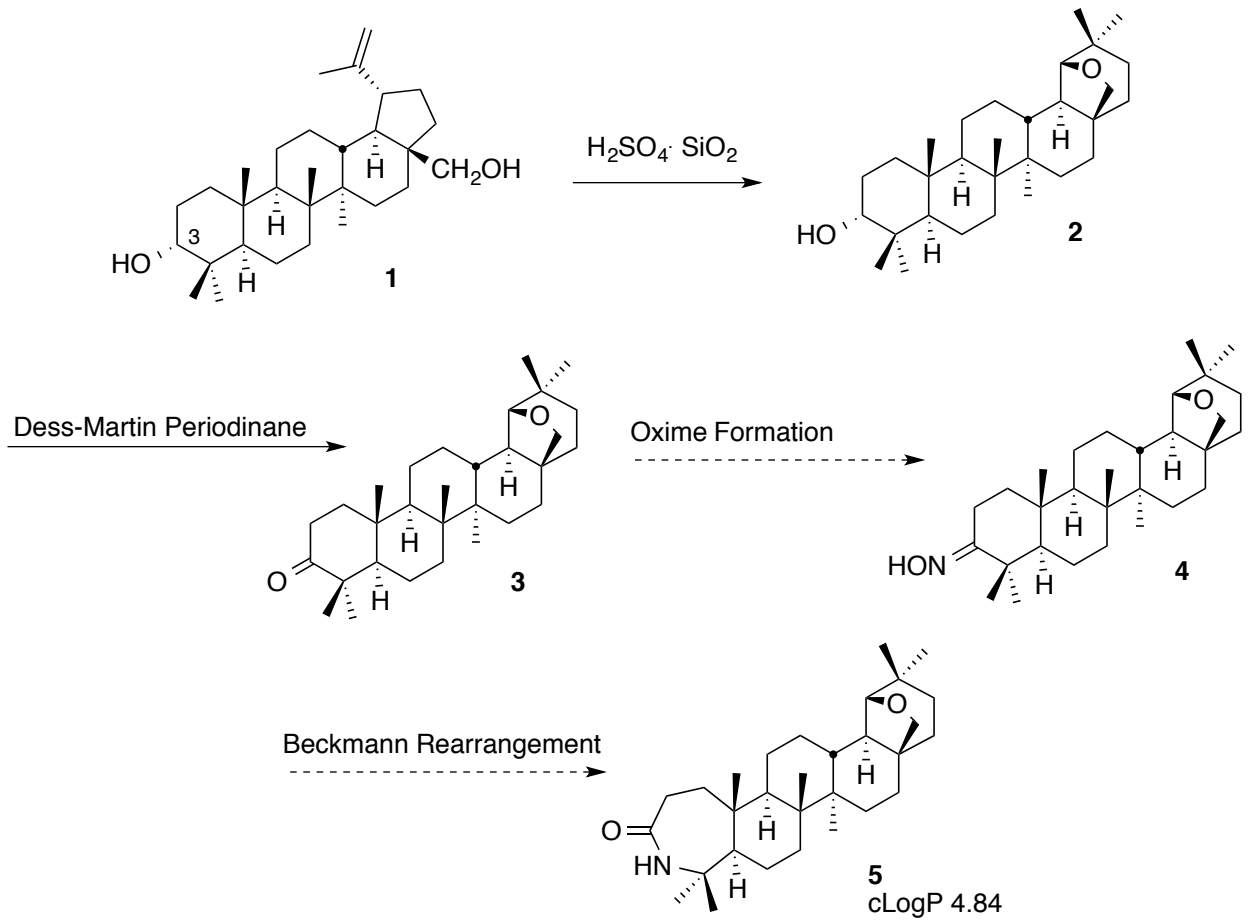


cLogP 7.09
EC_{50} HIV: 6.6 X 10^{-4} μM
IC_{50} cytotox.: 14.2 μM
Therapeutic Index: 21,515

Last Year's Progress



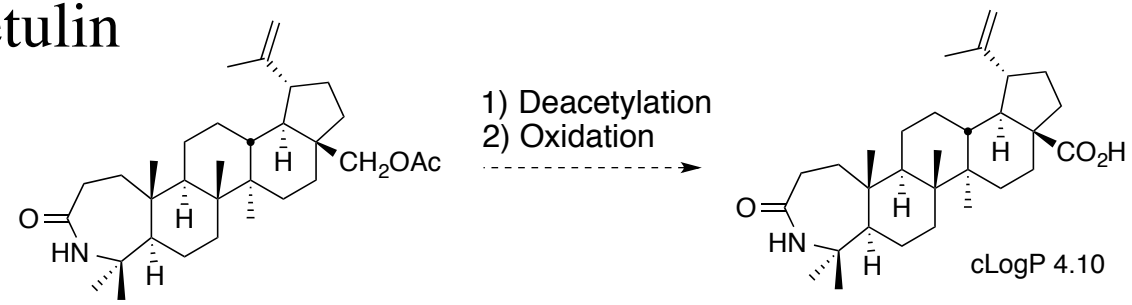
Allobetulin Analogues



Five Experiments to here!

Ultimate Targets

From Betulin



From Allobetulin