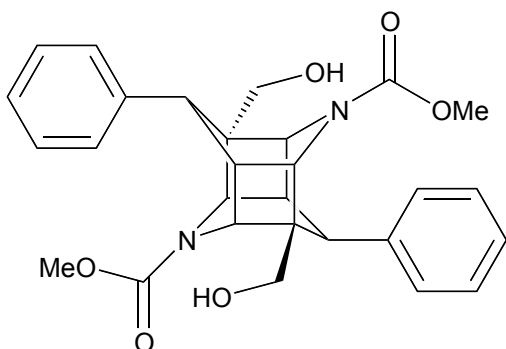


Trauner Group Meeting

Date: October 8, 2002

Speaker: Matthew Banghart (Novel Synthesis of Cyclopentenones and Photoswitchable Ion Channel Ligands).

• Molecule of the Week:



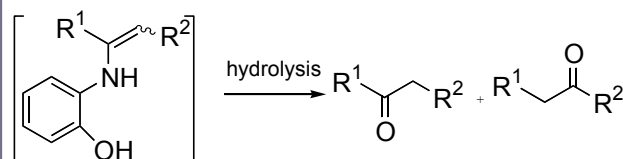
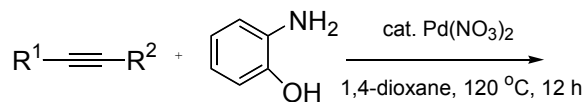
Hydroxymethyl-substituted 3,9-Diazatetraasteranes

Novel MDR modulators of rigid, symmetrical form support "symmetry hypothesis" about structure of binding region.

A. Hilgroth et al, *Angew. Chem. Int. Ed.* **2002**, *41*, 3623.

• Reaction/Method of the Week:

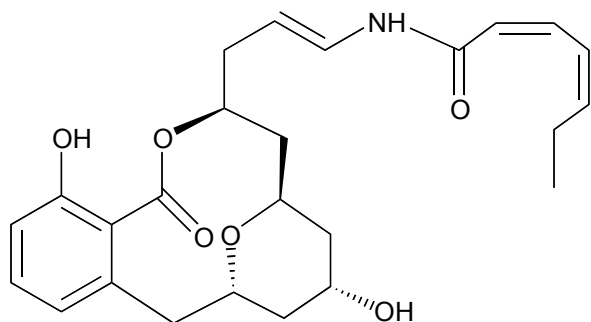
Palladium-Catalyzed Intermolecular Hydoramination of Alkynes



Ortho hydroxy chelation to palladium as source of rate enhancement.

T. Shimada, Y. Yamamoto, *J. Am. Chem. Soc.* **2002**, ASAP.

• Synthesis of the Week:



Apicularen A

Nicolaou et al, *Angew. Chem. Int. Ed.* **2002**, *41*, 3701.

- 10-membered ring lactone, doubly unsaturated acylenamine side chain
- Allylation-ozonolysis sequence mimics polyacetate biosynthetic pathway
- Takai iodo-olefination, then acylenamine formation

• Numbers of the Week:

Essential Conversion:

$$4.186 \text{ kJ} = 1 \text{ kcal}$$

NOE Intensity is proportional to:

$$1/r^6$$

Enthalpies of H Bond Formation (kcal/mol):

Methanol (OH - O) - 9.3 (inter)

Methanol-Pyridine (OH - N) - 9.1 (inter)

Water-Acetone (OH - O=C) - 2.5 (inter)

Phenol-Fluoroalkane (OH - F) - 2.1 (inter)

Phenol-Hexamethylbenzene (OH - π) - 1.7 (inter)

2-Methoxybenzoic acid (OH - O) - 3.3 (intra)

H Bond Strengths and Bond Energies (kcal/mol):

Strong: Proton Sponges, HF Complexes (14-29)

Moderate: Acids, Alcohols, Biomolecules (4-14)

Weak: CH - H bonds, OH - π bonds (< 3)

• Future order: Aubry Miller, Professor Dirk Trauner.