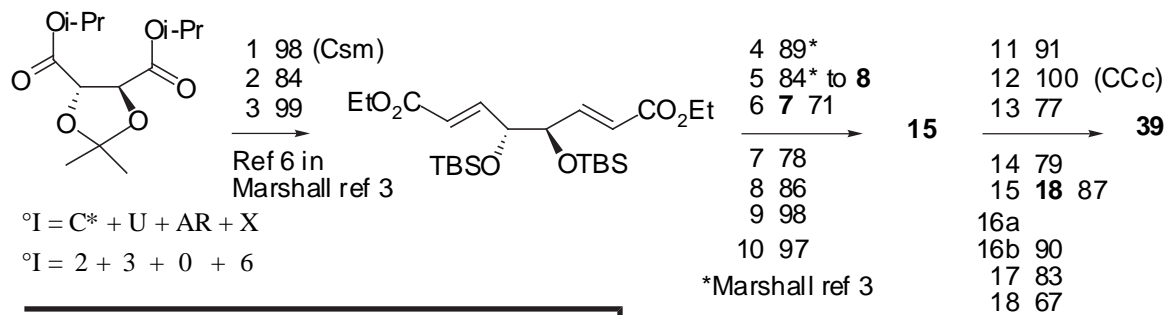


Supplemental Material
Increase in Intricacy—a Tool for Evaluating Organic Syntheses
 P. L. Fuchs
 Department of Chemistry, Purdue University, West Lafayette, IN 47907

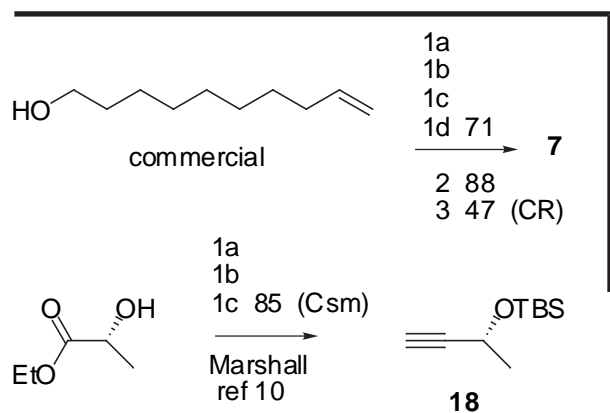
Target	Page #
Asimicin	2
Elaiolide	3
Fumagillol	4
Dysidoilide	5
Australine	6
Phorbol	7
Fluvirucin B1	8
Narciclasine	9
Isocrambescidin 800	10
Deoxycrispolide	11
Ptilocaulin	12
Pinnatoxin A	13
Croomine	14
Picrotoxinin	15
Digitoxigenin	16
Chlorothricolide	17
Roflamycoin	18
Pancreatistatin	19
Isopulo'upone	20
Callystatin A	21
Aplysiapyranoid C	22
Dynemicin A	23
Aegiceradienol	24
Mannostatin A	25
Steganone	26
Epothiolone A	27
Stipiamide	28
Discodermolide	29
Quassin	30
Methyl Phenidate	31
Amabiline	32
A58365A	33
Castanospermine	34
Decarestrictine D	35
Ricinelaic Acid	36
A26771B	37
K252a	38
MDL 28,726	39
Mappicine	40
U-106305	41

Asimicin



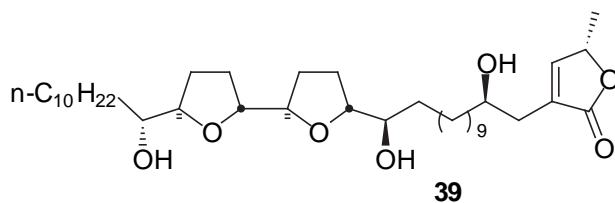
$$^{\circ}I = C^* + U + AR + X$$

$$^{\circ}I = 2 + 3 + 0 + 6$$



$$^{\circ}I = C^* + U + AR + X$$

$$^{\circ}I = 1 + 1 + 0 + 3$$



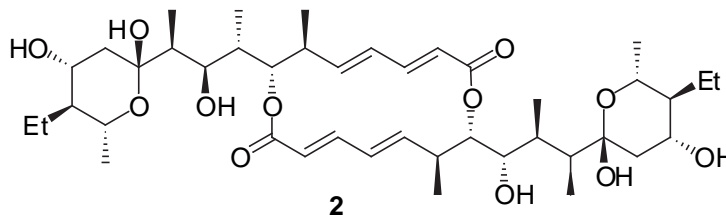
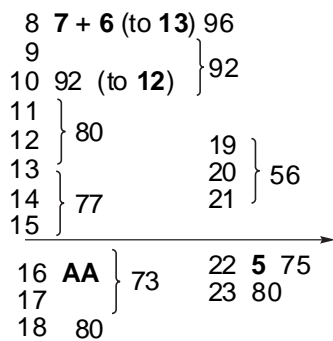
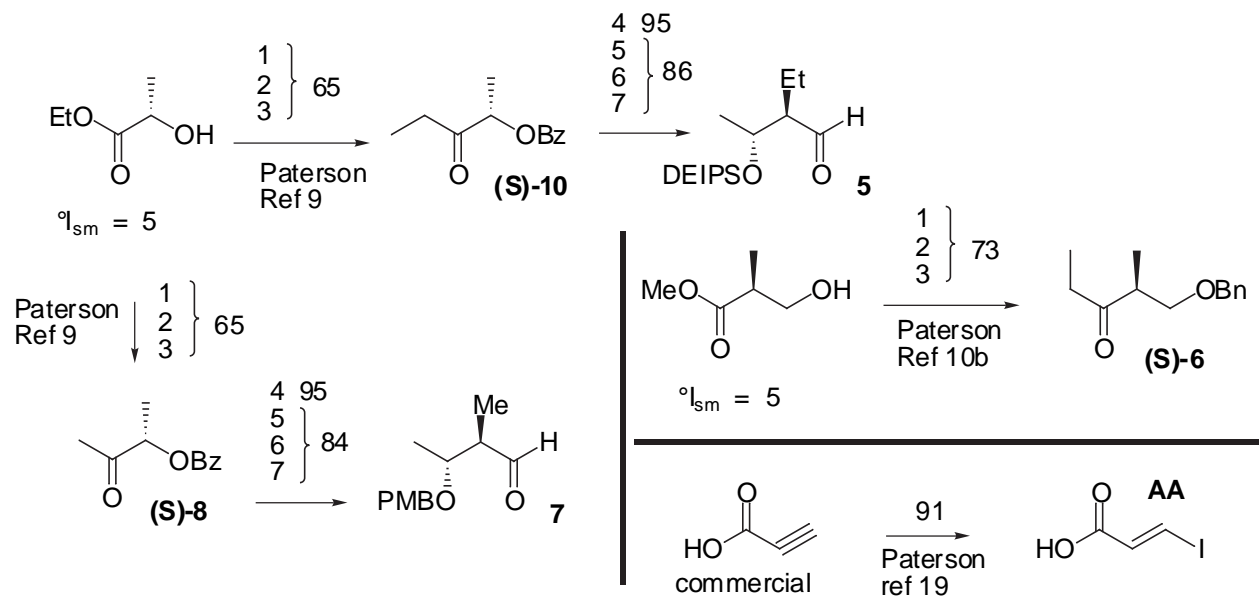
$$^{\circ}I = C^* + U + AR + X$$

$$^{\circ}I = 8 + 6 + 0 + 7$$

$$IQ = (21-14)/22 = 0.32$$

$$EQ = 84$$

Elaiolide



$$^{\circ}\text{I} = \text{C}^* + \text{U} + \text{AR} + \text{X}$$

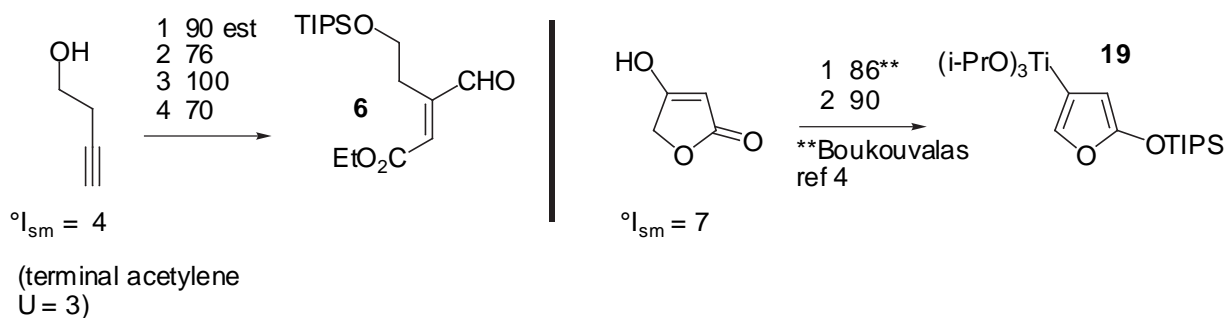
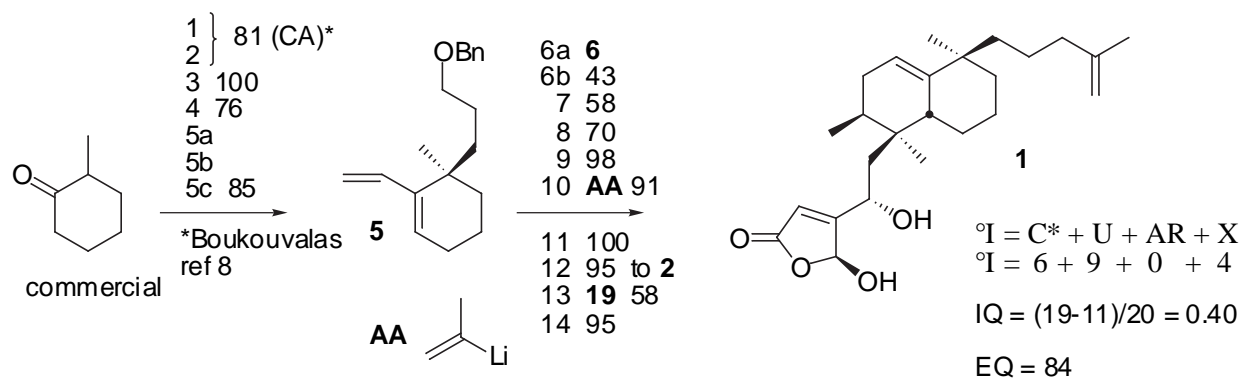
$$^{\circ}\text{I} = 18 + 13 + 0 + 12$$

$$^{\circ}\text{I} = 43/2 \text{ (symmetry axis decreases intricacy by half)}$$

$$\text{IQ} = (21.5 - 10)/33 = 0.35$$

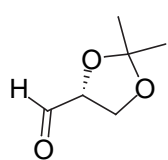
$$\text{EQ} = 82$$

4. Dysidiolide



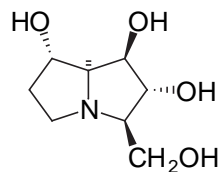
Australine

commercial,
but primary SM



1 } 63
2 }
3 } 74
White
ref 15

4	BB	93	10 99
5	96		11 84
6	62		12 75
7	90		13 99
8	76		14 99
9	97		



$$^{\circ}I = C^* + U + AR + X$$

$$^{\circ}I = 5 + 2 + 0 + 5$$

$$IQ = (12-6)/15$$

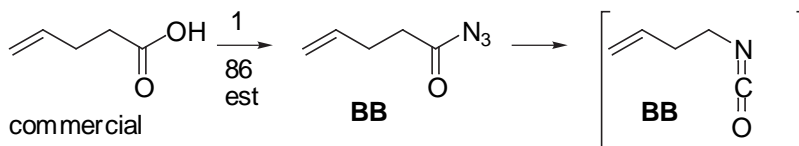
$$= 0.40$$

$$EQ = 86$$

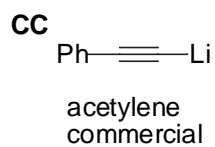
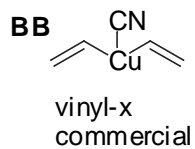
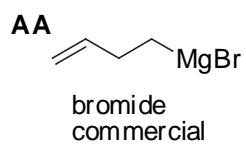
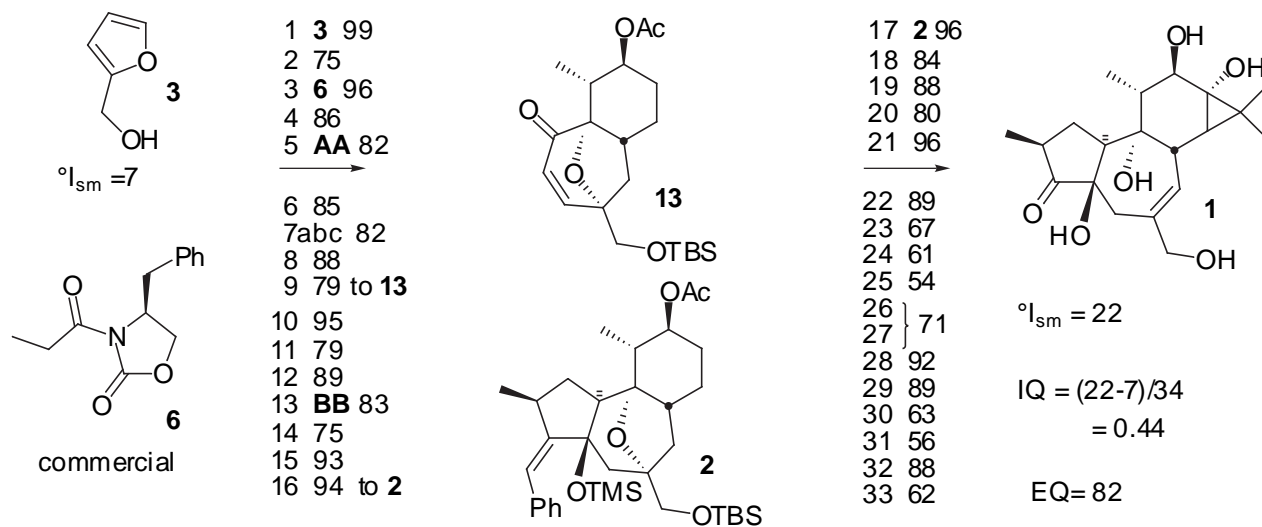
$$^{\circ}I = C^* + U + AR + X$$

$$^{\circ}I = 1 + 2 + 0 + 3$$

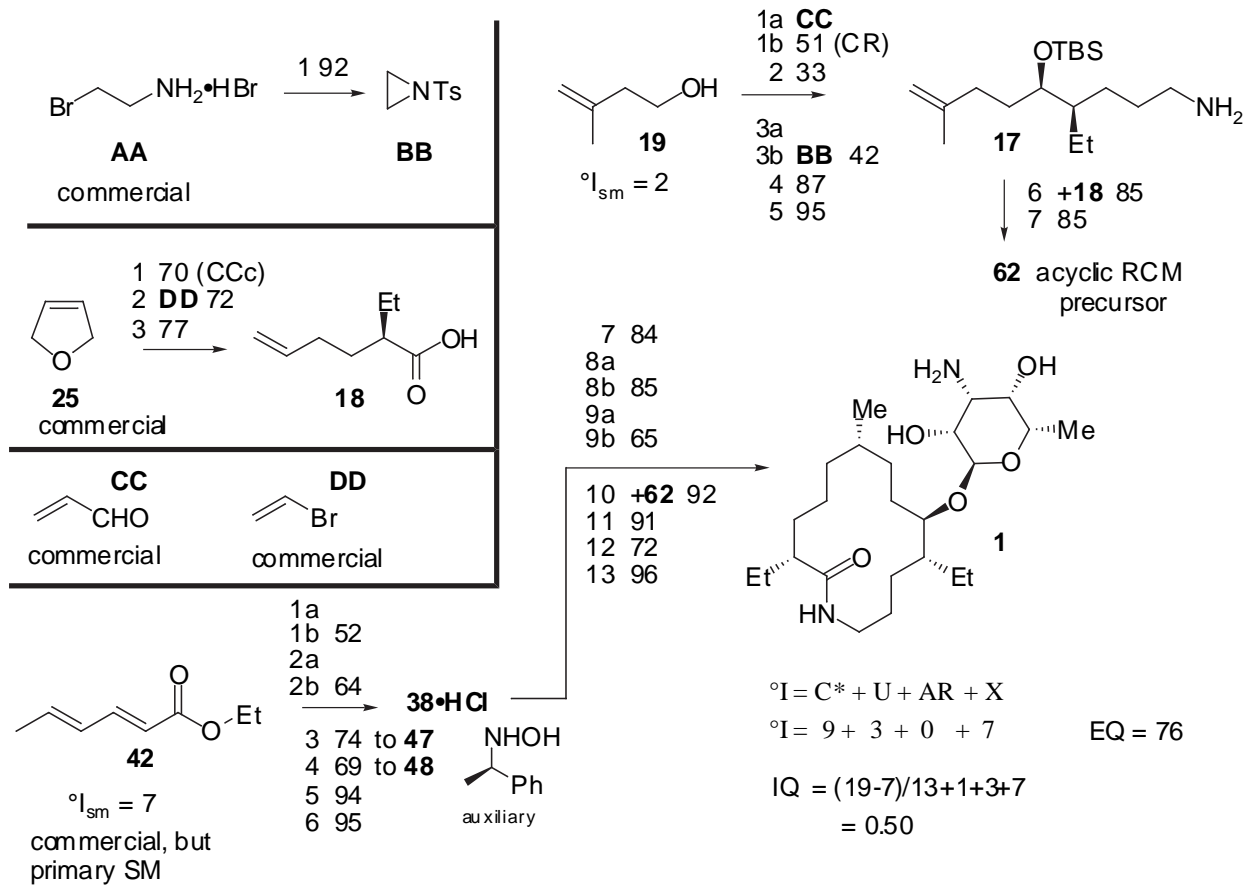
Australine



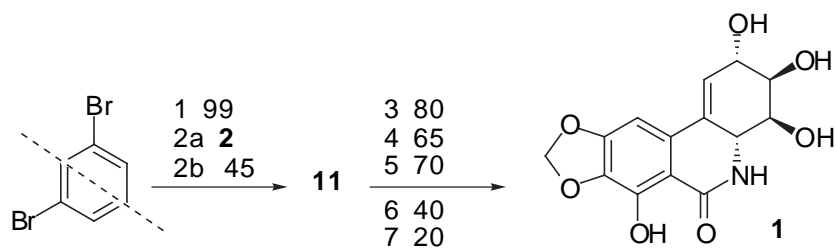
Phorbol



Fluvirucin B1



Narciclasine

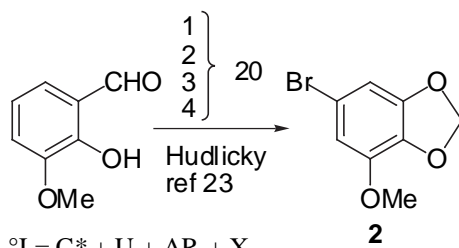


$$^{\circ}I = C^* + U + AR + X$$

$$^{\circ}I = 0 + 5 + 2 + 2$$

$$^{\circ}I = C^* + U + AR + X$$

$$^{\circ}I = 4 + 13 + 5 + 8$$



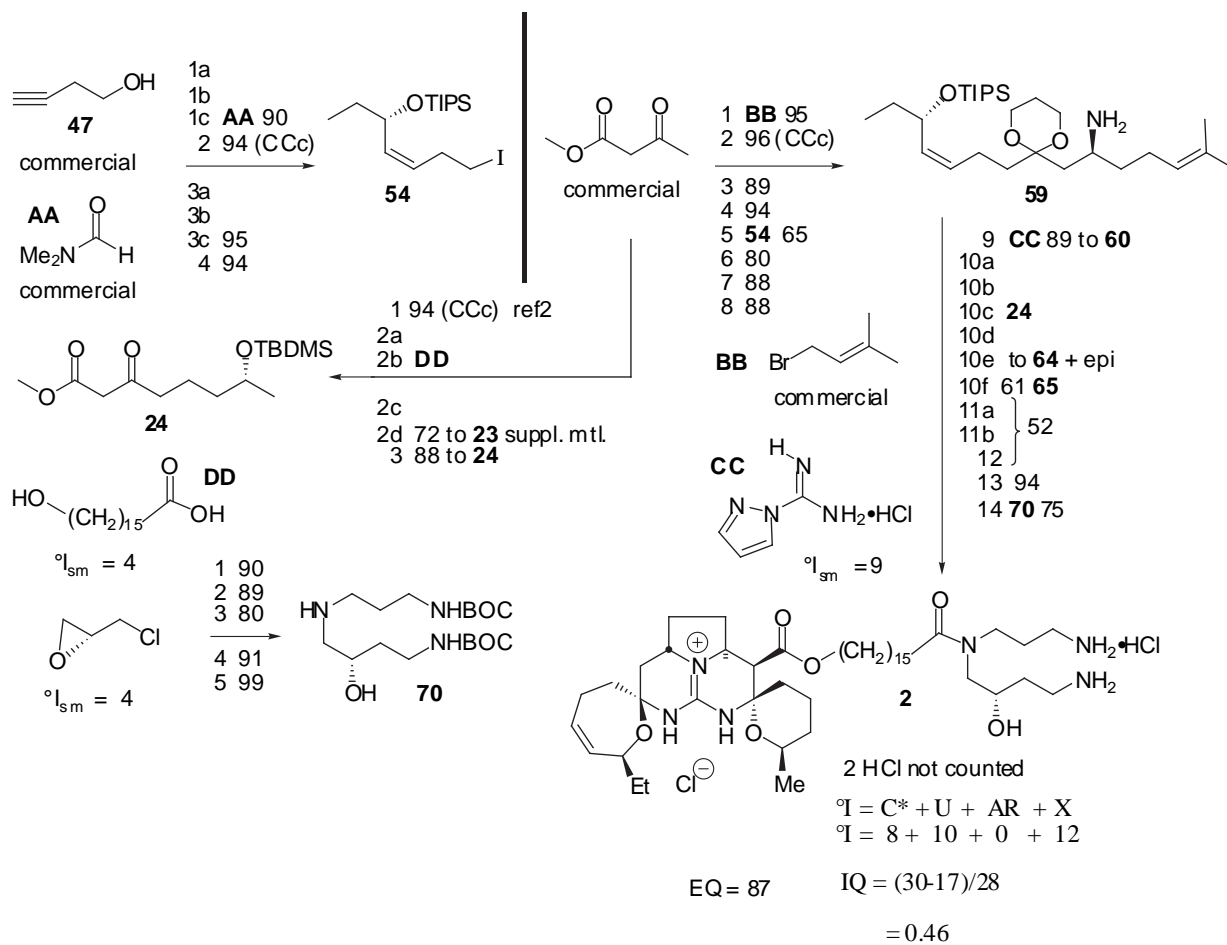
$$^{\circ}I = C^* + U + AR + X$$

$$^{\circ}I = 0 + 8 + 3 + 3$$

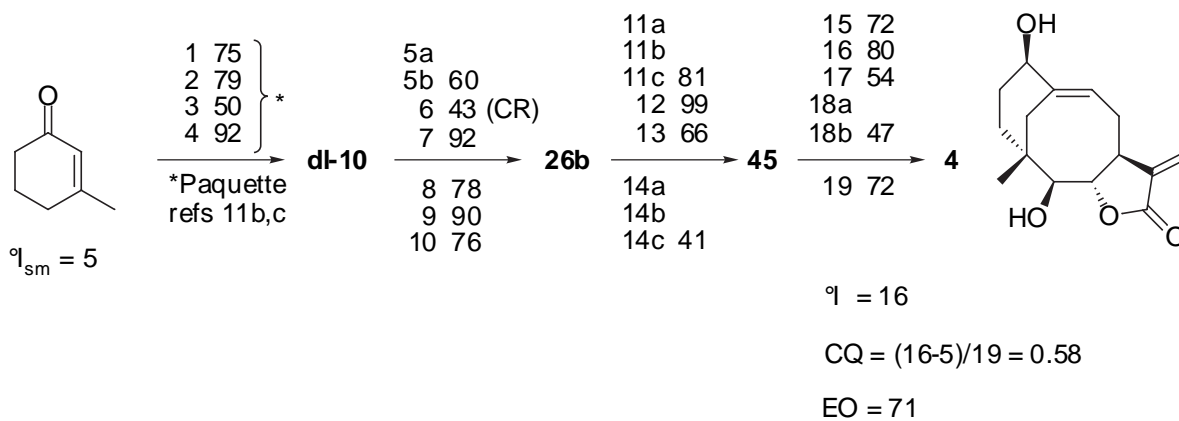
$$IQ = (30-23)/11 = 0.64$$

$$EQ = 62$$

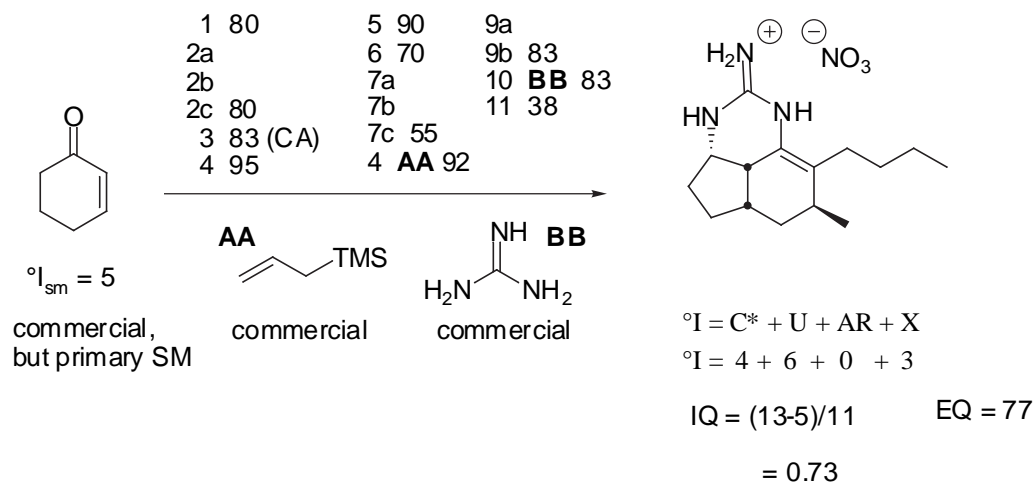
Isocrambescidin 800



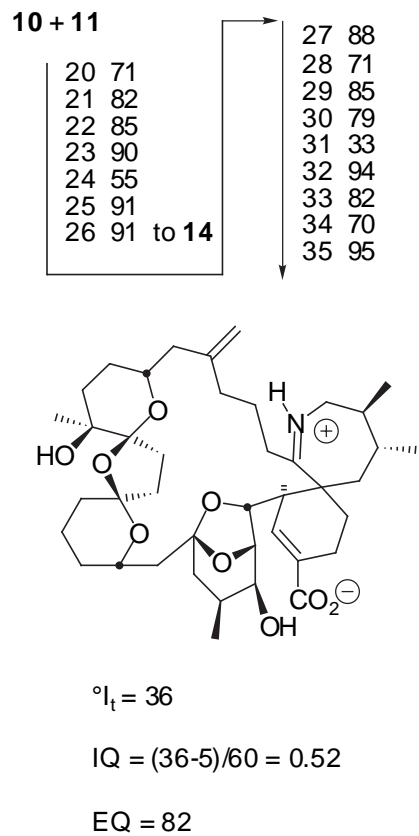
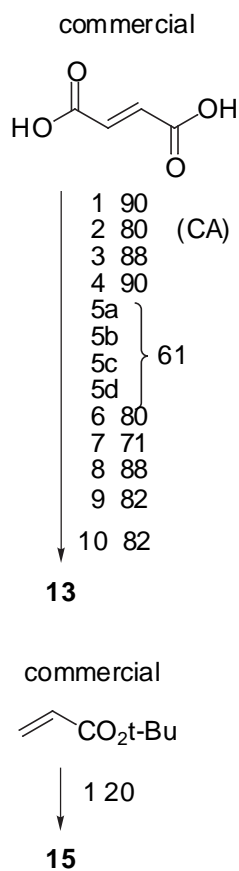
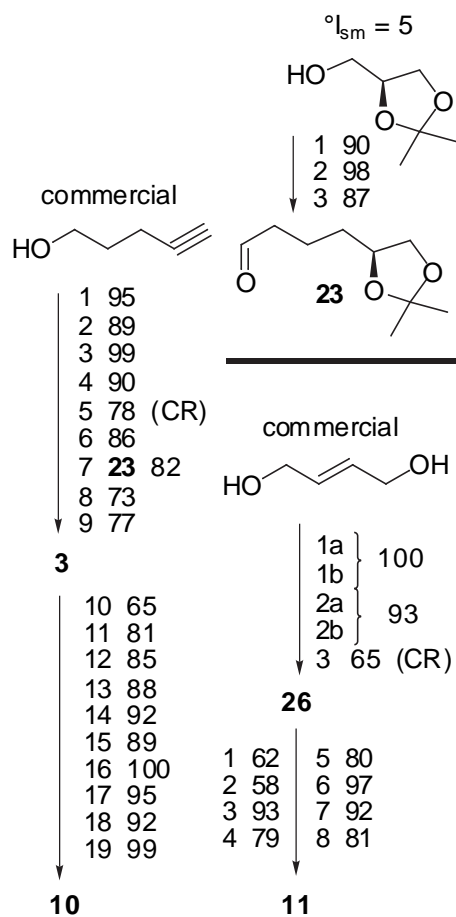
Deoxycrispolide



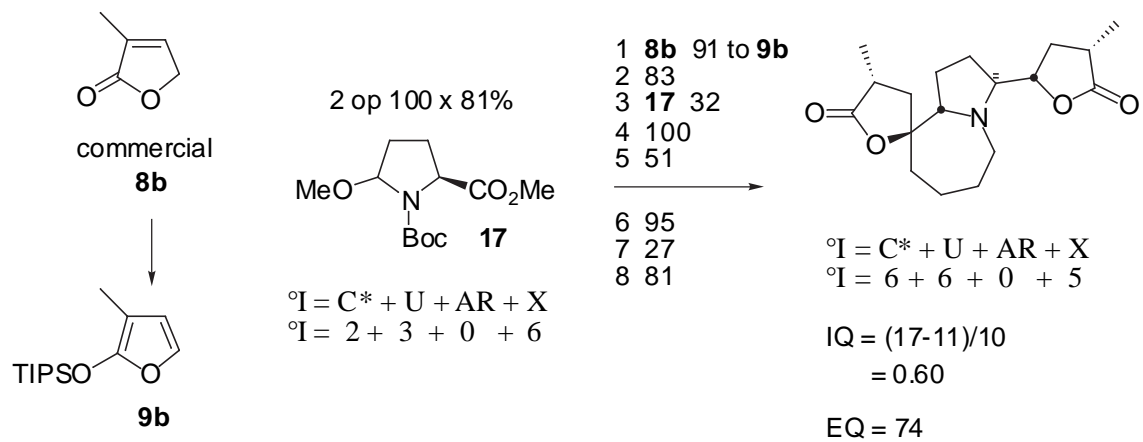
Ptilocaulin



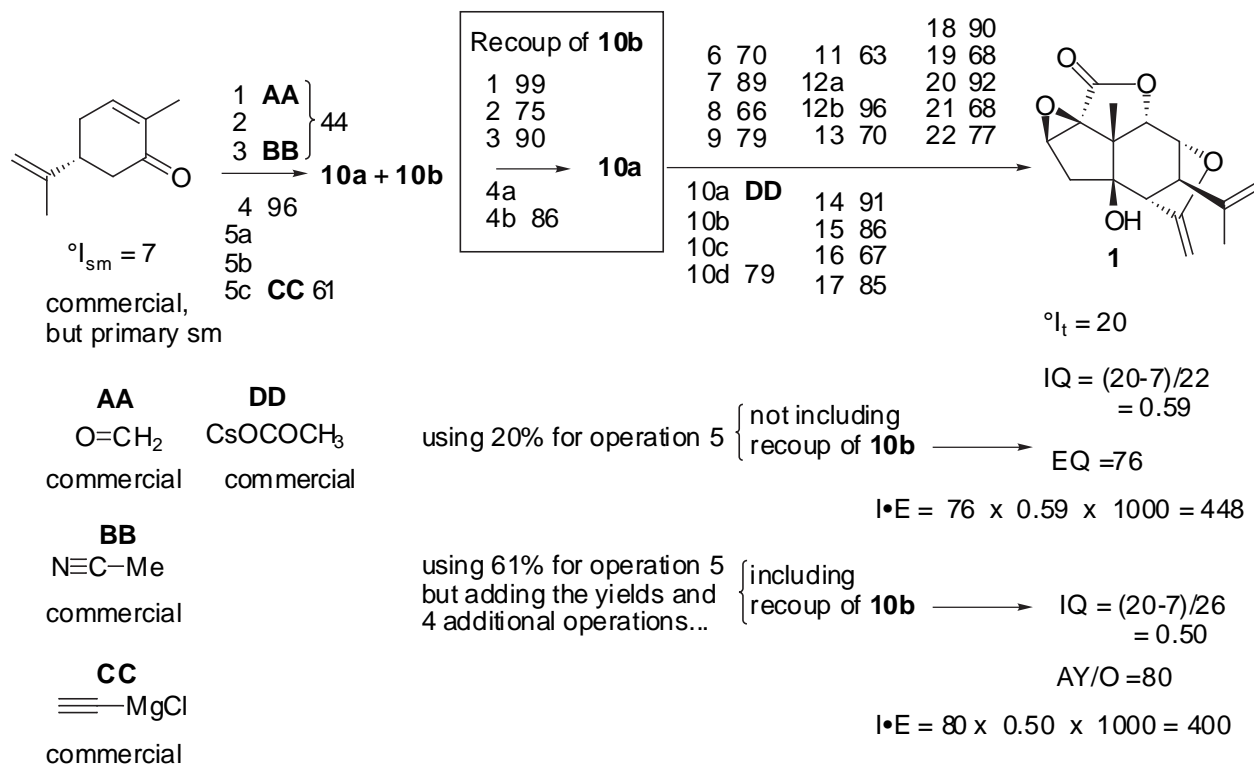
Pinnatoxin A



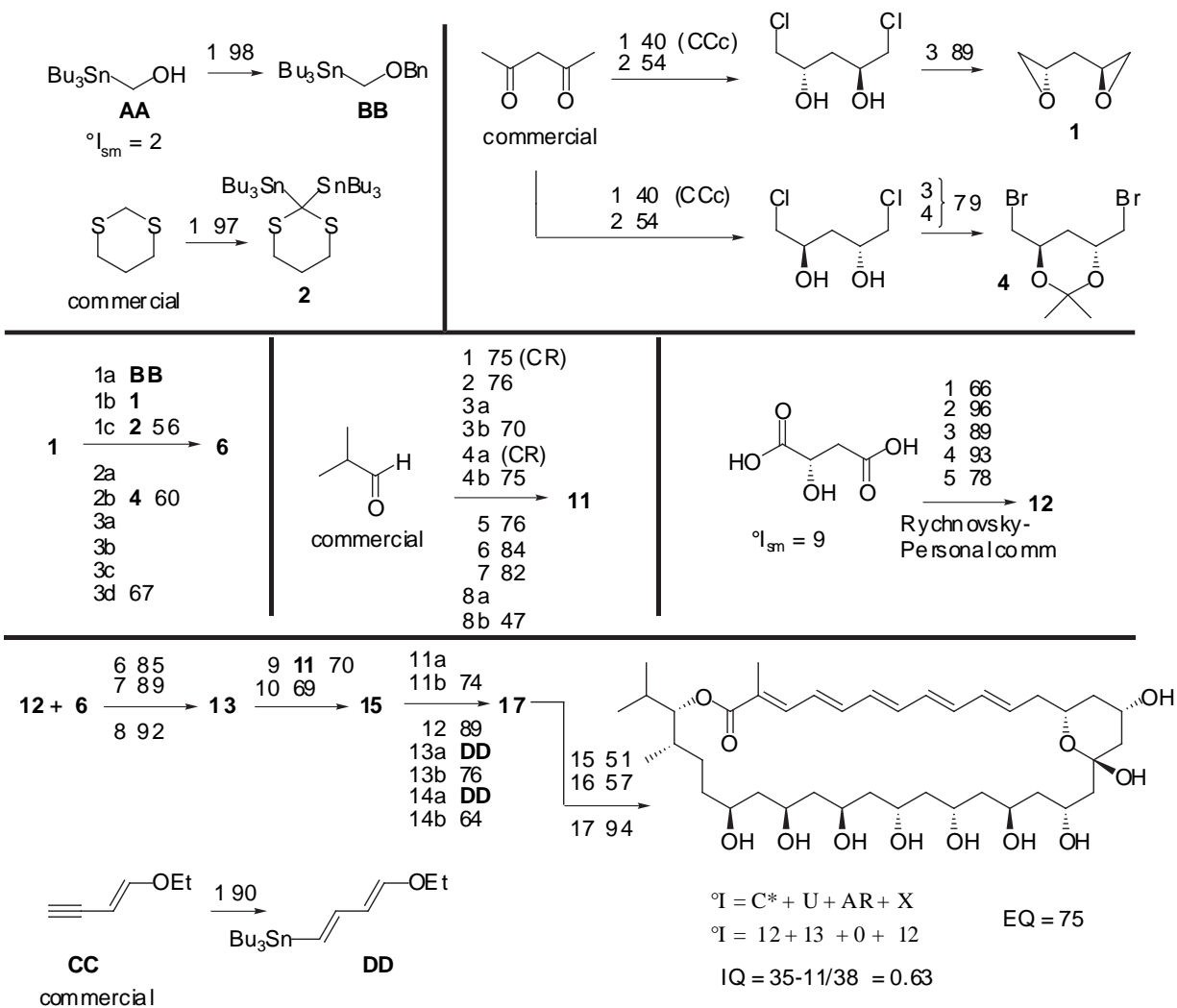
Croomine



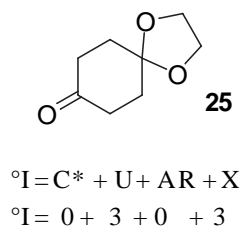
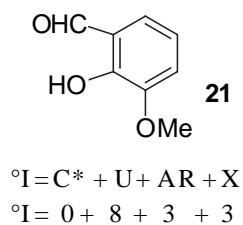
Picrotoxinin



Roflamycoin

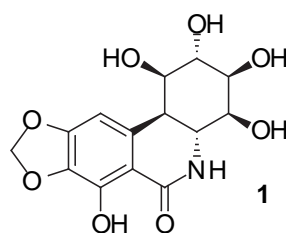
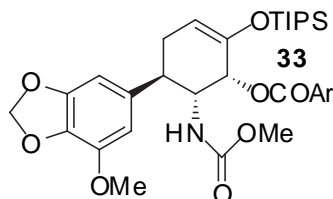
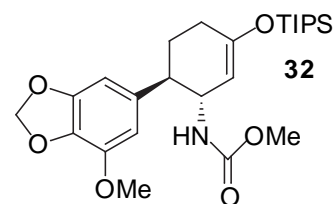
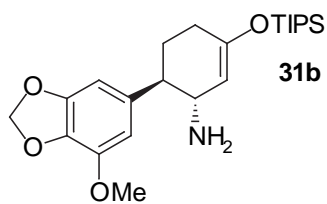


Pancratistatin



1 **21** 86
 2 89
 3 85
 4 **25** 85
 5 97

6 87
 7 89
 8 95 (CR)
 9 95 to **31b**
 10 56 to **32**
 11 83 to **33**
 12 88
 13 91
 14abc 85
 15ab 63
 16ab 60
 17 60
 18 73
 19 87 to **1**



$$^{\circ}I = C^* + U + AR + X$$

$$^{\circ}I = 6 + 11 + 5 + 9$$

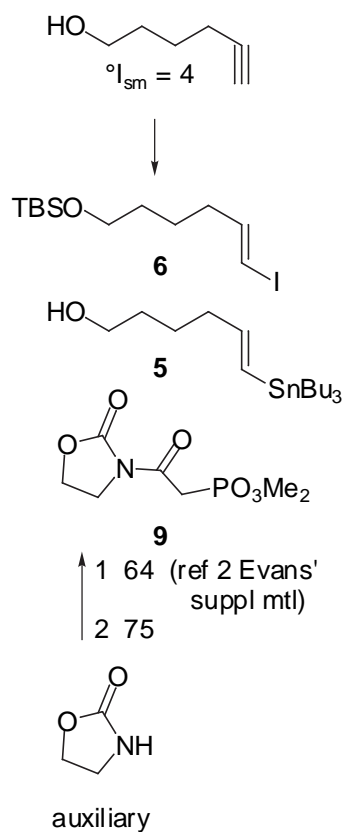
$$IQ = (31-20)/19$$

$$= 0.58$$

$$EQ = 82$$

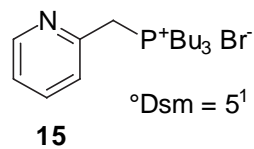
Isopulo'upone

terminal acetylene U = 3

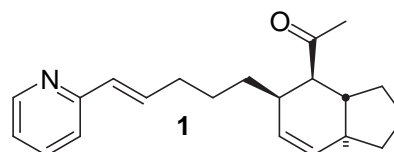
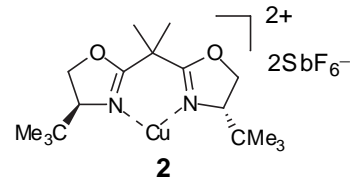
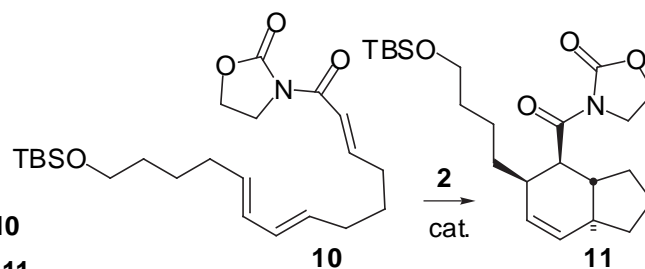


1 97
 2 } 69 to **6**
 3 }
 4 } 98 **6** to **5**
 5 }

6 **5** + **6** 72
 7 } 77 to **10**
 8 **9** }
 9 81 (CCc) to **11**
 10 90
 11 } 75
 12 }
 13 }
 14 }
 15 **15** 90 to **1**



$\text{°I} = \text{C}^* + \text{U} + \text{AR} + \text{X}$
 $\text{°I} = 0 + 6 + 1 + 2$
 + 2 op; 41%
 (Evans' Suppl material)

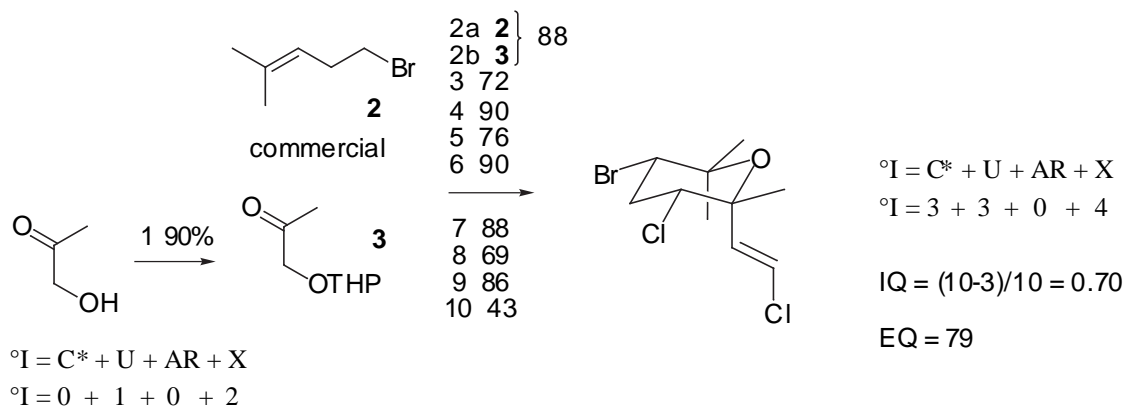


$\text{°I} = \text{C}^* + \text{U} + \text{AR} + \text{X}$
 $\text{°I} = 4 + 13 + 1 + 2$

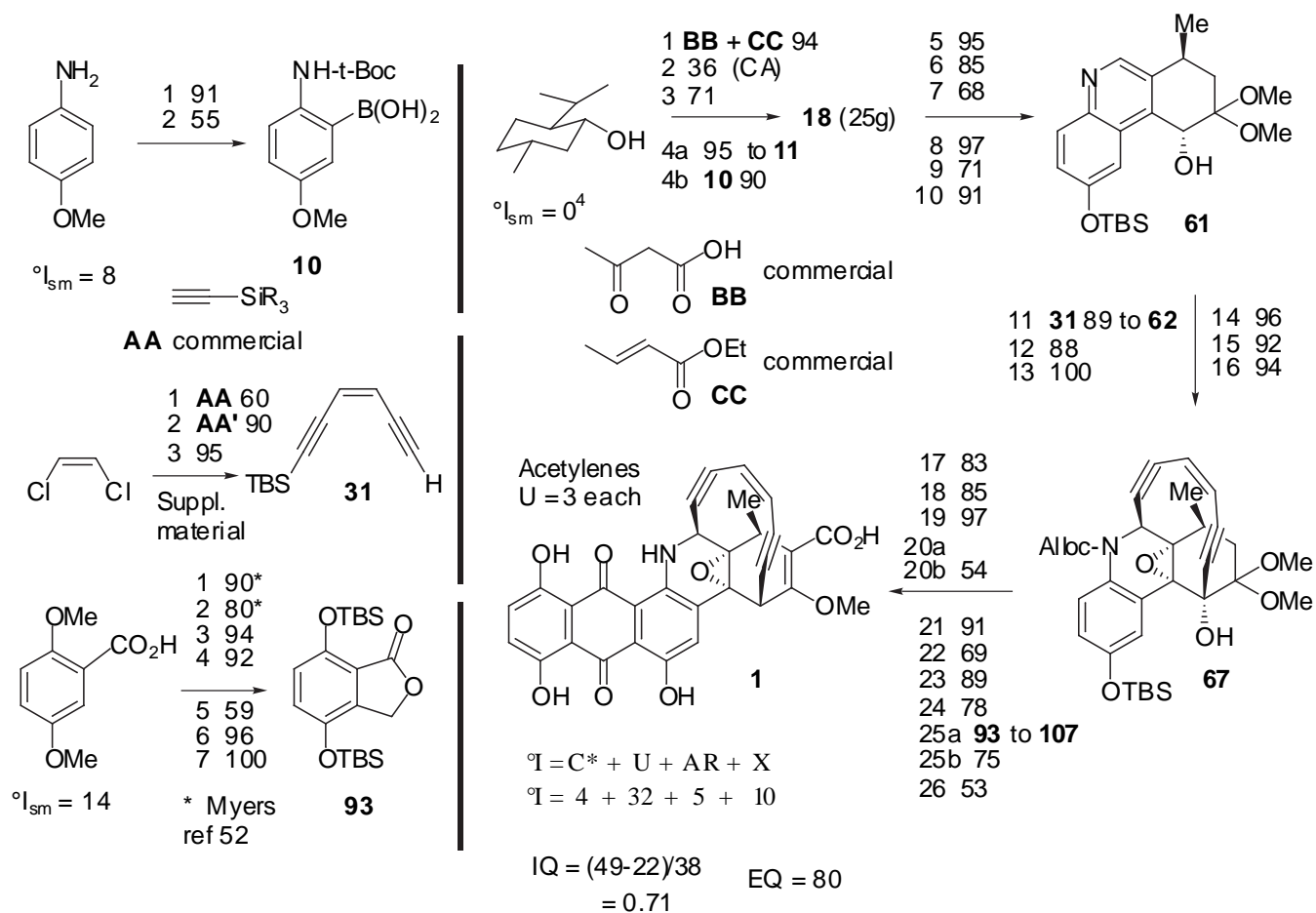
$\text{IQ} = (20-9)/15+2+2$
 $= 0.58$

EQ = 86

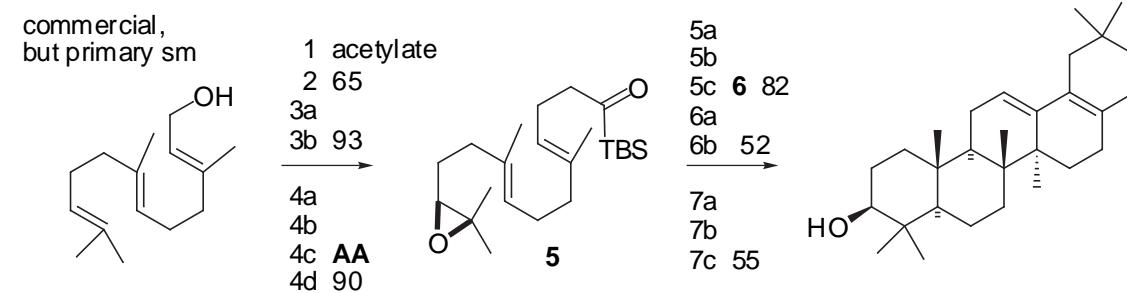
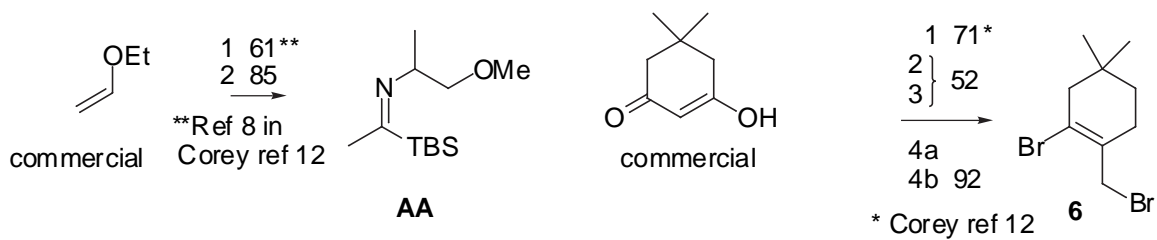
Aplysiapyranoid C



Dymericin A



23. Aegiceradienol



$$^{\circ}I = C^* + U + AR + X$$

$$^{\circ}I = 0 + 5 + 0 + 1$$

(dimethylolefin only U=1)

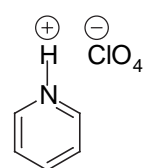
$$^{\circ}I = C^* + U + AR + X$$

$$^{\circ}I = 6 + 9 + 0 + 1$$

$$IQ = (16-6) / 13 = 0.77$$

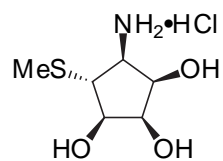
$$EQ = 75$$

24. Mannostatin A



$$^{\circ}I_{sm} = 4$$

1a	
1b	42
2	68 (CCb)
3	97
4	100
→	
5	90
6	91 borsm
7	100
8	65
9	74
10	100



$$IQ = (11-4)/10$$

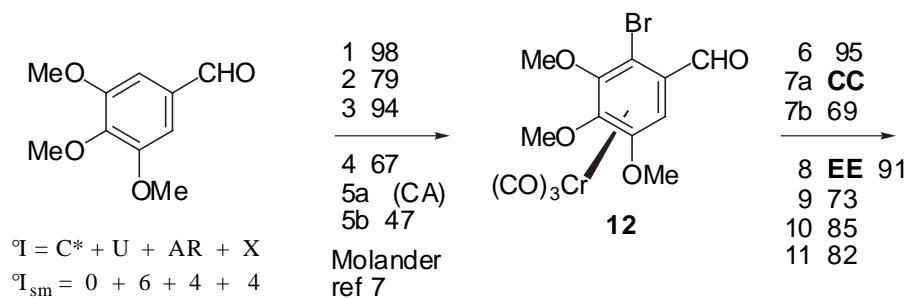
$$= 0.7$$

$$EQ = 83$$

$$^{\circ}I = C^* + U + AR + X$$

$$^{\circ}I = 5 + 1 + 0 + 5$$

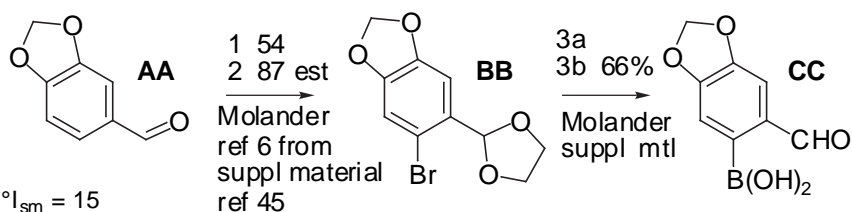
25. Steganone



$$^{\circ}I = C^* + U + AR + X$$

$$^{\circ}I_{sm} = 0 + 6 + 4 + 4$$

U = 4 prochiral
unsat, 1 C=O, 1 ring



$$^{\circ}I_{sm} = 15$$

U = 6 prochiral
unsat, C=O, 2 ring

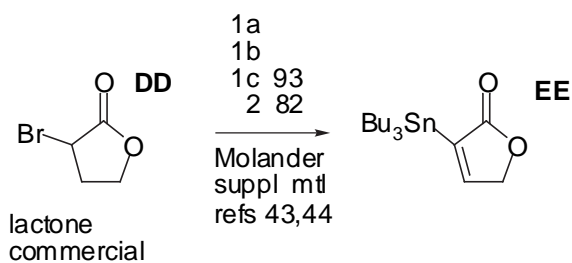
$$^{\circ}I_t = C^* + U + AR + X$$

$$^{\circ}I_t = 3 + 19 + 9 + 8$$

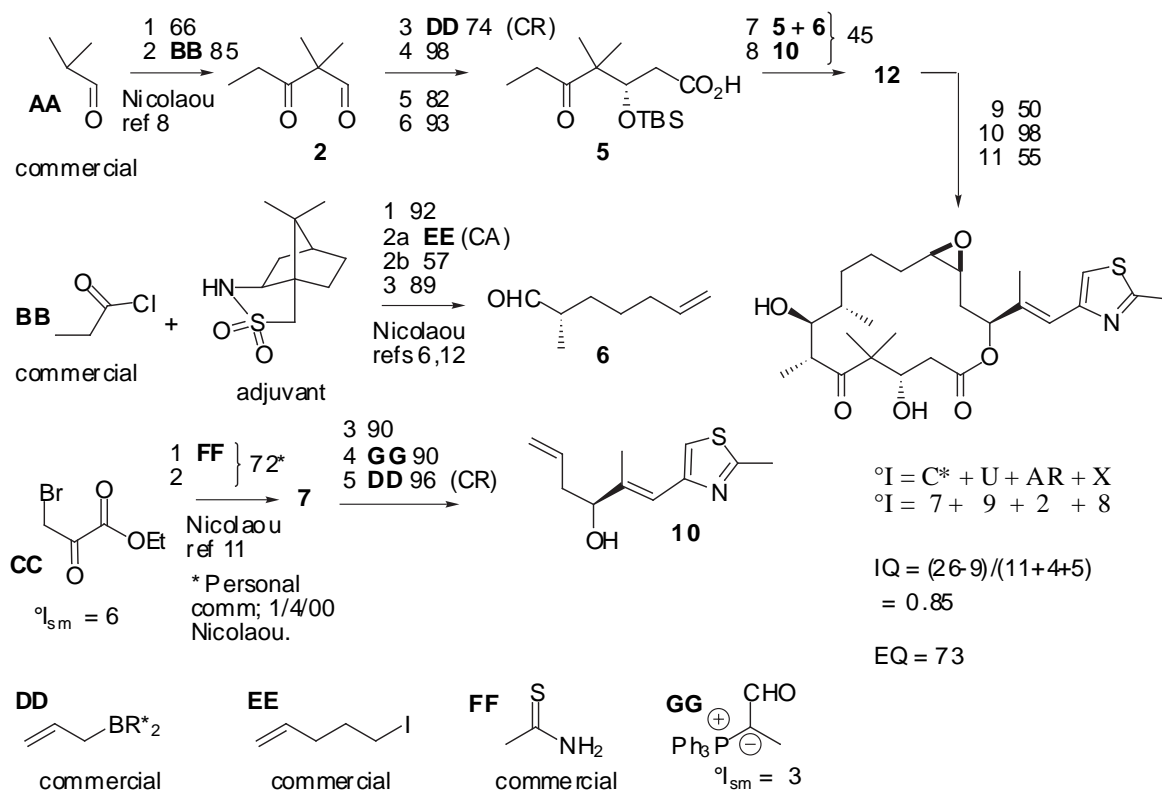
(C* includes atropisomer)

$$IQ = (41-29)/16 = 0.75$$

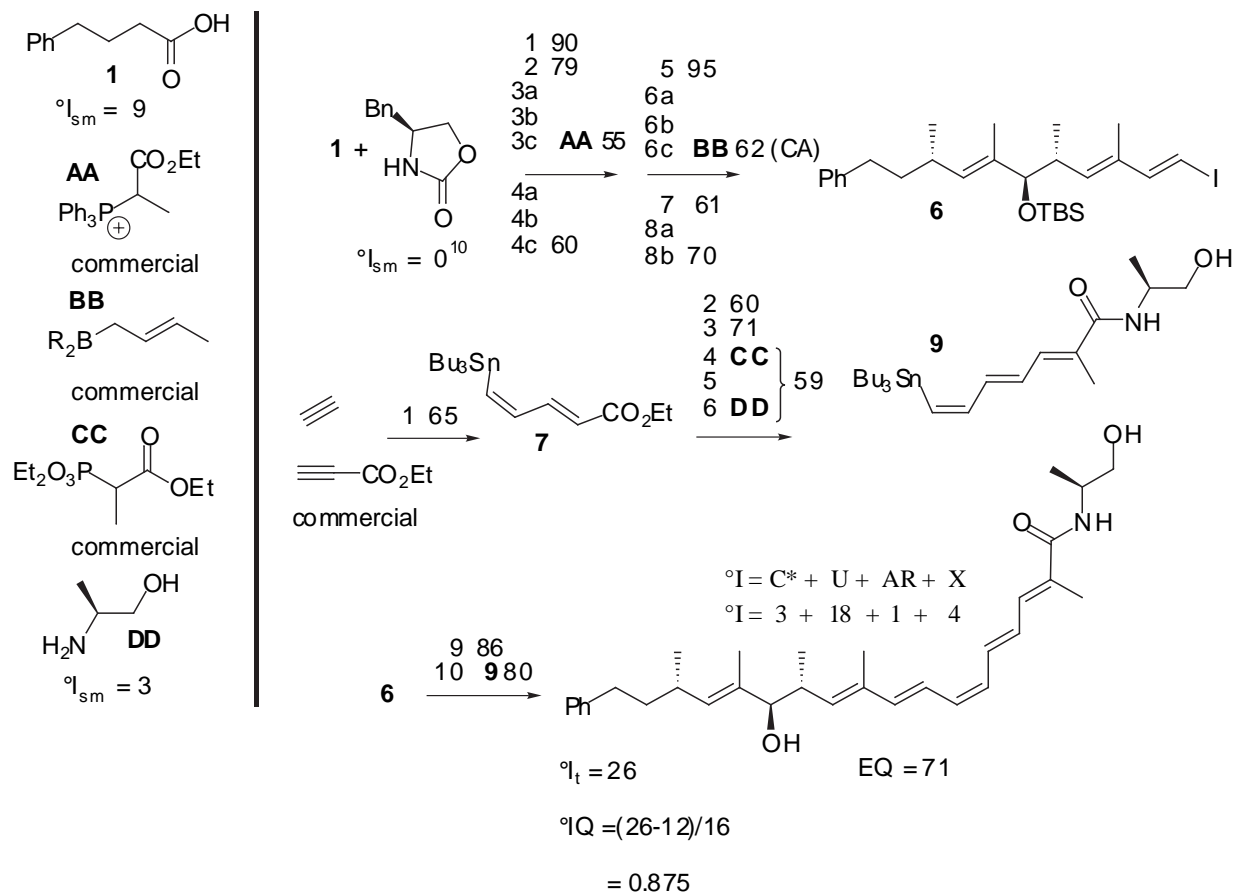
$$EQ = 79$$



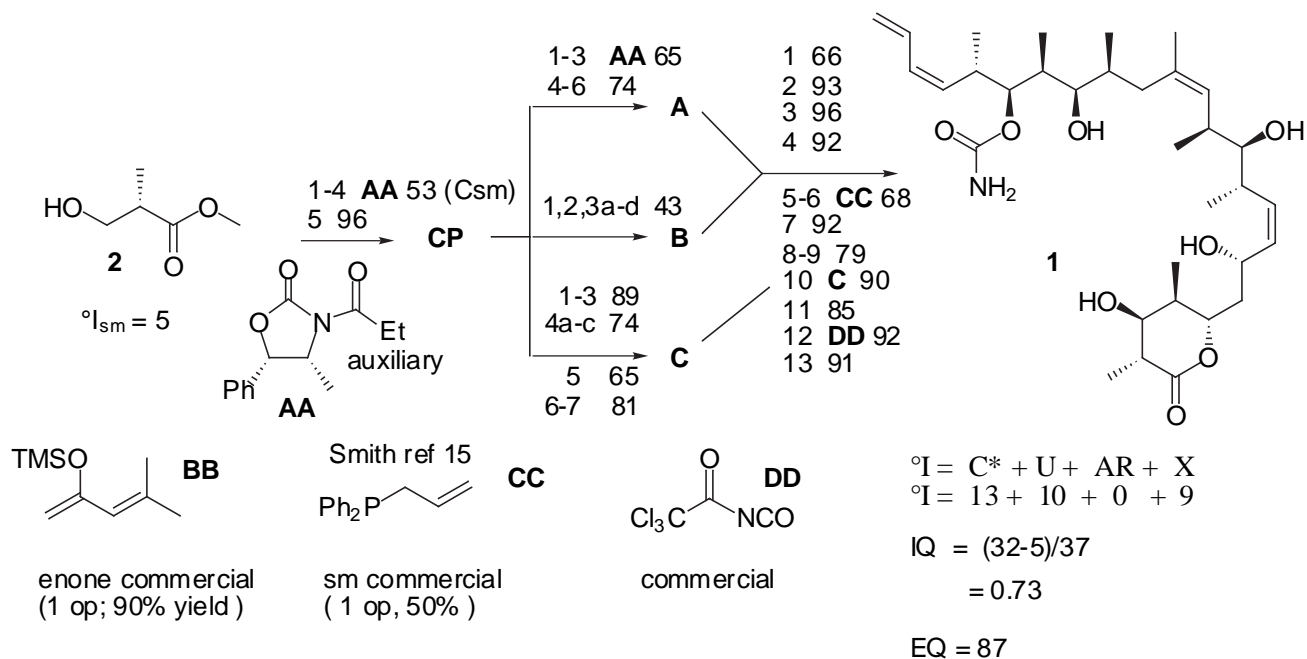
Epothiolone A



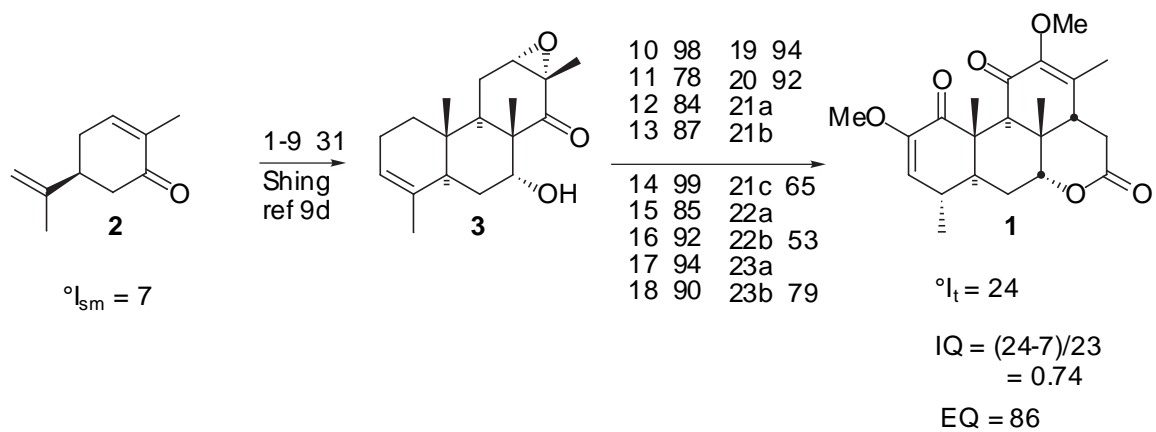
Stipiamide



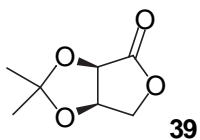
Discodermolide



Quassin

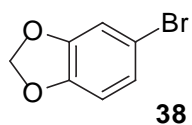


Amabiline



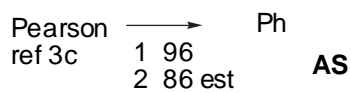
$$^{\circ}I = C^* + U + AR + X$$

$$^{\circ}I = 2 + 3 + 0 + 4$$



$$^{\circ}I = C^* + U + AR + X$$

$$^{\circ}I = 0 + 9 + 3 + 3$$



$$^{\circ}I = C^* + U + AR + X$$

$$^{\circ}I = 0 + 5 + 2 + 2$$

$$1a \text{ } \mathbf{38 + 39}$$

$$1b \text{ } 99$$

$$2a$$

$$2b$$

$$2c \text{ } 83$$

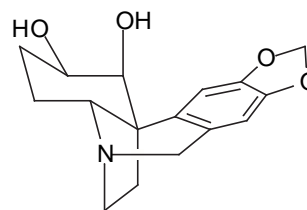
$$3a \text{ } \mathbf{AS}$$

$$3b$$

$$3c \text{ } 62$$

$$4a$$

$$4b \text{ } 85$$



$$^{\circ}I = C^* + U + AR + X$$

$$^{\circ}I = 4 + 11 + 4 + 5$$

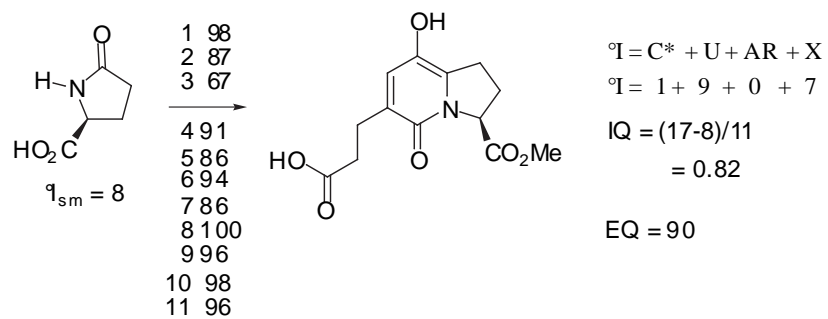
$$EQ = 85$$

$$IQ = (24-24)/6 = \mathbf{0 !!}$$
 from **38**

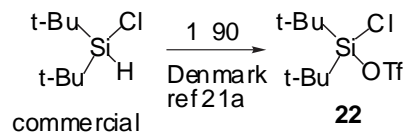
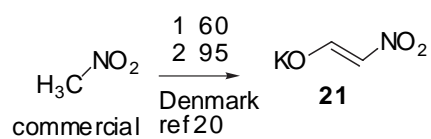
~~~~~

$$IQ = (24-18)/7 = 0.86$$
 from **MDB**

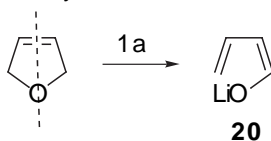
## A58365A



## Castanospermine

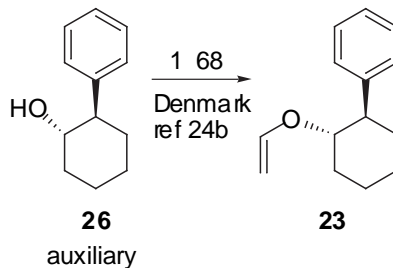


commercial.  
but primary SM



$$^{\circ}\text{I} = \text{C}^* + \text{U} + \text{AR} + \text{X}$$

$$^{\circ}\text{I} = 0 + 2 + 0 + 1$$



1b **22** to **27** 73  
2a **21**  
2b **23** 40 (CA)

**31**

3 86 (CCc)

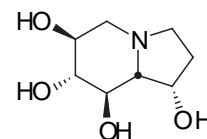
4a

4b 73

5a

5b 88

**26**



$$^{\circ}\text{I} = \text{C}^* + \text{U} + \text{AR} + \text{X}$$

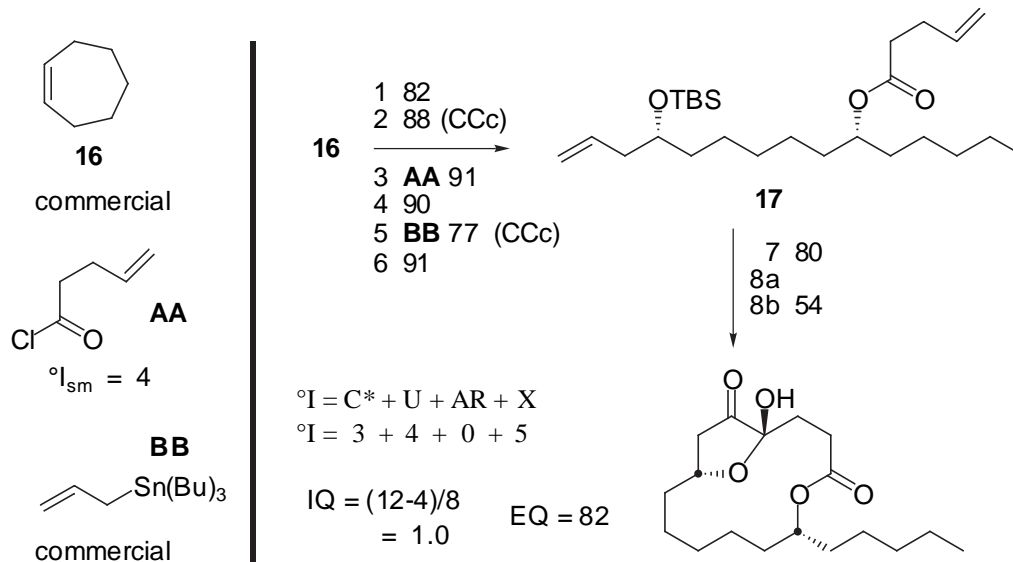
$$^{\circ}\text{I} = 5 + 2 + 0 + 5$$

$$\text{IQ} = (12-3)/9 \quad \text{EQ} = 75$$

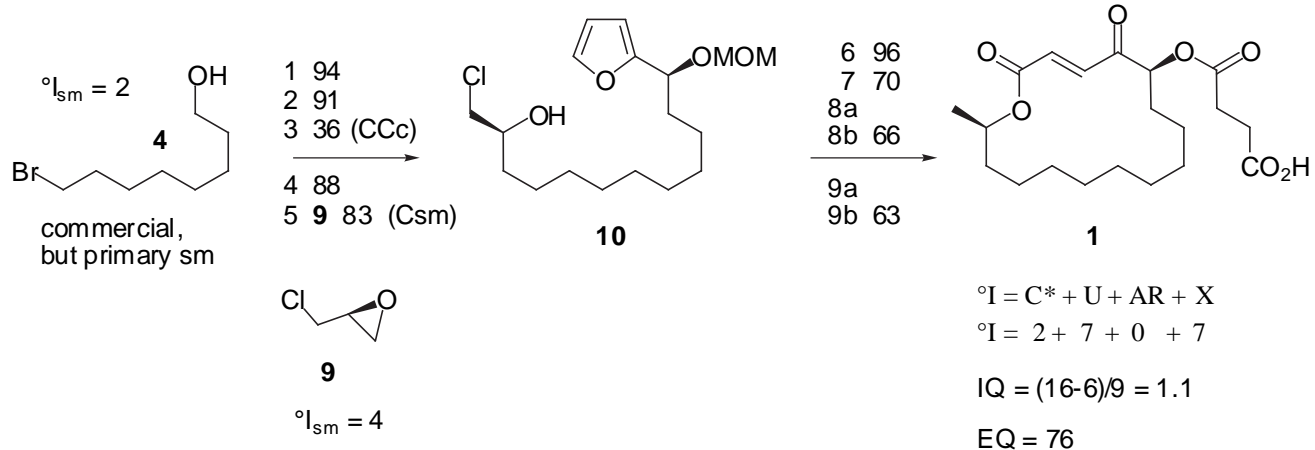
$$= 1.0$$



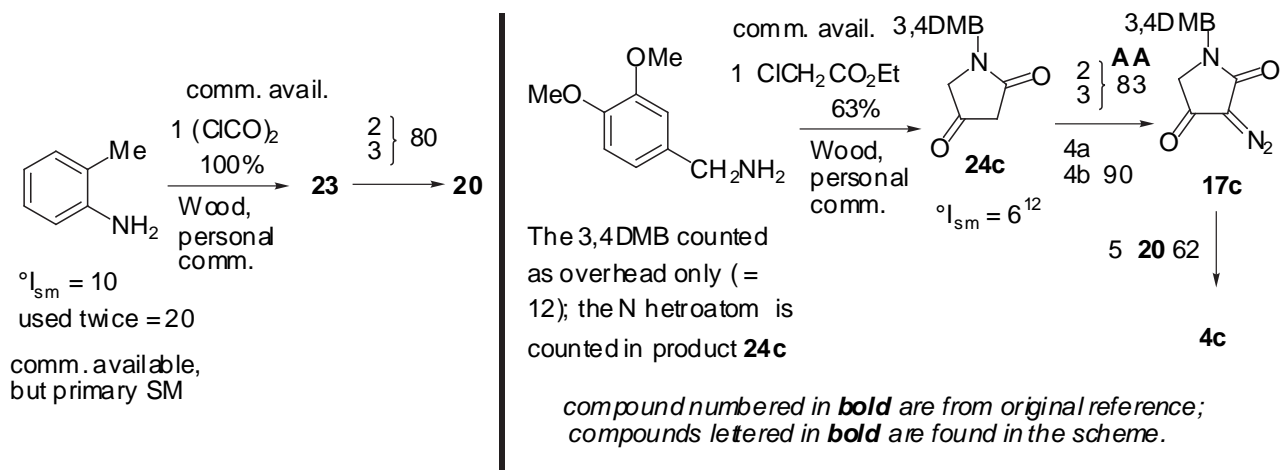
## Ricinelaiddic Acid



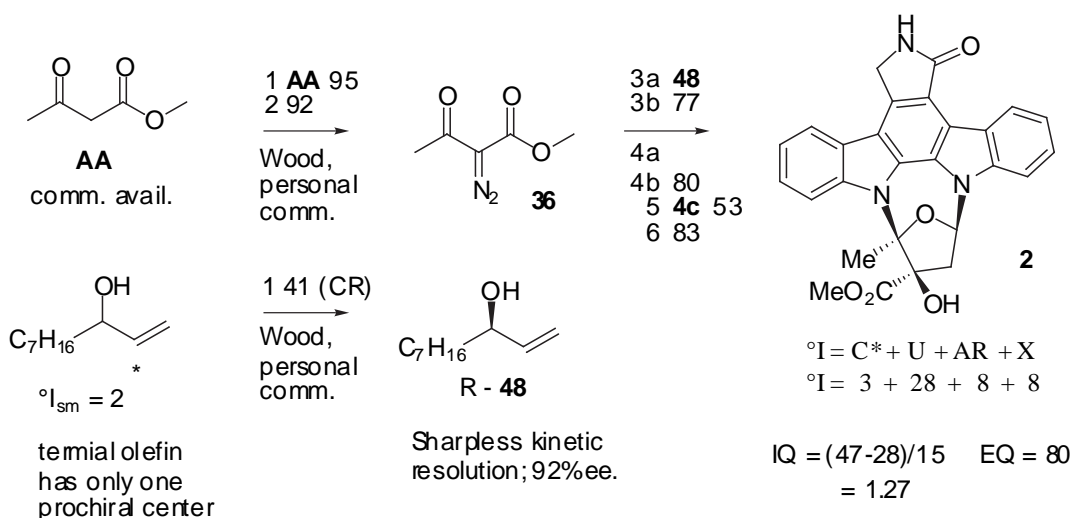
## A26771B



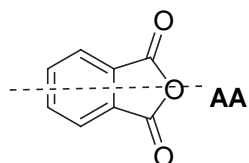
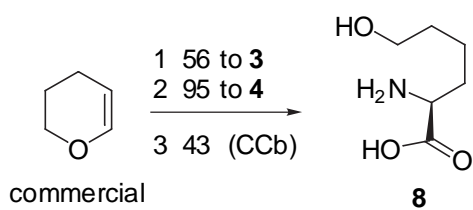
## K252a



(eq 19)

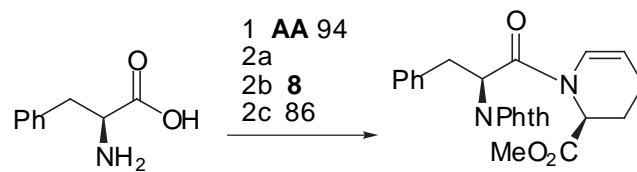


## MDL 28,726



$$\begin{aligned} \circ I &= C^* + U + AR + X \\ \circ I &= 0 + 6 + 2 + 3 \end{aligned}$$

(counted because NPhth is part of final structure)

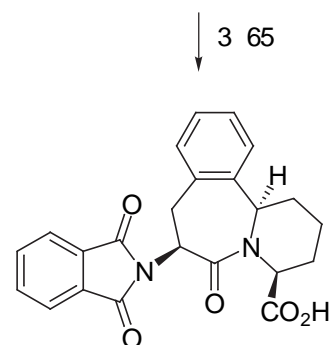


$$\begin{aligned} \circ I &= C^* + U + AR + X \\ \circ I &= 1 + 6 + 1 + 3 \end{aligned}$$

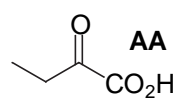
$$\begin{aligned} \circ I &= C^* + U + AR + X \\ \circ I &= 3 + 17 + 4 + 7 \end{aligned}$$

$$IQ = (31-22)/6 = 1.50$$

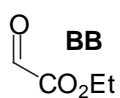
$$EQ = 73$$



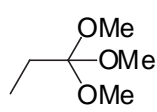
## Mappicine



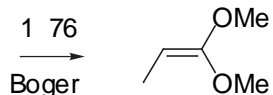
commercial



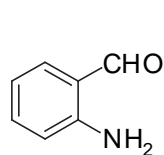
commercial



commercial



1 76  
Boger  
Ref 19;  
personal  
comm.

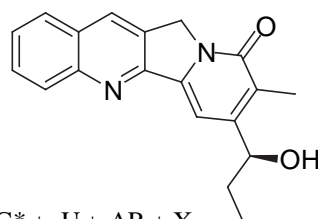


1 **AA** } 74  
2  
3 78

4 89  
5 98  
6 **BB** 78

7a  
7b **DD**  
7c 64

8 79  
9 88  
10 73 (CR)



$$^{\circ}I = C^* + U + AR + X$$

$$^{\circ}I = 0 + 8 + 2 + 2$$

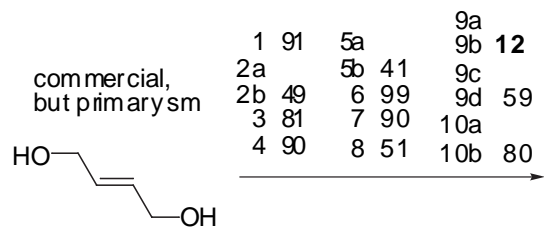
$$^{\circ}I = C^* + U + AR + X$$

$$^{\circ}I = 1 + 18 + 4 + 4$$

$$IQ = (27 - 12) / 11 \quad EQ = 82$$

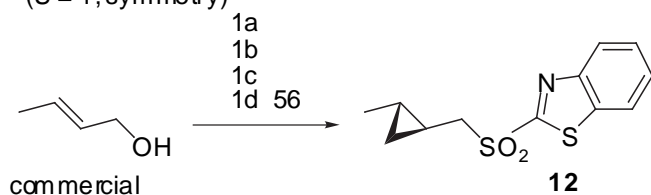
$$= 1.36$$

## U-106,305

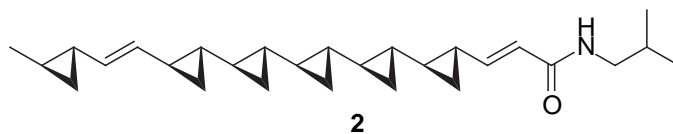


$$^{\circ}I_{sm} = 3$$

(U = 1, symmetry)



commercial



$$^{\circ}I = C^* + U + AR + X$$

$$^{\circ}I = 12 + 11 + 0 + 2$$

$$IQ = (25-3)/12$$

$$= 1.83$$

$$EQ = 72$$