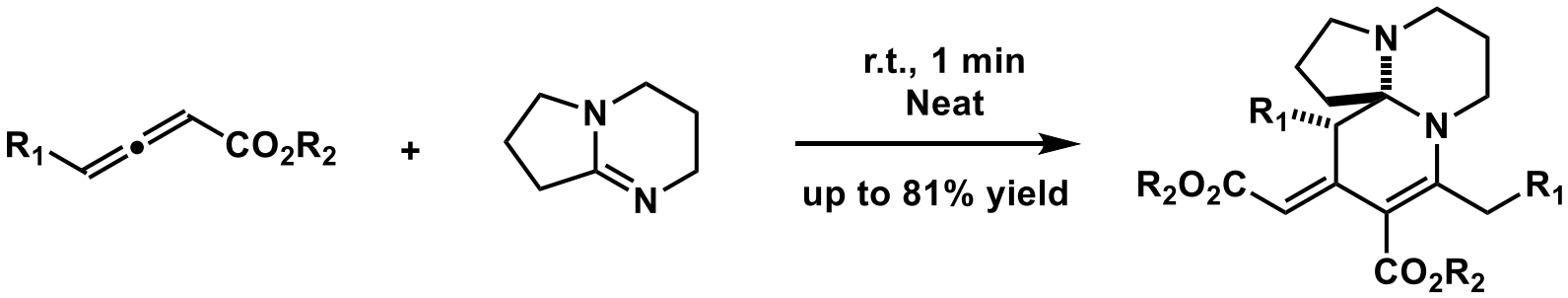
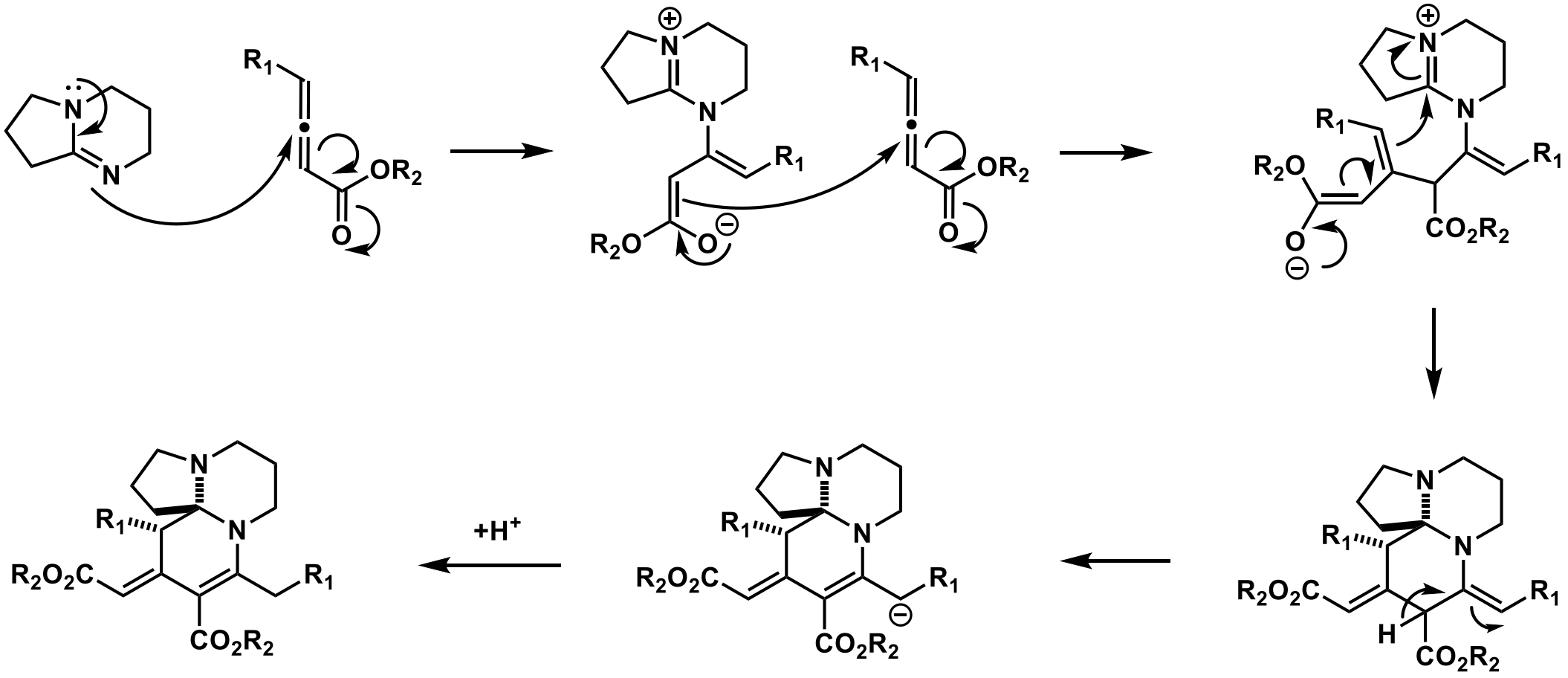
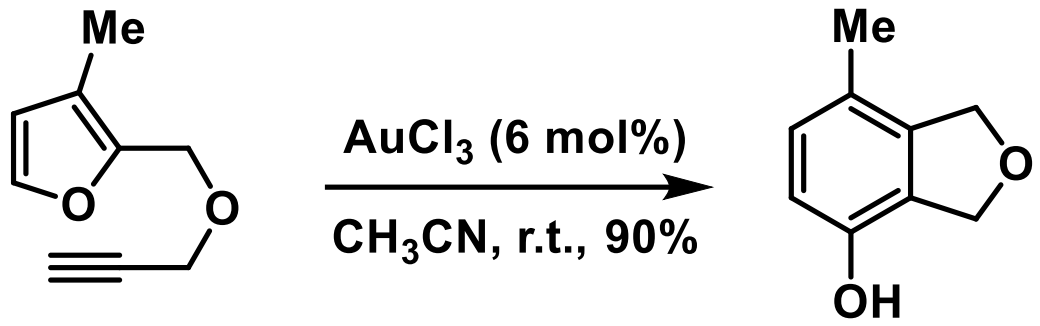
1.



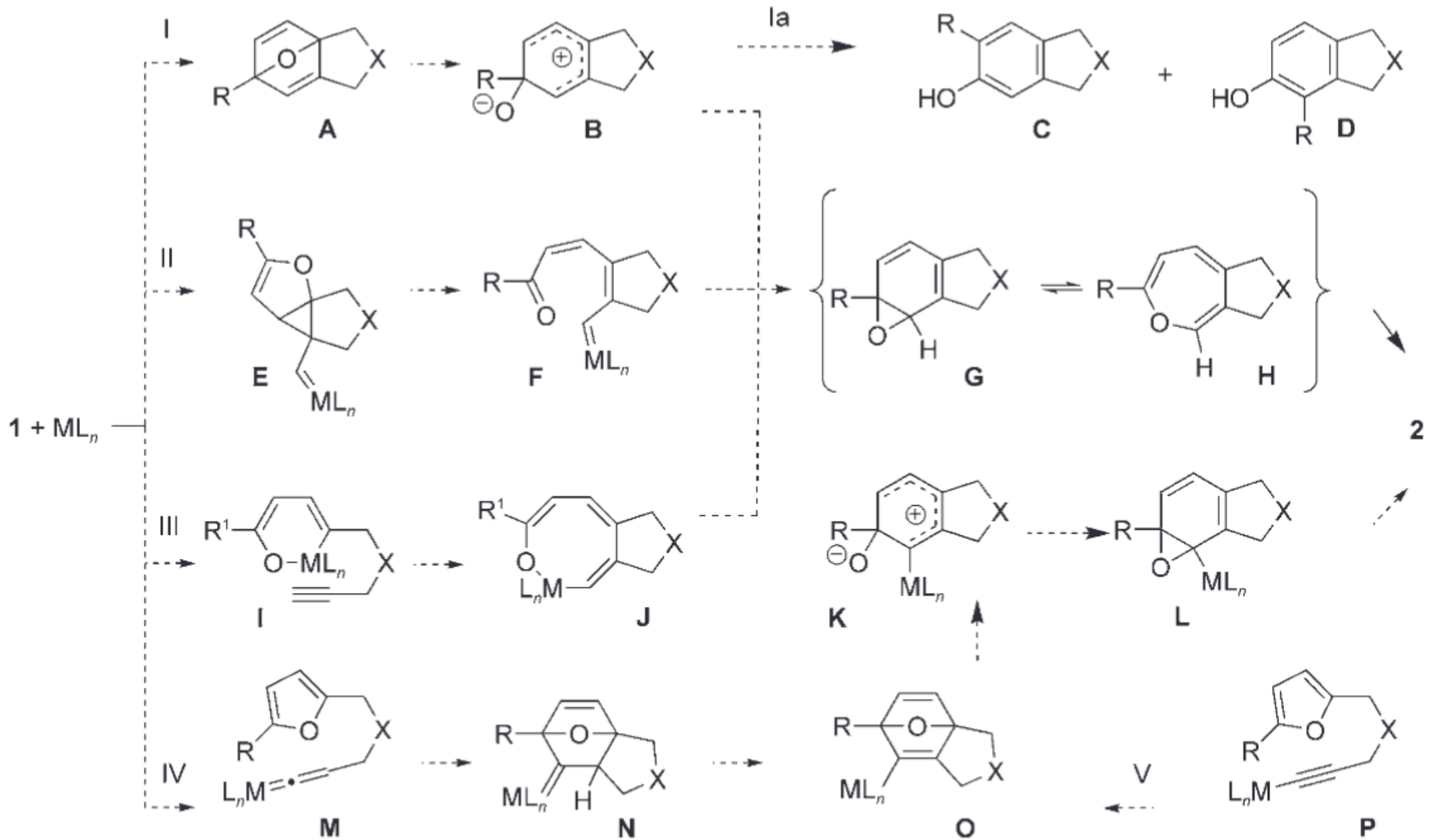
Org. Lett., **2023**, *25*, 7711.


R1
N
OR2
O
R2O
CO2R2
H
+H+
R2O2C

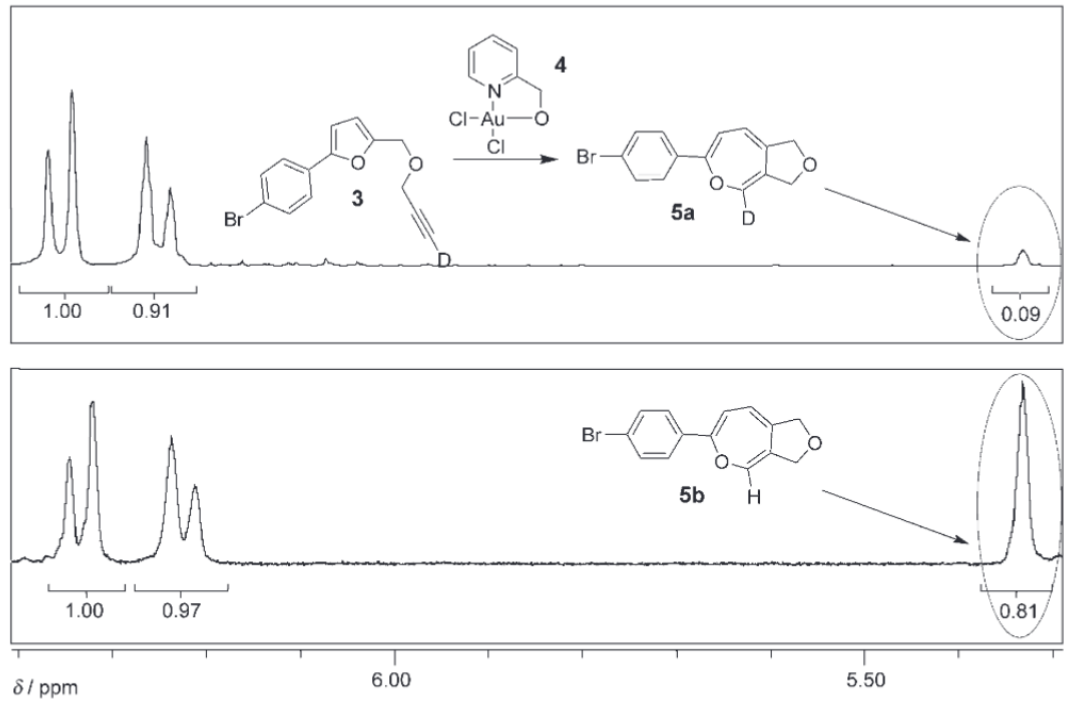
2.

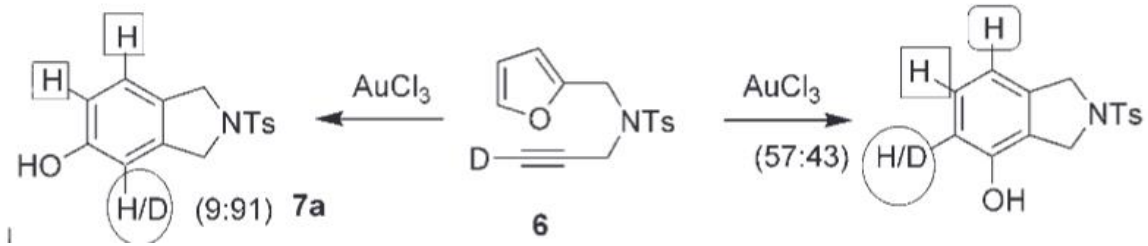


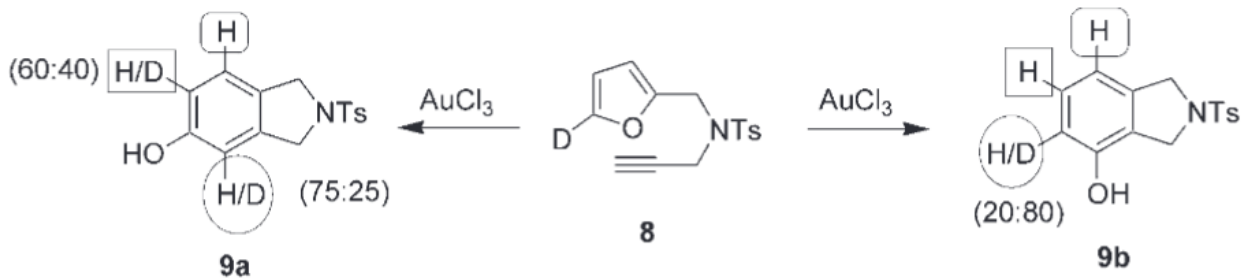
Chem. Eur. J., **2008**, *14*, 3703.



Scheme 2. Possible pathways of the gold-catalyzed phenol synthesis.


4
Cl–Au–O
Cl
3
Br
D
5a
D
1.00
0.91
0.09
5b
H
1.00
0.97
0.81
δ / ppm
6.00
5.50


H
H
NTs
HO
H/D
(9:91)
7a
AuCl3
O
NTs
D
6
AuCl3
(57:43)
H
H
NTs
H/D
OH


(60:40)
H/D
H
NTs
HO
H/D
(75:25)
9a
AuCl3
D
O
NTs
8
AuCl3
H
H
NTs
H/D
OH
(20:80)
9b

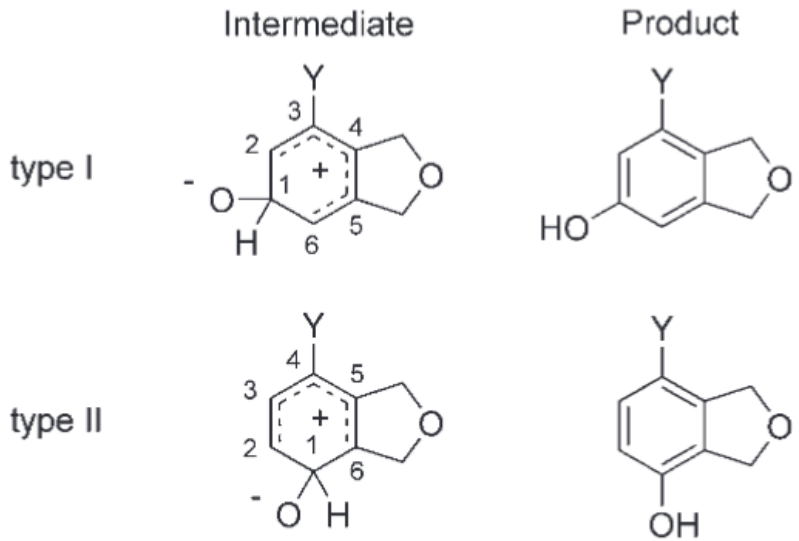
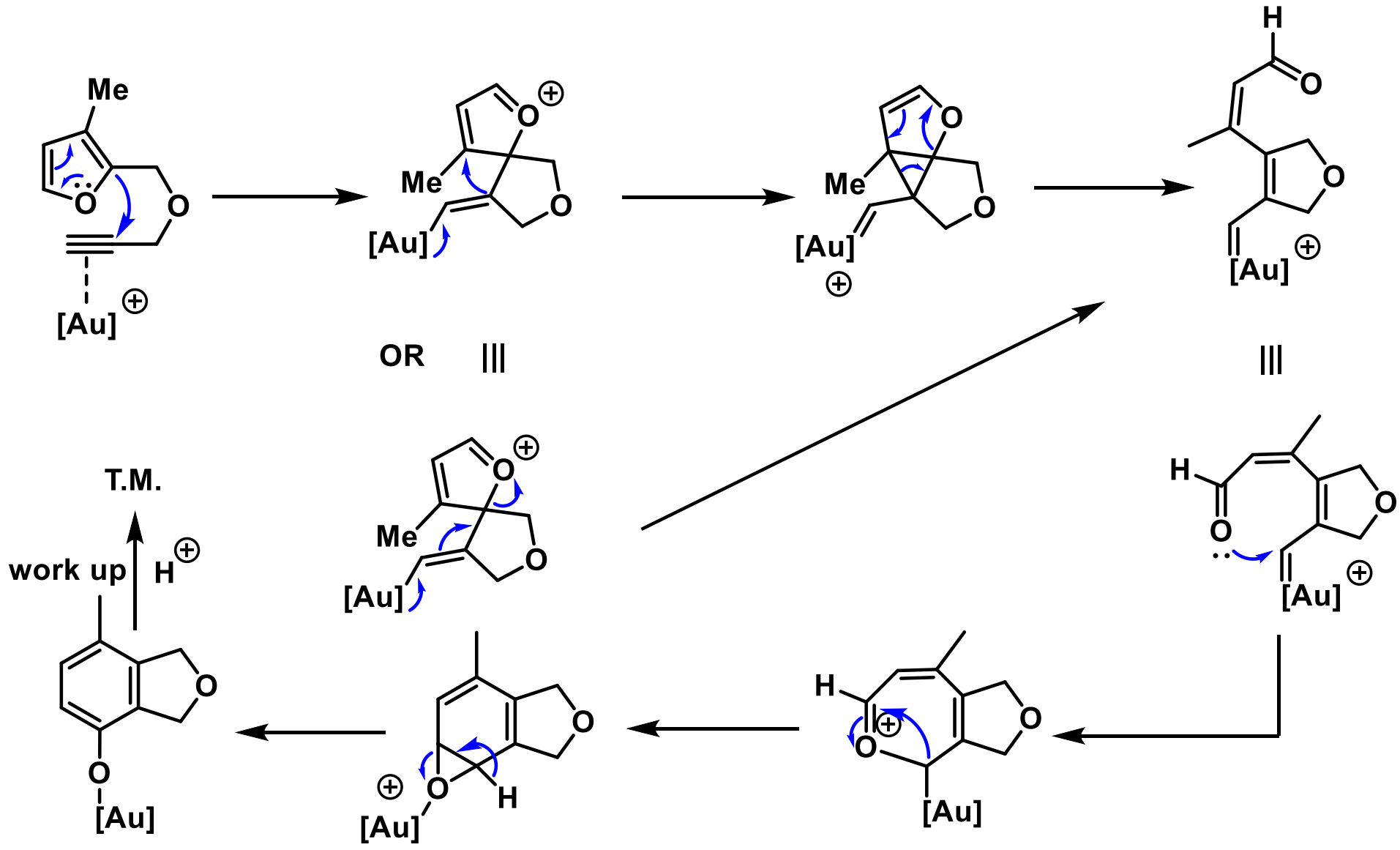


Figure 5. Molecular structures of the intermediates and products (Y = H, CH_3).

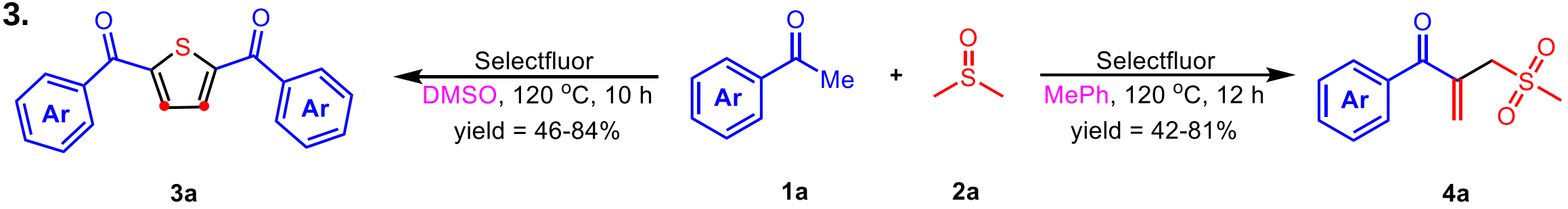
Table 1. Comparison of energy differences[a] of the intermediates (ΔE_{int}) and the products (ΔE_{pr}) between structures of type I and II in Figure 5.

	Y = H		Y = CH_3	
	ΔE_{int}[b]	ΔE_{pr}[b]	ΔE_{int}[b]	ΔE_{pr}[b]
gas phase	−2.03 (−1.89)	−0.82 (−0.69)	−5.13 (−4.68)	−0.07 (0.05)
PCM[c]	−0.59 (−0.41)	−0.42 (−0.36)	−4.17 (−3.97)	0.82 (0.93)

[a] Energy differences are shown in kcal mol^{-1}. Relative energies with ZPE corrected are shown in parentheses. [b] $\Delta E = E$(structure of type II) − E(structure of type I). [c] PCM model calculation with $\varepsilon = 78.6$ (water).

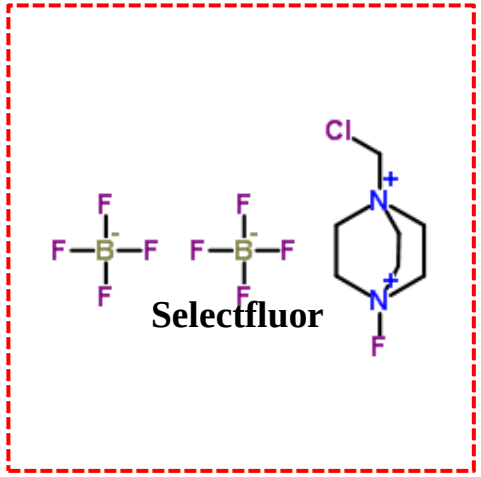

Me
O
O
[Au]
Me
O
O
[Au]
OR
Me
O
[Au]
H
O
O
[Au]
H
O
O
[Au]
T.M.
work up
H
O
[Au]
Me
O
[Au]
O
H
[Au]
H
O
O
[Au]
H
O
O
[Au]

3.

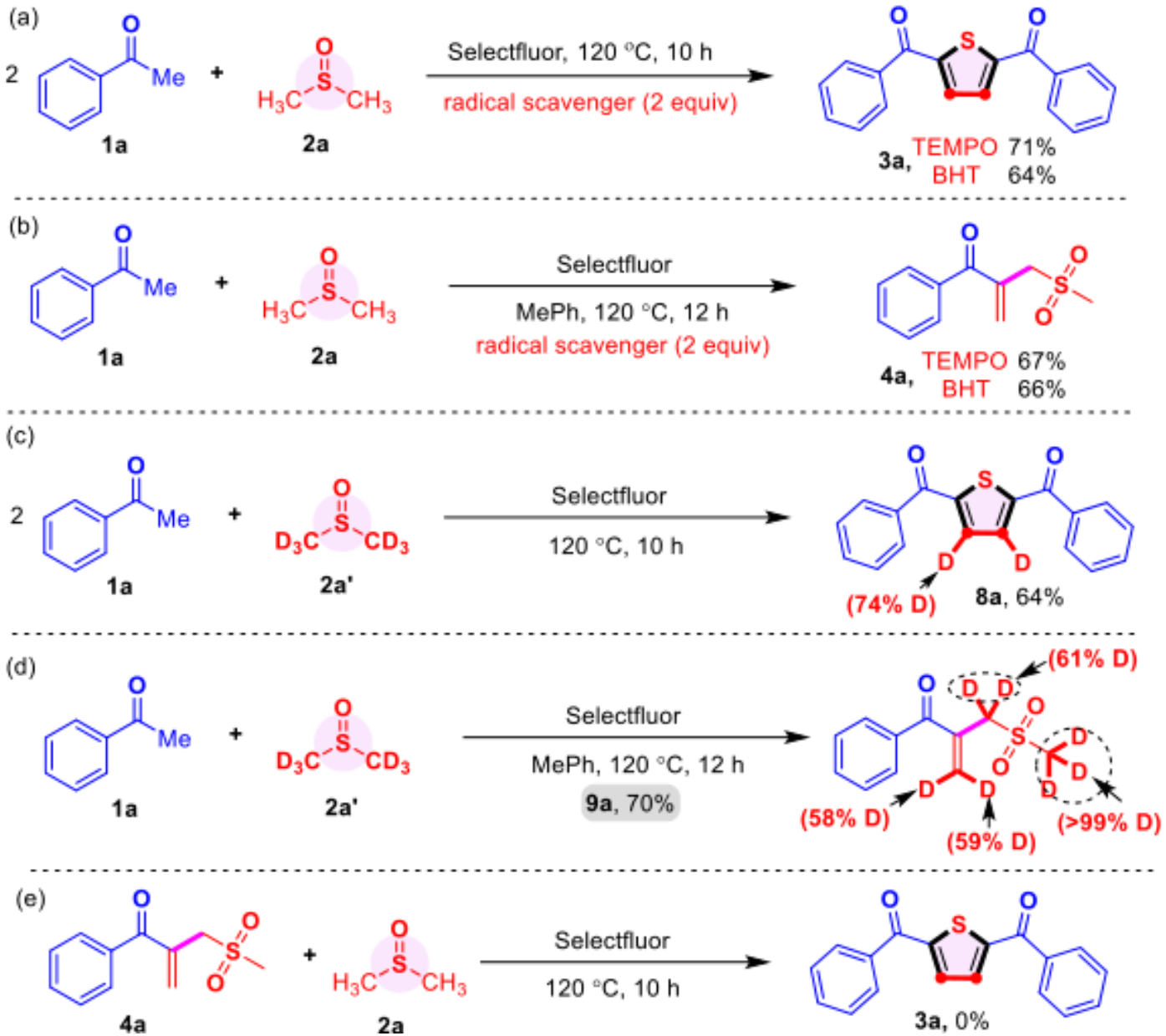


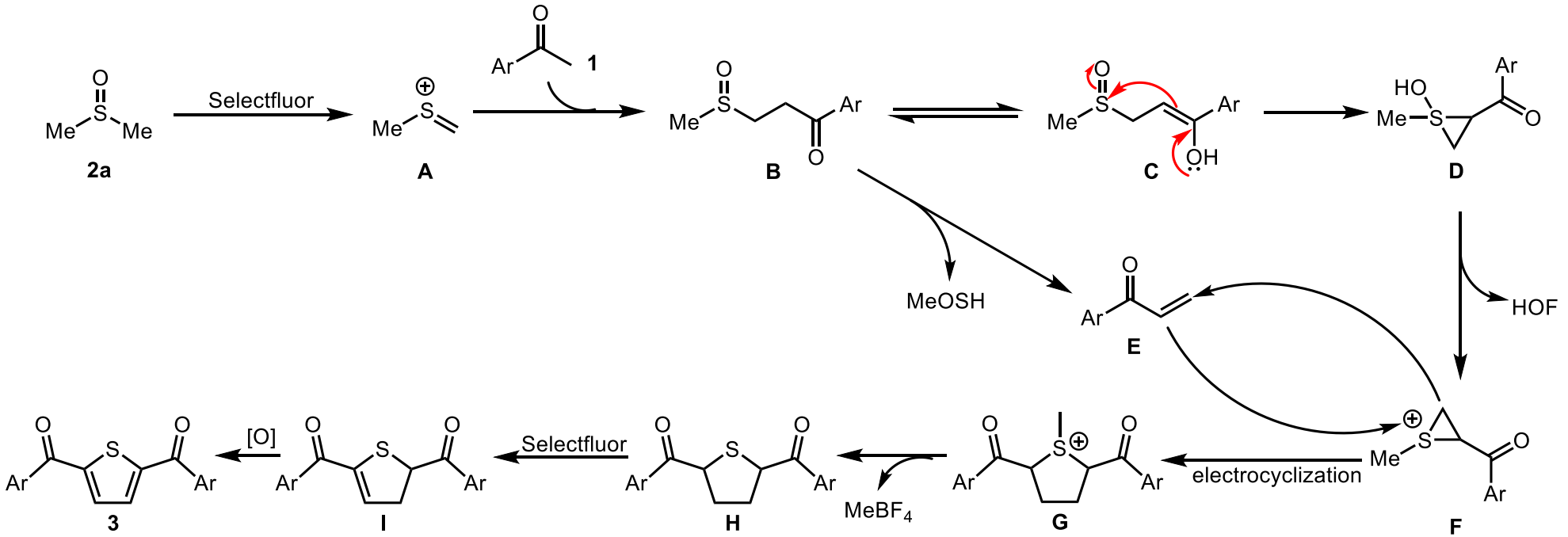
3a **1a** **2a** **4a**

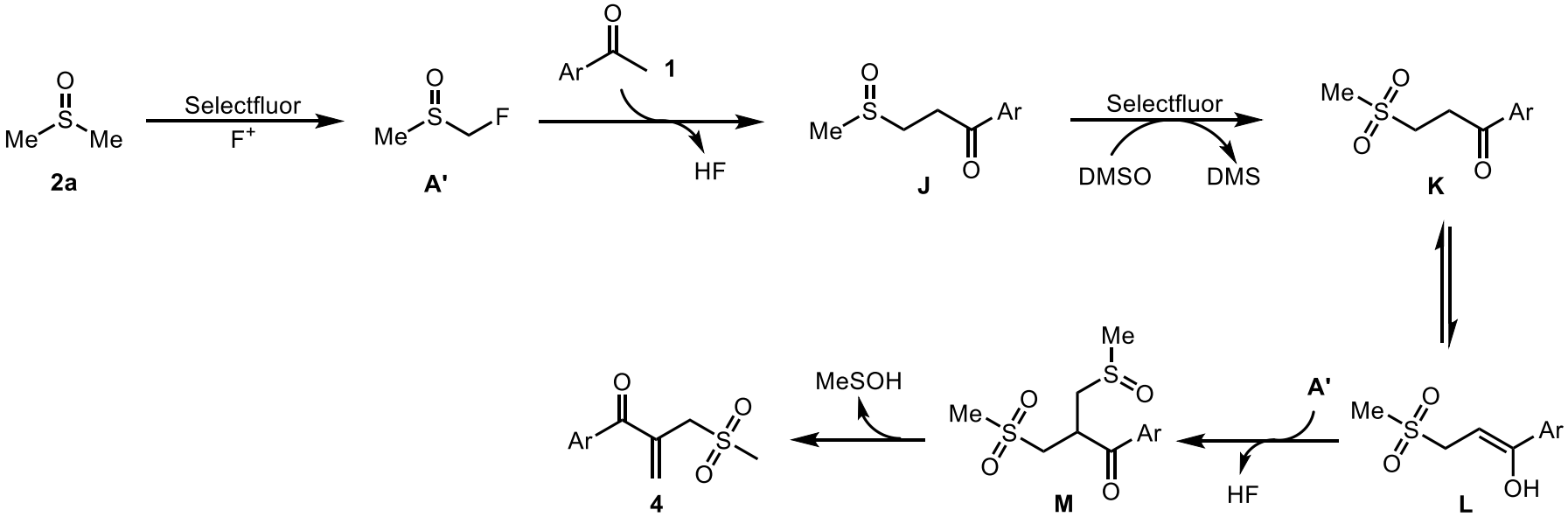
Org. Lett., **2023**, *25*, 389.



Scheme 5. Control Experiments




Selectfluor
2a
A
1
B
C
D
MeOSH
HOF
E
F
electrocyclization
G
MeBF4
H
Selectfluor
I
[O]
3


Selectfluor
F+
2a
A'
1
HF
J
Selectfluor
DMSO
DMS
K
L
A'
HF
M
MeSOH
4