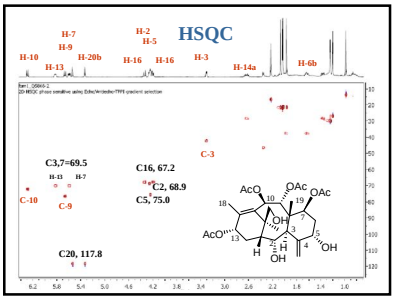
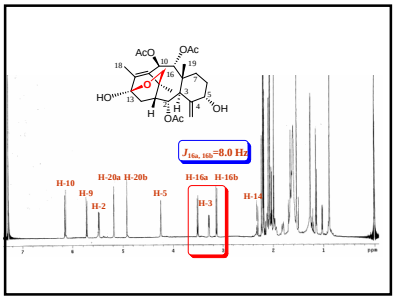
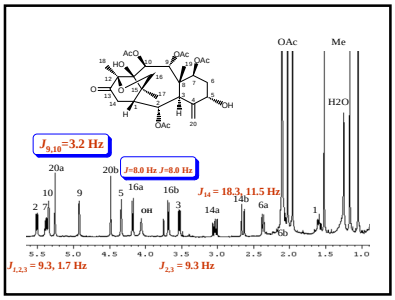
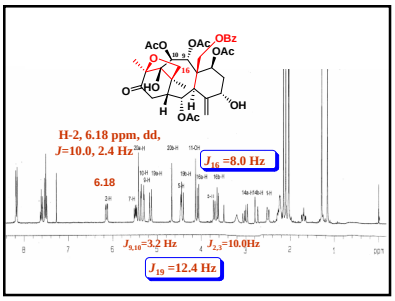
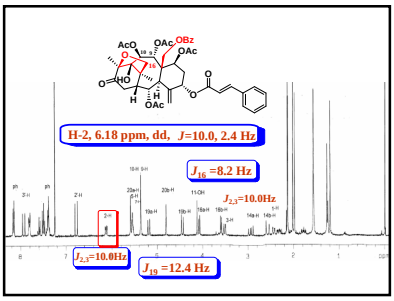
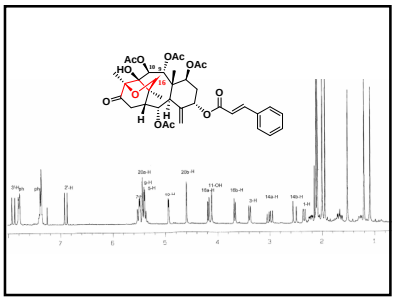

HSQC
H-7
H-9
H-10
H-13
H-20b
H-2
H-5
H-16
H-16
H-3
H-14a
H-6b
C-3
C3,7=69.5
C16, 67.2
C2, 68.9
C5, 75.0
C-10
C-9
C20, 117.8

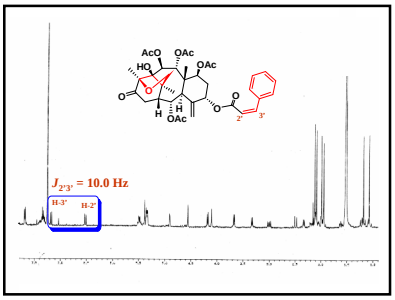

$J_{16a,\ 16b}$=8.0 Hz
H-10
H-9
H-2
H-20a
H-20b
H-5
H-16a
H-16b
H-3
H-14

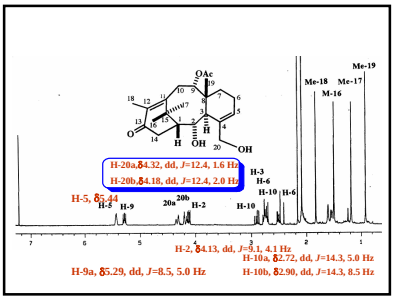

OAc
Me
H2O
$J_{9,10}$=3.2 Hz
J=8.0 Hz J=8.0 Hz
J_{14} = 18.3, 11.5 Hz
$J_{1,2,3}$ = 9.3, 1.7 Hz
$J_{2,3}$ = 9.3 Hz

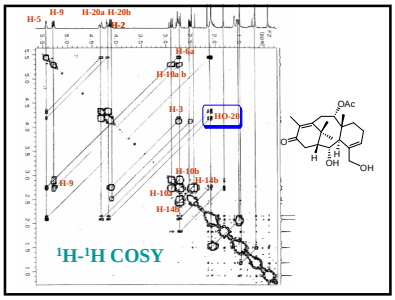

H-2, 6.18 ppm, dd,
J=10.0, 2.4 Hz
6.18
J_{16} =8.0 Hz
$J_{9,10}$=3.2 Hz
$J_{2,3}$=10.0Hz
J_{19} =12.4 Hz

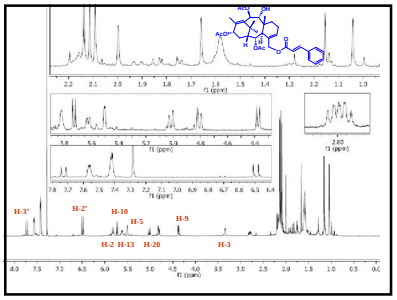

H-2, 6.18 ppm, dd, J=10.0, 2.4 Hz
J_{16} =8.2 Hz
$J_{2,3}$=10.0Hz
$J_{2,3}$=10.01Hz
J_{19} =12.4 Hz

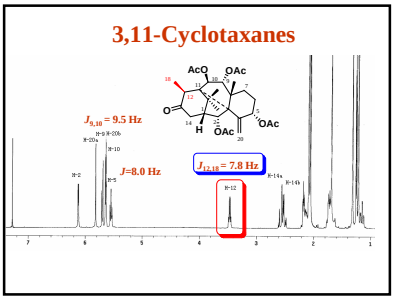


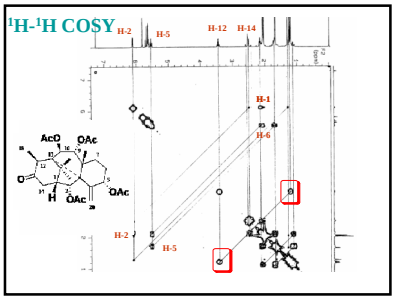

$J_{2'3'}$ = 10.0 Hz
H-3'
H-2'

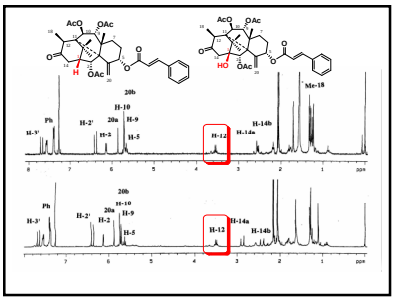

Me-19
Me-18
Me-17
M-16
H-20a, δ4.32, dd, J=12.4, 1.6 Hz
H-20b, δ4.18, dd, J=12.4, 2.0 Hz
H-5, δ5.44
H-3
H-6
H-10
H-6
H-2, δ4.13, dd, J=9.1, 4.1 Hz
H-10a, δ2.72, dd, J=14.3, 5.0 Hz
H-9a, δ5.29, dd, J=8.5, 5.0 Hz
H-10b, δ2.90, dd, J=14.3, 8.5 Hz

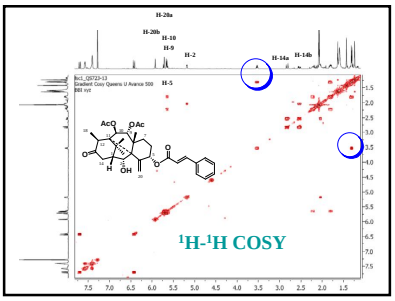

^{1}H-^{1}H COSY

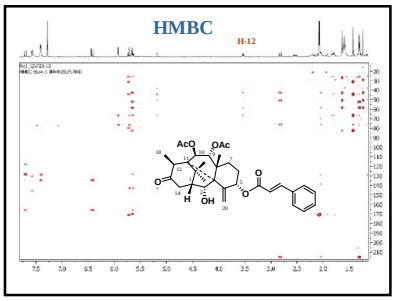

H-3'
H-2'
H-10
H-5
H-9
H-2 H-13 H-20
H-3

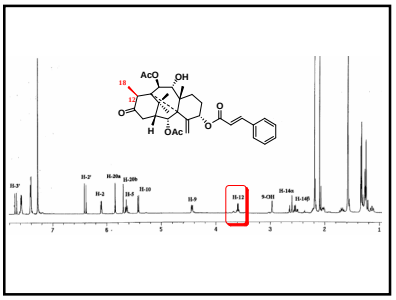

3,11-Cyclotaxanes
$J_{9,10}$ = 9.5 Hz
J=8.0 Hz
$J_{12,13}$ = 7.8 Hz

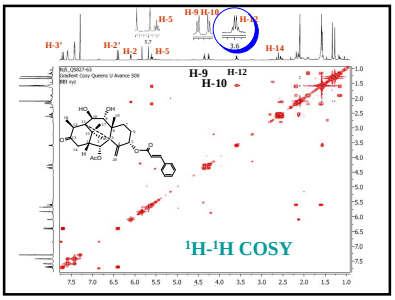

^{1}H-^{1}H COSY
H-2
H-5
H-12
H-14
H-1
H-6
H-2
H-5

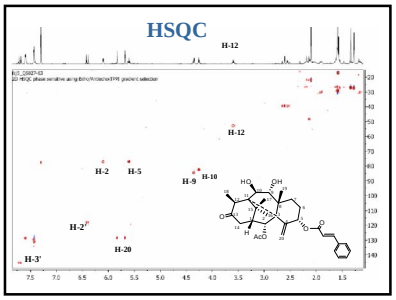

Me-18
H-12
H-14a
H-14b

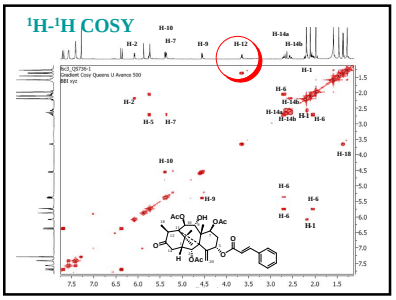

^{1}H-^{1}H COSY

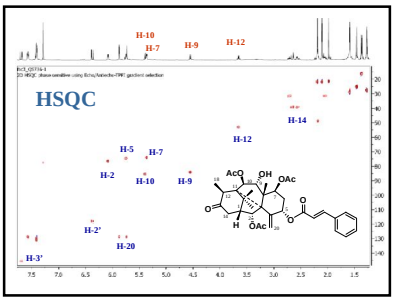

HMBC
H-12

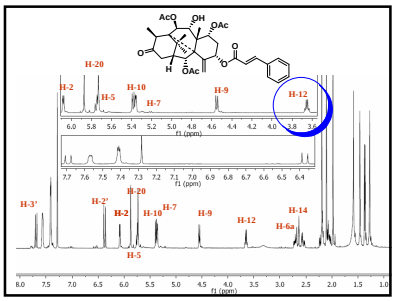


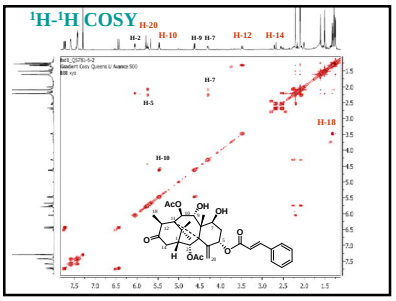

H-9
H-10
H-12
^{1}H-^{1}H COSY

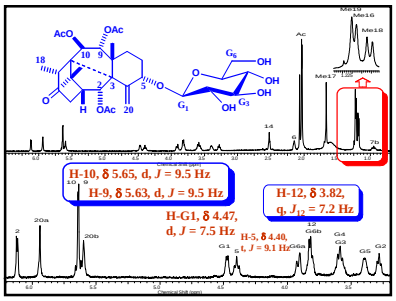

HSQC
H-12
H-2
H-5
H-9
H-10
H-20
H-3'

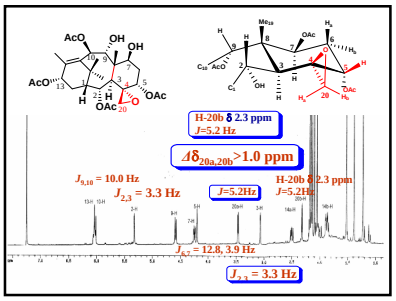

¹H-¹H COSY
H-10
H-7
H-2
H-9
H-12
H-14a
H-14b
H-1
H-6
H-5
H-18
AcO
OH
OAc
H
ÖAc

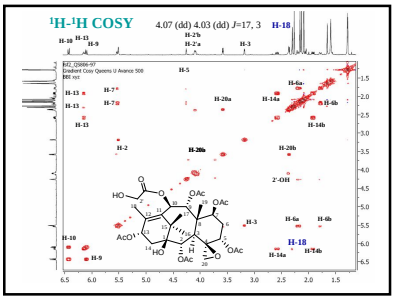

HSQC
H-10
H-7
H-9
H-12
H-14
H-5
H-2
H-2'
H-20
H-3'
AcO
OH
OAc
H
ÖAc

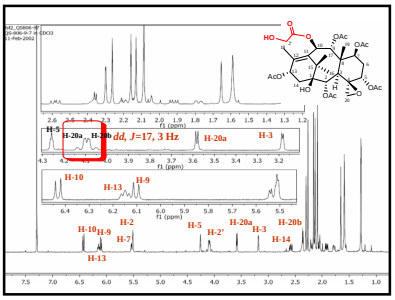

AcO
OH
OAc
H
ÖAc
H-20
H-2
H-5
H-10
H-7
H-9
H-12
H-3'
H-2'
H-14
H-6a
f1 (ppm)

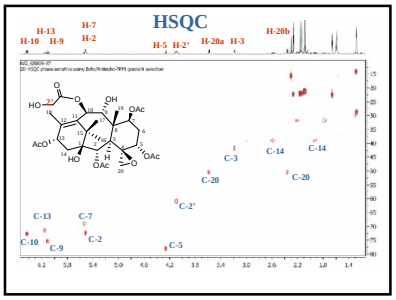

¹H-¹H COSY
H-20
H-2
H-10
H-9
H-7
H-12
H-14
H-5
H-18
AcO
OH
OAc
H
ÖAc

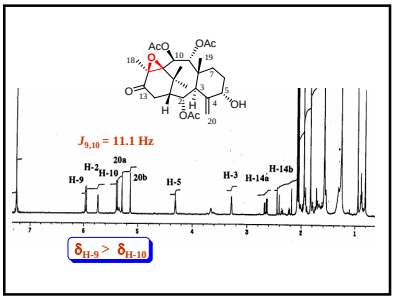

AcO
OAc
OH
OH
OH
OH
H
ÖAc
H-10, δ 5.65, d, J = 9.5 Hz
H-9, δ 5.63, d, J = 9.5 Hz
H-G1, δ 4.47, d, J = 7.5 Hz
H-5, δ 4.40, t, J = 9.1 Hz
H-12, δ 3.82, q, J12 = 7.2 Hz

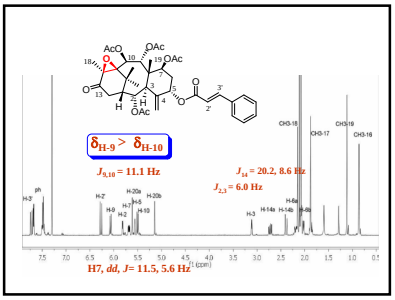

AcO
OH
OAc
H
ÖAc
H-20b δ 2.3 ppm
J=5.2 Hz
Δδ20a,20b>1.0 ppm
J9,10 = 10.0 Hz
J2,3 = 3.3 Hz
J=5.2Hz
H-20b δ 2.3 ppm
J=5.2Hz
J9,8 = 12.8, 3.9 Hz
J2,3 = 3.3 Hz

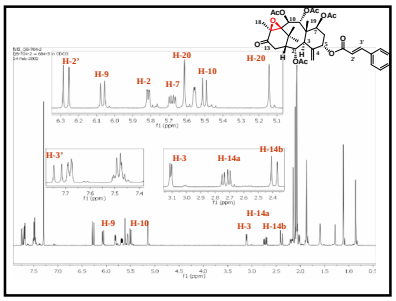

¹H-¹H COSY
4.07 (dd) 4.03 (dd) J=17, 3
H-18
H-10
H-13
H-9
H-2b
H-2a
H-3
H-5
H-7
H-20a
H-14a
H-6a
H-6b
H-14b
H-20b
H-2
2'-OH
HO
OAc
AcO
H
ÖAc

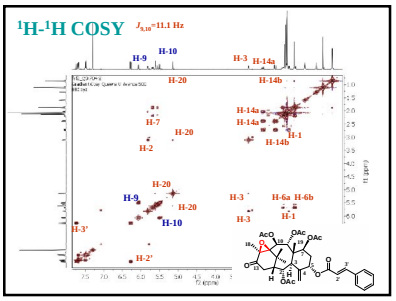

H-5
H-20a
H-20b
dd, J=17, 3 Hz
H-20a
H-3
H-10
H-13
H-9
H-2
H-7
H-5
H-2'
H-20a
H-3
H-20b
H-14
f1 (ppm)

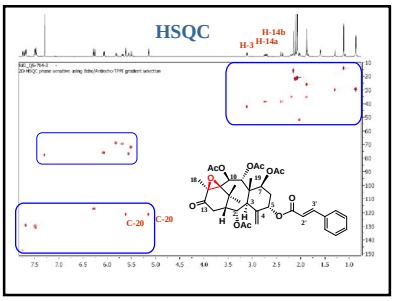

HSQC
H-13
H-10
H-9
H-7
H-2
H-5
H-2'
H-20a
H-3
H-20b
C-3
C-14
C-14
C-20
C-20
C-2'
C-13
C-7
C-10
C-9
C-2
C-5

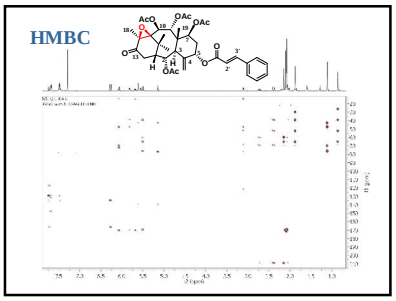

$J_{9,10}$ = 11.1 Hz
H-9
H-2
H-10
20a
20b
H-5
H-3
H-14a
H-14b
$\delta_{H-9} > \delta_{H-10}$

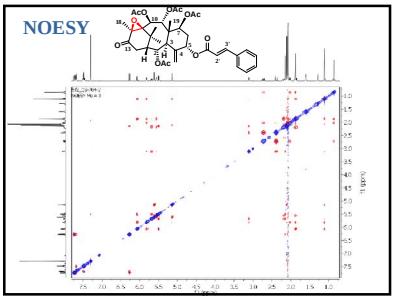

$\delta_{H-9} > \delta_{H-10}$
$J_{9,10}$ = 11.1 Hz
J_{14} = 20.2, 8.6 Hz
$J_{2,3}$ = 6.0 Hz
H7, dd, J= 11.5, 5.6 Hz

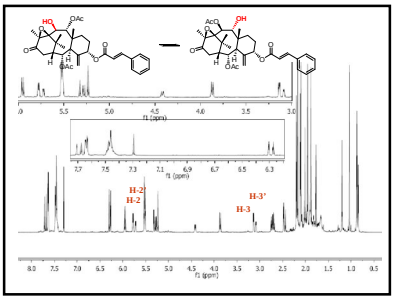

H-2'
H-9
H-2
H-7
H-10
H-20
H-3'
H-3
H-14a
H-14b
H-9
H-10
H-14a
H-3
H-14b

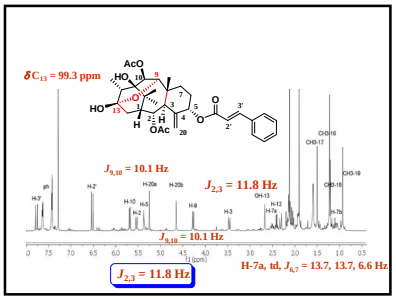

^{1}H-^{1}H COSY
$J_{9,10}$=11.1 Hz
H-9
H-10
H-3
H-14a
H-20
H-14b
H-7
H-14a
H-14a
H-20
H-1
H-2
H-14b
H-20
H-9
H-20
H-3
H-6a H-6b
H-10
H-1
H-3
H-3'
H-2'

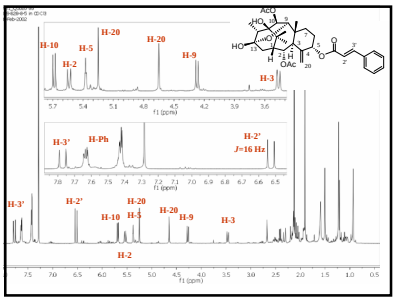

HSQC
H-14b
H-3 H-14a
C-20
C-20

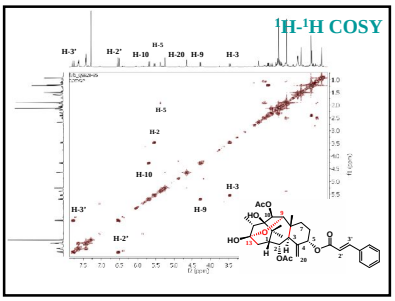

HMBC

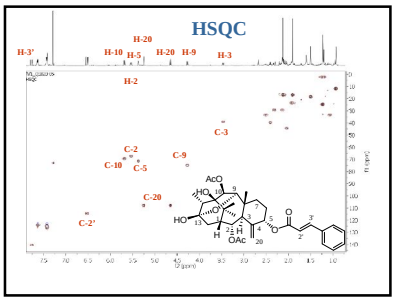

NOESY

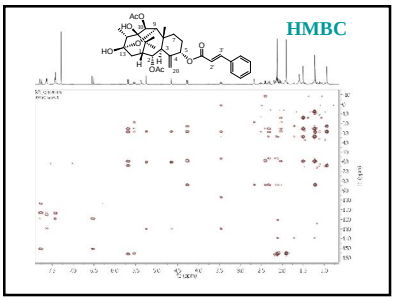

H-2
H-2
H-3'
H-3

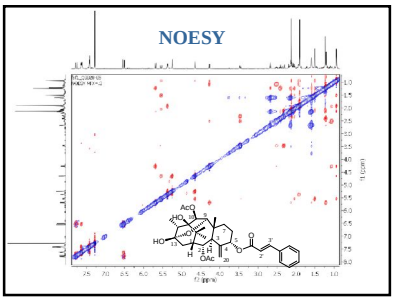

δC_{13} = 99.3 ppm
$J_{9,10}$ = 10.1 Hz
$J_{2,3}$ = 11.8 Hz
$J_{9,10}$ = 10.1 Hz
$J_{2,3}$ = 11.8 Hz
H-7a, td, $J_{6,7}$ = 13.7, 13.7, 6.6 Hz


H-10
H-2
H-5
H-20
H-20
H-9
H-3
H-3'
H-Ph
H-2'
J=16 Hz
H-3'
H-2'
H-10
H-5
H-20
H-20
H-9
H-3
H-2


^{1}H-^{1}H COSY
H-3'
H-2'
H-5
H-10
H-20
H-9
H-3
H-5
H-2
H-10
H-3
H-9
H-3'
H-2'


HSQC
H-3'
H-20
H-10
H-5
H-20
H-9
H-3
H-2
C-3
C-2
C-10
C-5
C-9
C-20
C-2'


HMBC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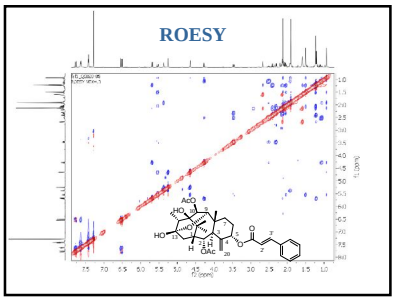
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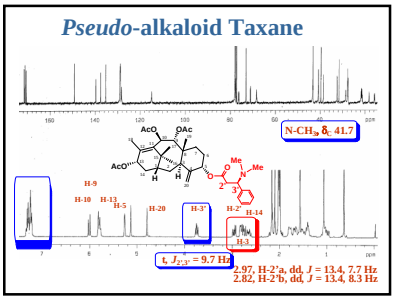
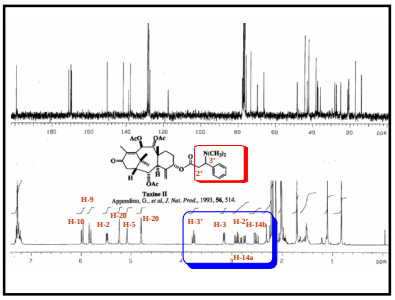
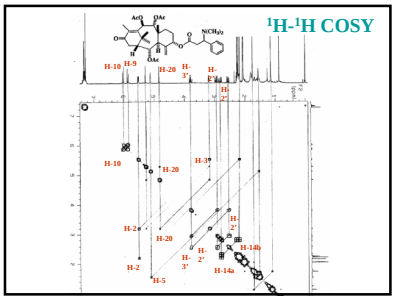
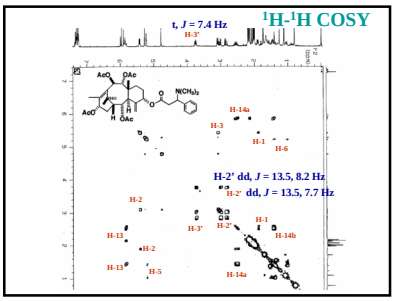
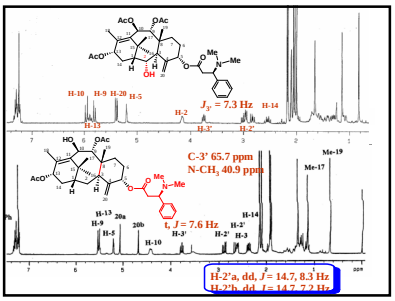
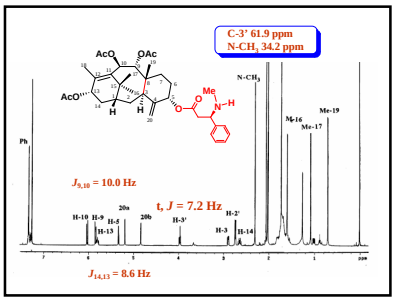

Pseudo-alkaloid Taxane
N-CH$_3$ δ$_C$ 41.7
H-9
H-10
H-13
H-5
H-20
H-3'
H-2
H-14
H-3
t, $J_{2'-3'}$ = 9.7 Hz
2.97, H-2'a, dd, J = 13.4, 7.7 Hz
2.82, H-2'b, dd, J = 13.4, 8.3 Hz

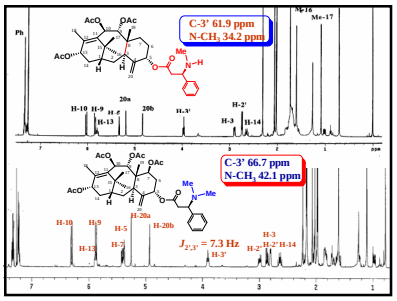

Taxine II
Appendino, G., et al, J. Nat. Prod., 1993, 56, 514.
H-9
H-10
H-2
H-20
H-5
H-20
H-3'
H-3
H-2'
H-14b
H-14a

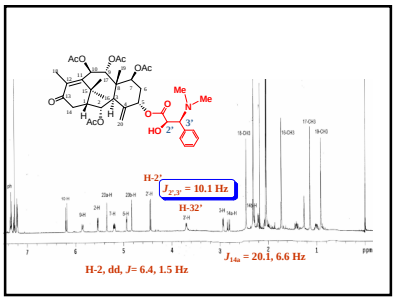

^{1}H-^{1}H COSY
H-10
H-9
H-20
H-3'
H-2'
H-10
H-20
H-3'
H-2'
H-20
H-14b
H-2
H-3'
H-14a
H-2
H-5

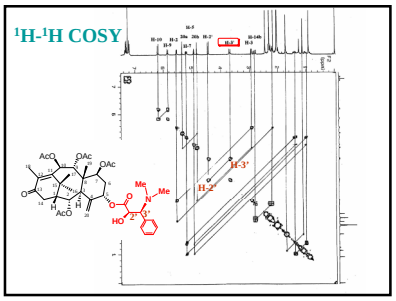


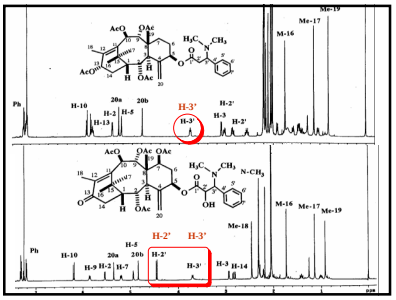




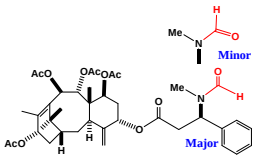


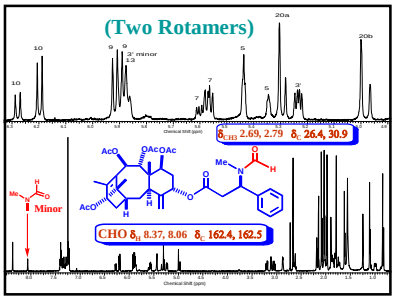


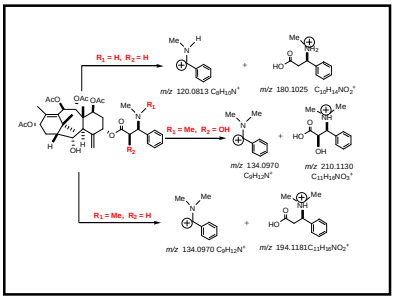


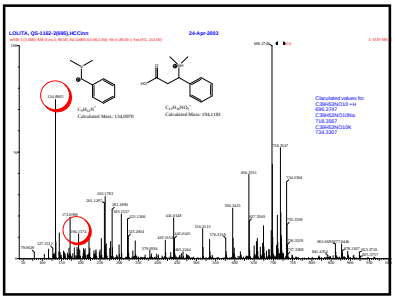


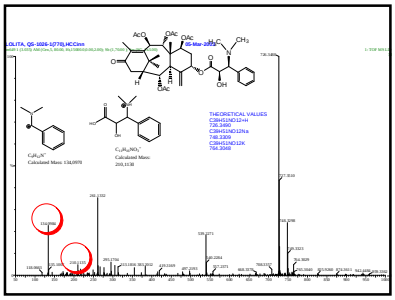
Pseudo-alkaloid Taxane With Two Rotamers

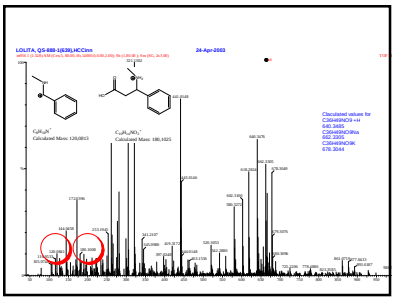
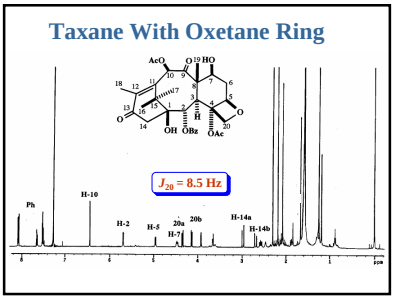
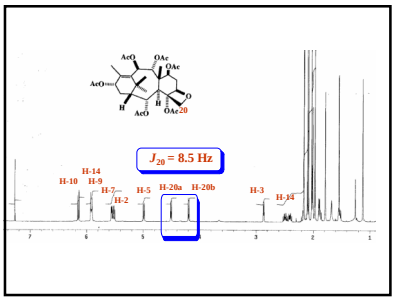












Taxane With Oxetane Ring