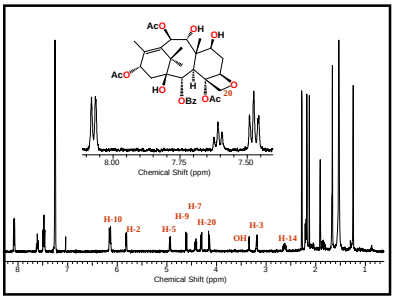
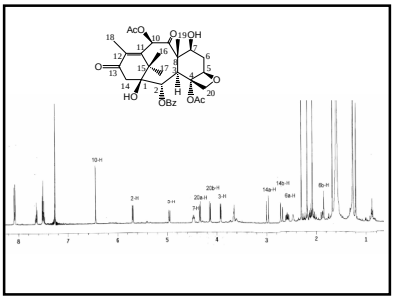
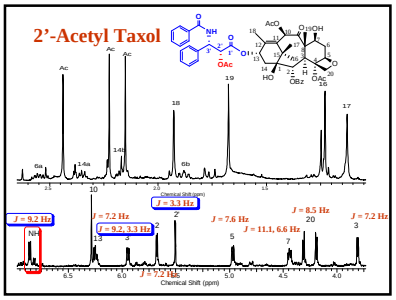
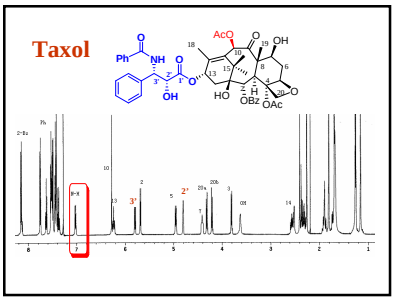
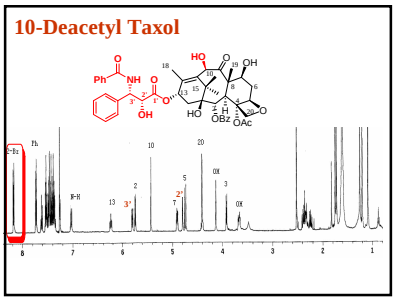
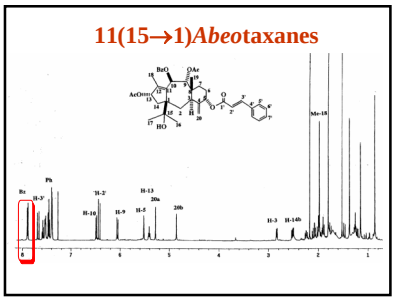

H-10
H-2
H-5
H-9
H-7
H-20
OH
H-3
H-14
Chemical Shift (ppm)

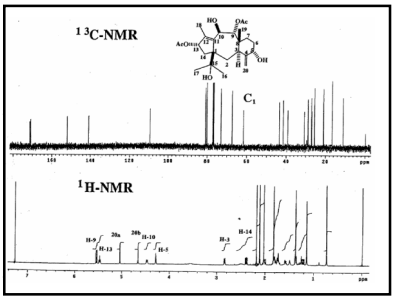


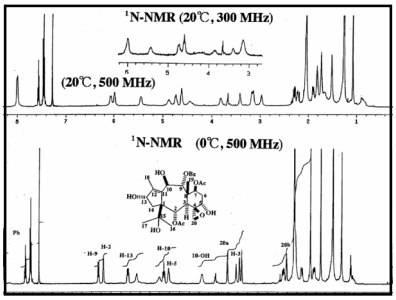

2'-Acetyl Taxol
J = 9.2 Hz
J = 7.2 Hz
J = 9.2, 3.3 Hz
J = 3.3 Hz
J = 7.6 Hz
J = 11.1, 6.6 Hz
J = 8.5 Hz
J = 7.2 Hz
Chemical Shift (ppm)

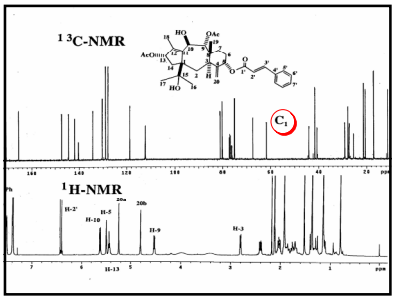

Taxol

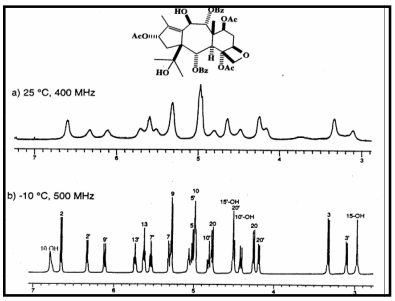

10-Deacetyl Taxol

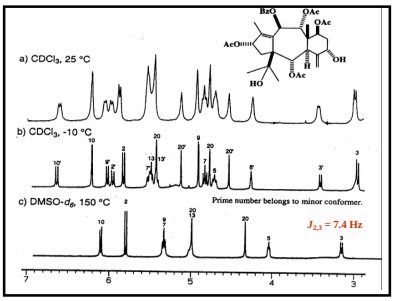

11(15→1)*Abeo*taxanes

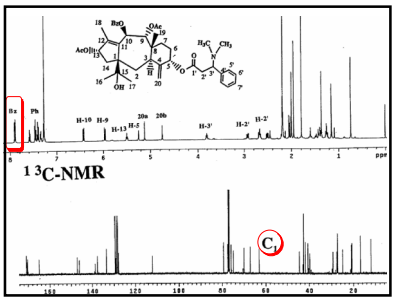

^{13}C-NMR
C_1
^{1}H-NMR

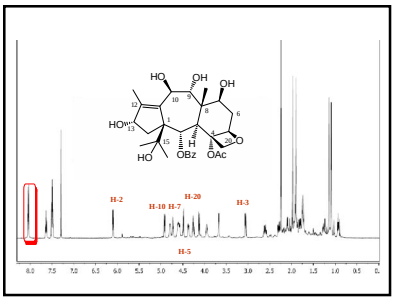

^{1}N-NMR (20℃, 300 MHz)
(20℃, 500 MHz)
^{1}N-NMR (0℃, 500 MHz)


^{13}C-NMR
C_1
^{1}H-NMR

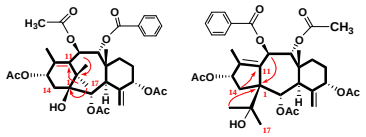






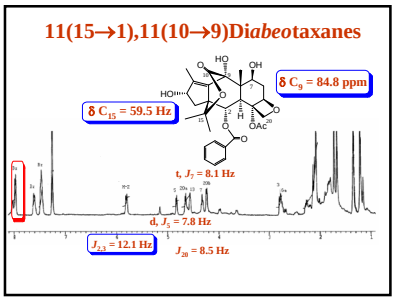


6/8/6-Ring Taxane and 11(15→1)*abeo*taxanes

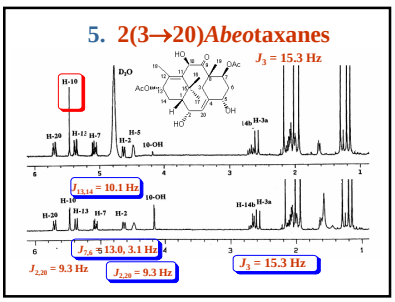


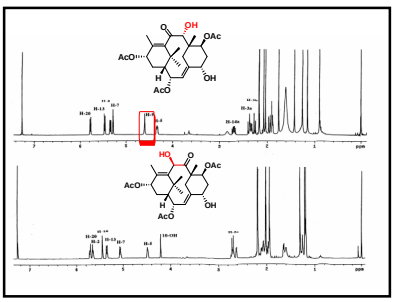
H-17 to C-11 **HMBC** H-17 to C-1

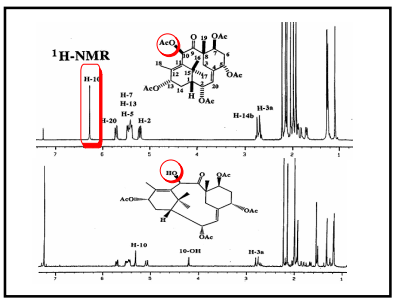
11(15→1),11(10→9)Di*abeo*taxanes

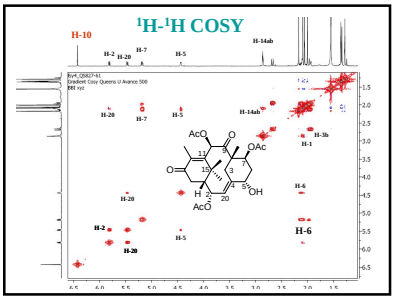


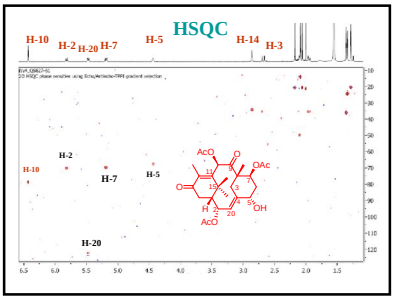
5. 2(3→20)*Abeo*taxanes

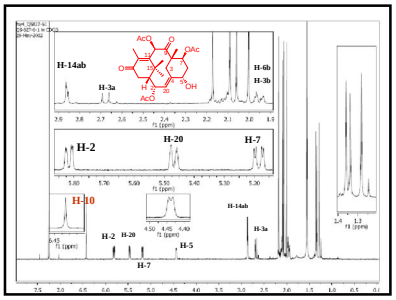


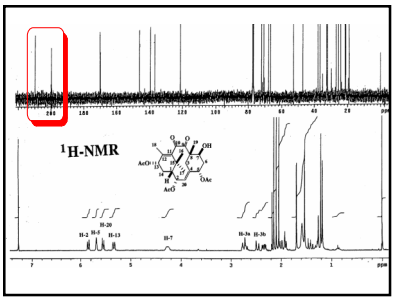


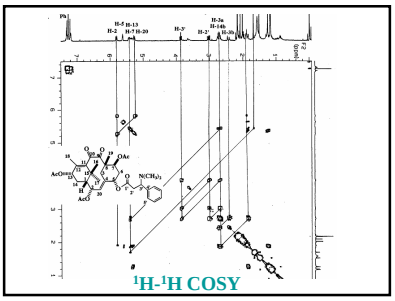


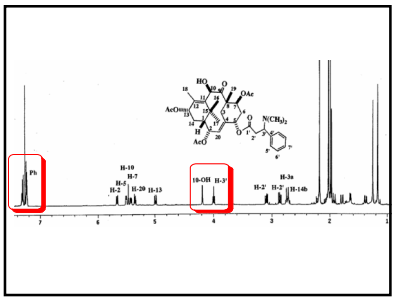

^{1}H-^{1}H COSY
H-10
H-14ab
H-20
H-7
H-5
H-3b
H-1
H-6
H-2

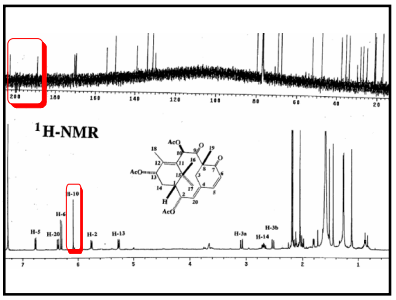

HSQC
H-10
H-2
H-20
H-7
H-5
H-14
H-3
H-20

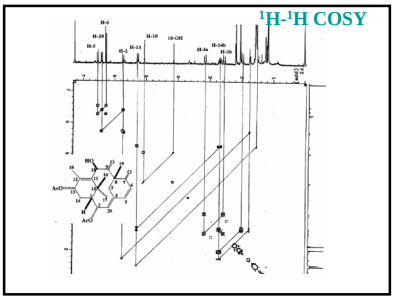

H-14ab
H-3a
H-6b
H-3b
H-2
H-20
H-7
H-10
H-5

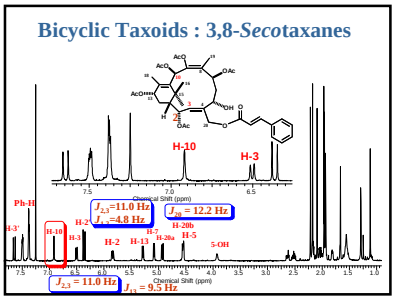

^{1}H-NMR
H-20
H-2
H-13
H-7
H-3a
H-3b

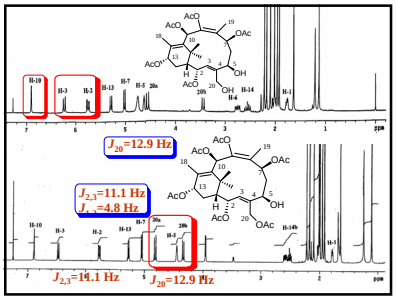

^{1}H-^{1}H COSY

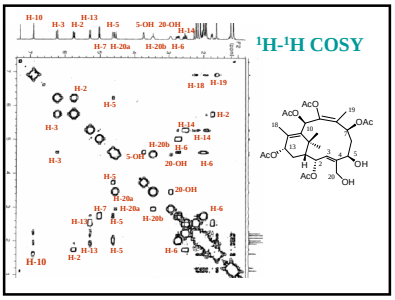

Ph
H-10
H-7
H-2
H-20
H-13
10-OH
H-3'
H-2'
H-3a
H-14b

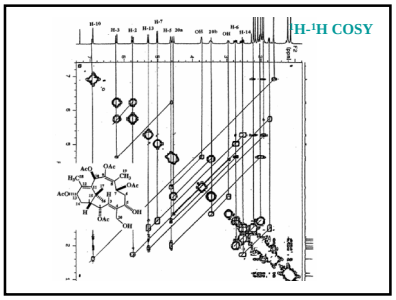

^{1}H-NMR
H-10
H-6
H-5
H-20
H-2
H-13
H-3a
H-3b
H-14

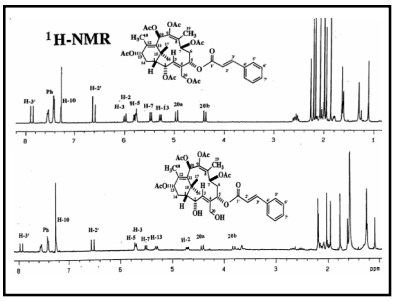

^{1}H-^{1}H COSY

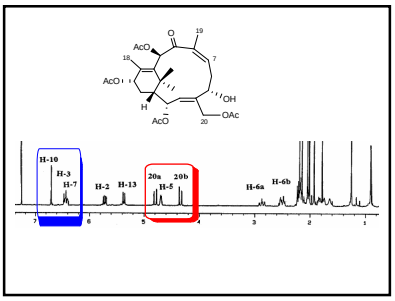

Bicyclic Taxoids : 3,8-*Seco*taxanes
H-10
H-3
Chemical Shift (ppm)
Ph-H
H-3'
H-10
H-2
H-13
H-20b
H-5
5-OH
$J_{2,3}$=11.0 Hz
$J_{3,4}$=4.8 Hz
J_{20} = 12.2 Hz
$J_{2,3}$ = 11.0 Hz
$J_{3,4}$ = 9.5 Hz

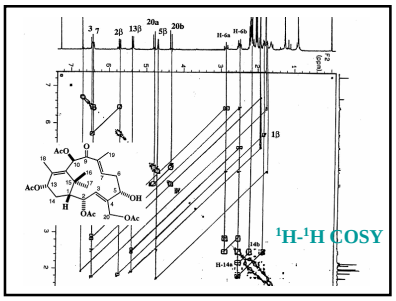

J_{20}=12.9 Hz
$J_{2,3}$=11.1 Hz
$J_{3,4}$=4.8 Hz
$J_{2,3}$=11.1 Hz
J_{20}=12.9 Hz

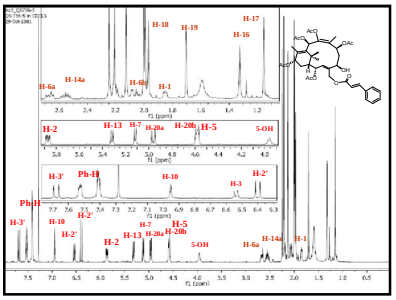

^{1}H-^{1}H COSY

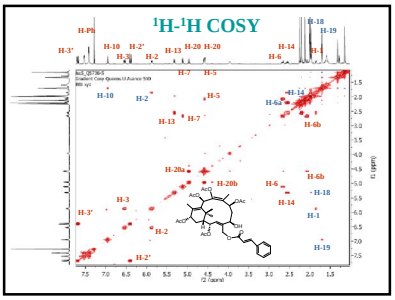

^{1}H-^{1}H COSY

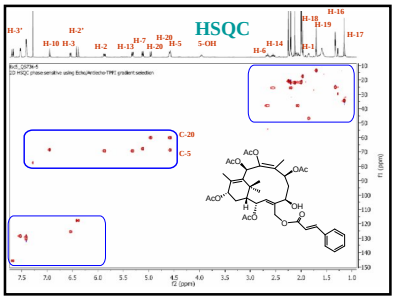

^{1}H-NMR

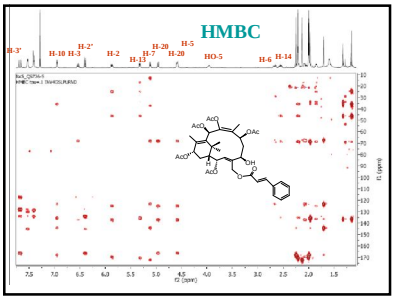


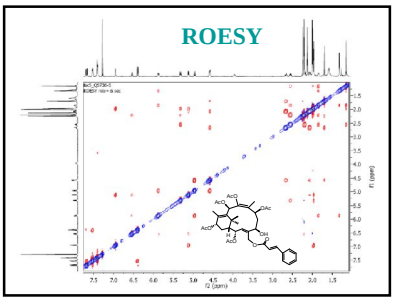

^{1}H-^{1}H COSY

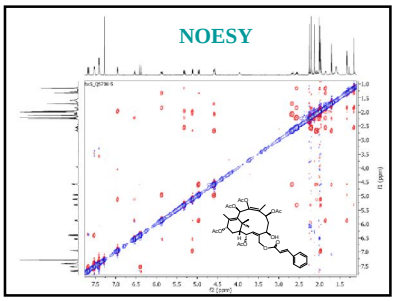


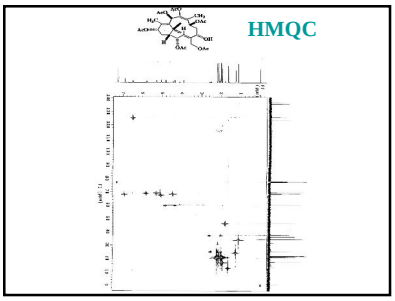

^{1}H-^{1}H COSY

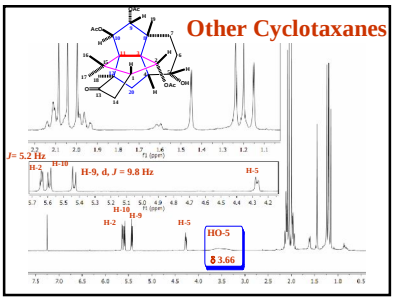

HSQC

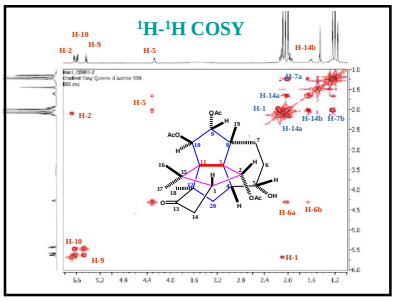

HMBC
H-3'
H-10 H-3
H-2'
H-2
H-13
H-7
H-20
H-20
H-5
HO-5
H-6
H-14

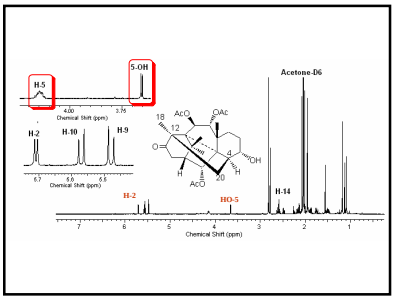

ROESY

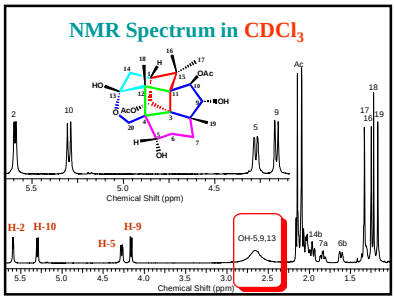

NOESY

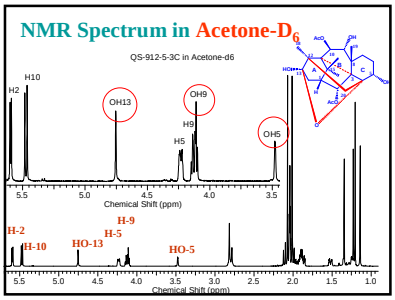

HMQC

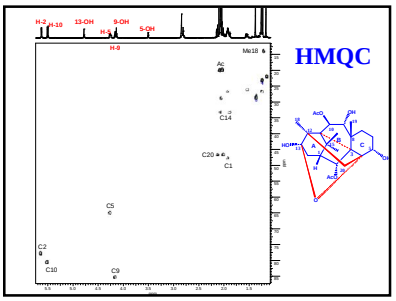

Other Cyclotaxanes
J= 5.2 Hz
H-2
H-10
H-9, d, J = 9.8 Hz
H-5
H-10
H-9
H-2
H-5
HO-5
δ 3.66

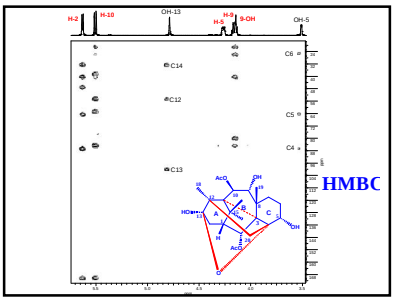

^{1}H-^{1}H COSY
H-10
H-2
H-9
H-5
H-14b
H-7a
H-14a
H-1
H-14b
H-7b
H-14a
H-2
H-5
H-6a
H-6b
H-10
H-9
H-1

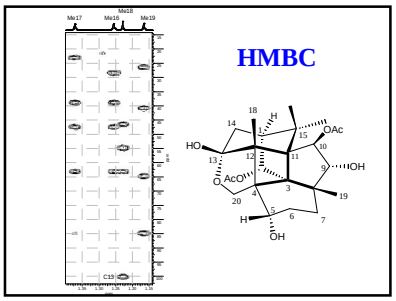

H-5
5-OH
Chemical Shift (ppm)
H-2
H-10
H-9
Chemical Shift (ppm)
Acetone-D6
H-2
HO-5
H-14
Chemical Shift (ppm)


NMR Spectrum in CDCl3
Chemical Shift (ppm)
H-2
H-10
H-9
H-5
OH-5,9,13
Chemical Shift (ppm)

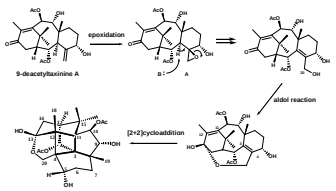

NMR Spectrum in Acetone-D6
QS-912-5-3C in Acetone-d6
H2
H10
OH13
OH9
H9
H5
OH5
Chemical Shift (ppm)
H-2
H-10
HO-13
H-9
H-5
HO-5
Chemical Shift (ppm)



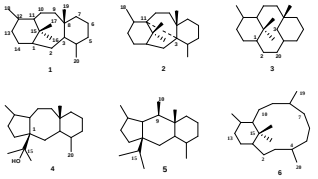




Hypothetical Biosynthetic Route



Summarization
Skeletons of Taxane Diterpenoids



骨 架	^{1}H NMR 特 征
1	H-3α (δ 2.57–3.27, d, *J* = 6.8 Hz)为其特征信号, 不同的亚类型有其不同的特征。
2	缺少H-3α的特征信号，Me-18 (δ 1.24–1.34, d, *J* = 7.0 Hz), H-12 α (δ 3.23–3.79, q, *J* = 7.0 Hz)
3	H-20 (δ 5.30-5.80, d, *J* = 9-10 Hz), H-3a (δ 2.52-2.82, d, *J* = 15.5 Hz), H-3b (δ 1.64-2.00, d, *J* = 15.5 Hz)
4	在氢谱中很难与相应的6/8/6骨架相区别，但在碳谱中C-1与其它不含杂原子的碳相比明显位于低场（δ_C 57-70）; Me-16（δ 1.01–1.39）。缺少从H–16到C–11的远程偶合。
5	缺少H-9β和H-10α的特征信号，但在碳谱中有C-10内酯羰基特征信号（δ_C 173）
6	H-10α (δ 6.83-7.31), H-3 (δ 5.59-6.47, d, *J* = 10-12 Hz) ; H-20a, H-20b为一组AB四重峰, *J* = 12.9-13.5 Hz, 当C-20为羟基时H-20a (4.40-4.60, d), H-20b (3.40-3.80, d); 当C-20为乙酰氧或肉桂酰氧基时H-20a (4.80-4.95，d), H-20b (4.10-4.55, d)

Thank You for Your Attention

谢　谢