Supporting Information

Convenient synthesis of *trans-syn-trans* perhydrobenz[*e*]indene triketone, a key intermediate for the total synthesis of stelletins

Yang Cao,[a] Xiaoyu Liu,[a] Zhe Wang,[a] Yuan Wang,[a] Xiaozhen Jiao,[a*] and Ping Xie[a*]

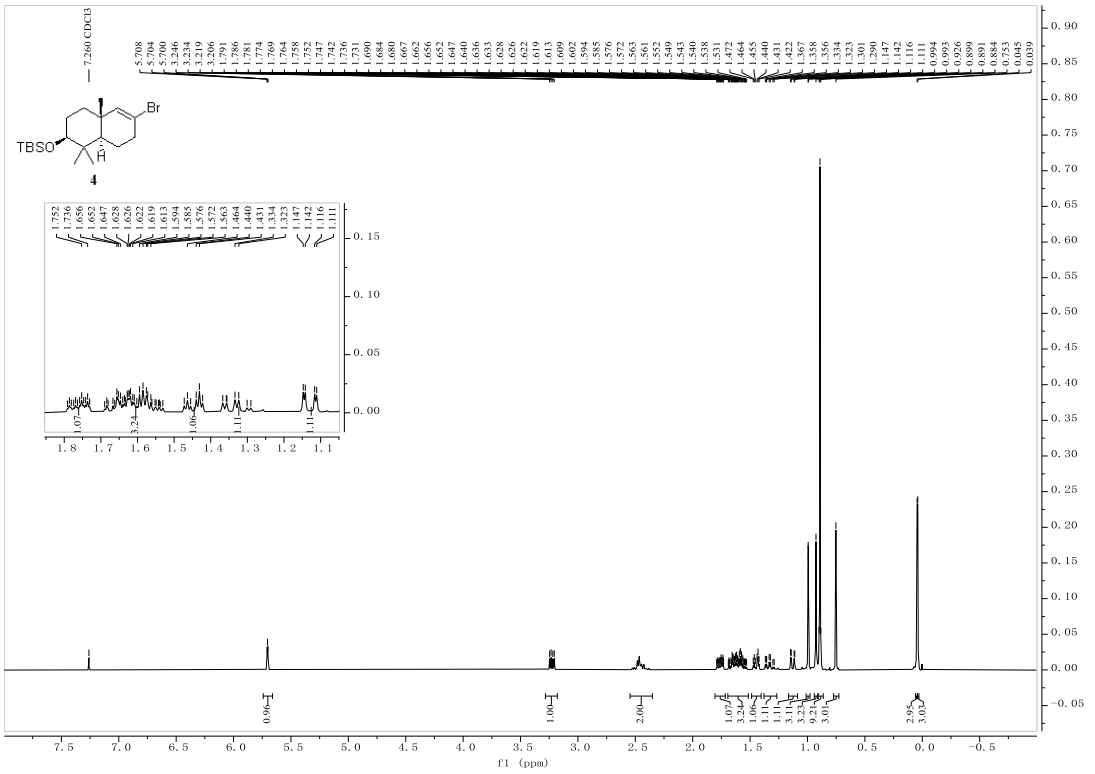
[a]*State Key Laboratory of Bioactive Substance and Function of Natural Medicines, Beijing Key Laboratory of Active Substances Discovery and Druggability Evaluation, Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing 100050, China.*

Fax: +86 10 63017757; Tel: +86 10 63165242

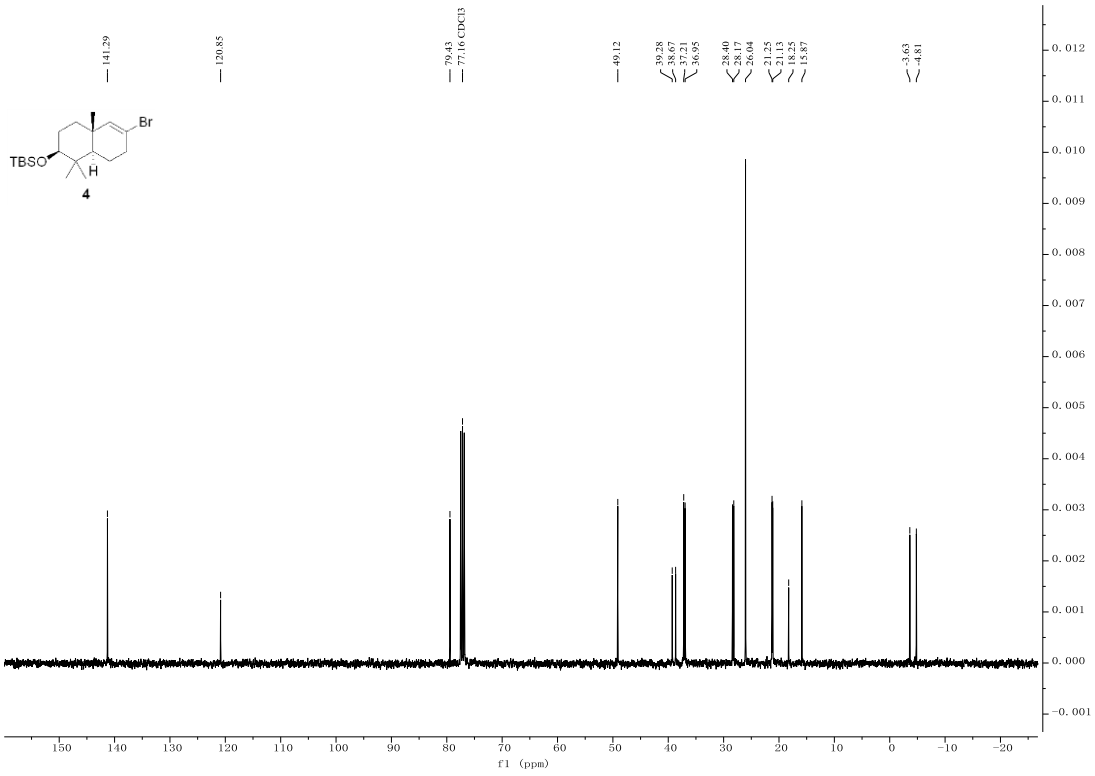
Email: jiaoxz@imm.ac.cn, xp@imm.ac.cn

Contents

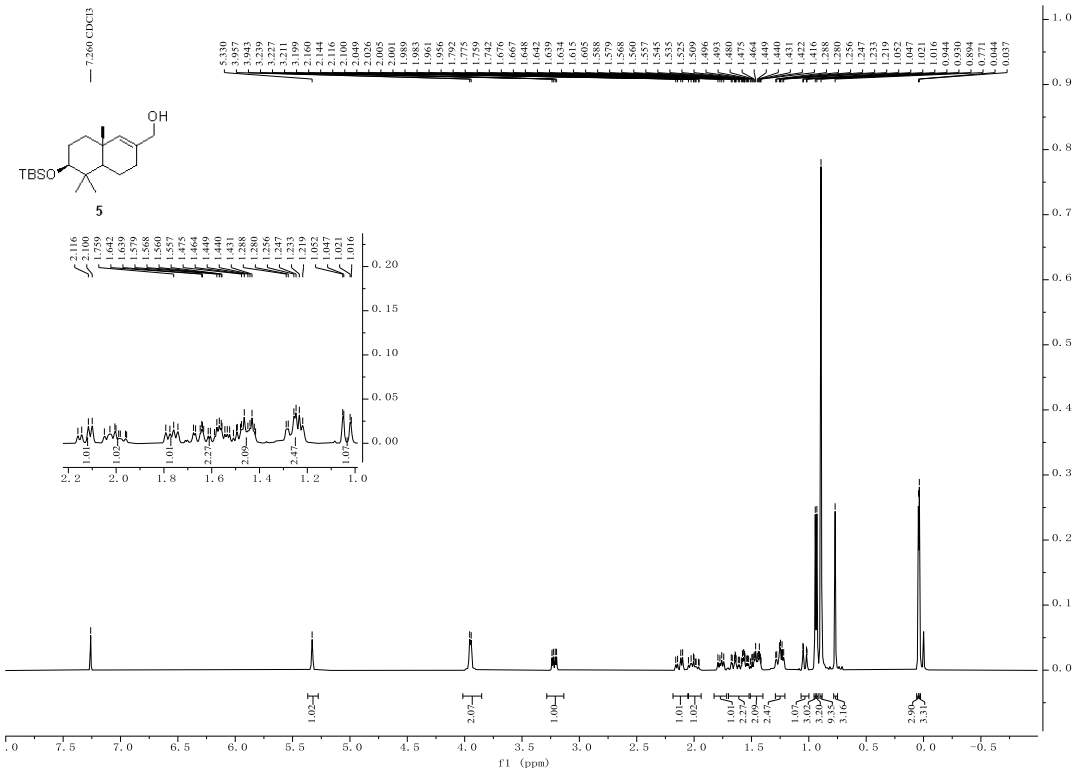
^{1}H NMR spectrum of compound **4**



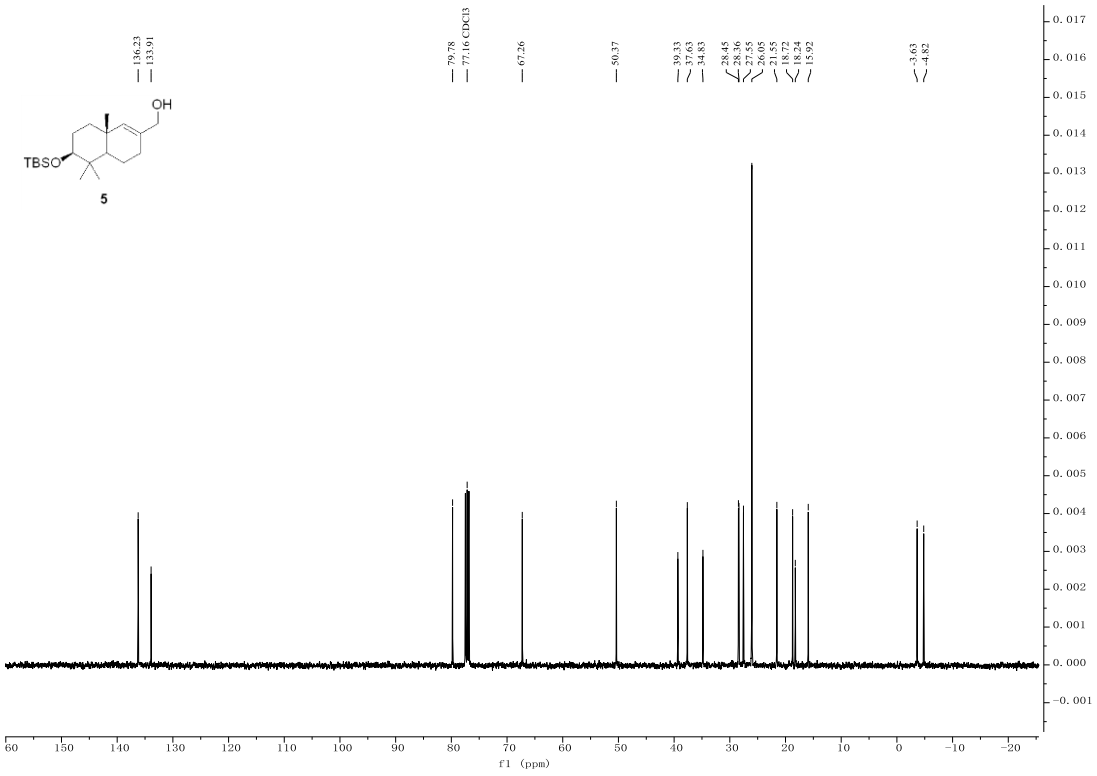
^{13}C NMR spectrum of compound **4**



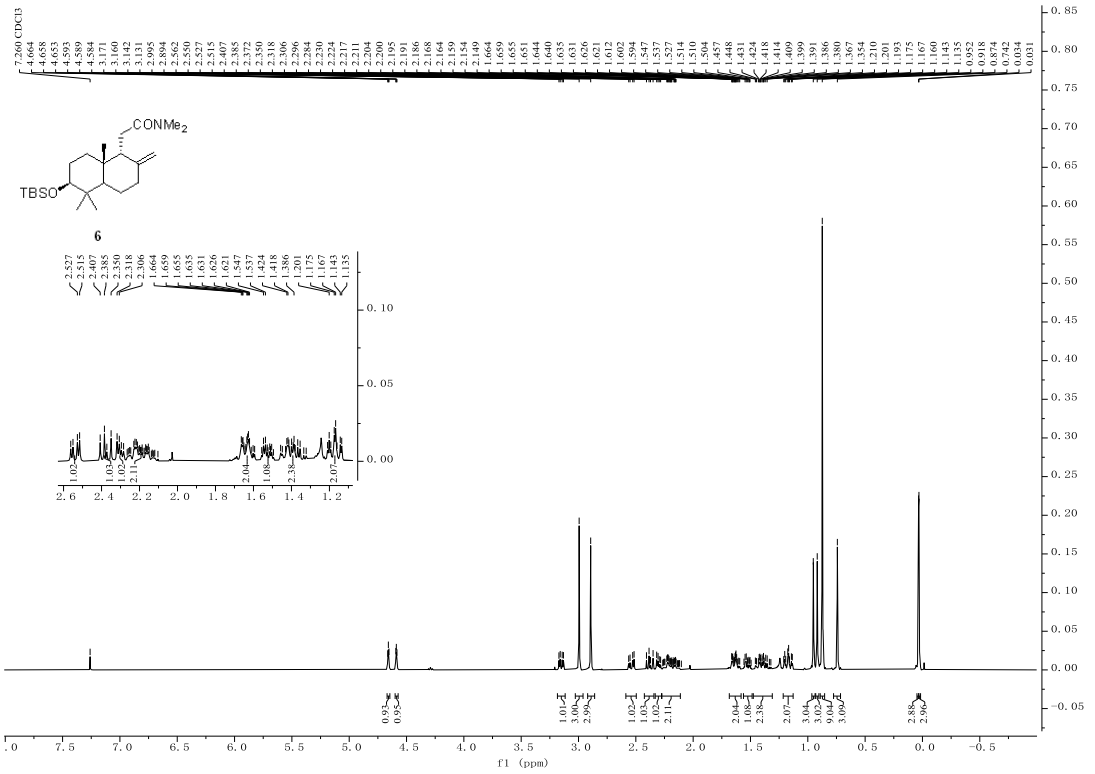
^{1}H NMR spectrum of compound **5**



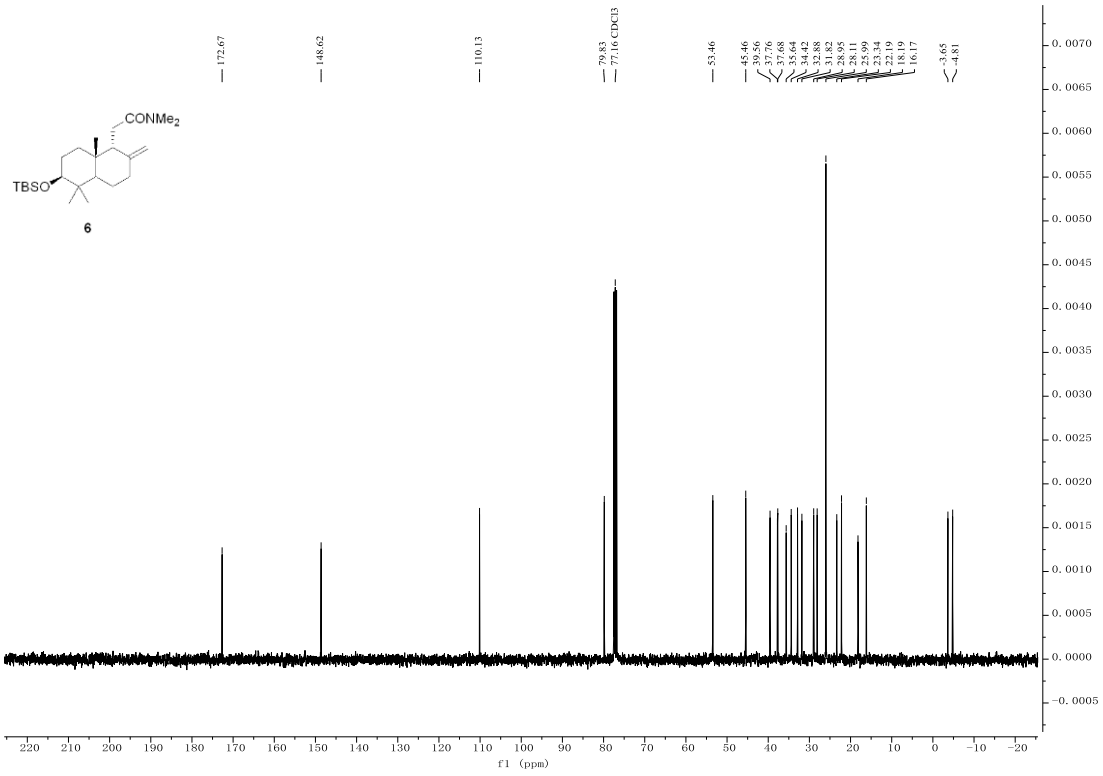
^{13}C NMR spectrum of compound **5**



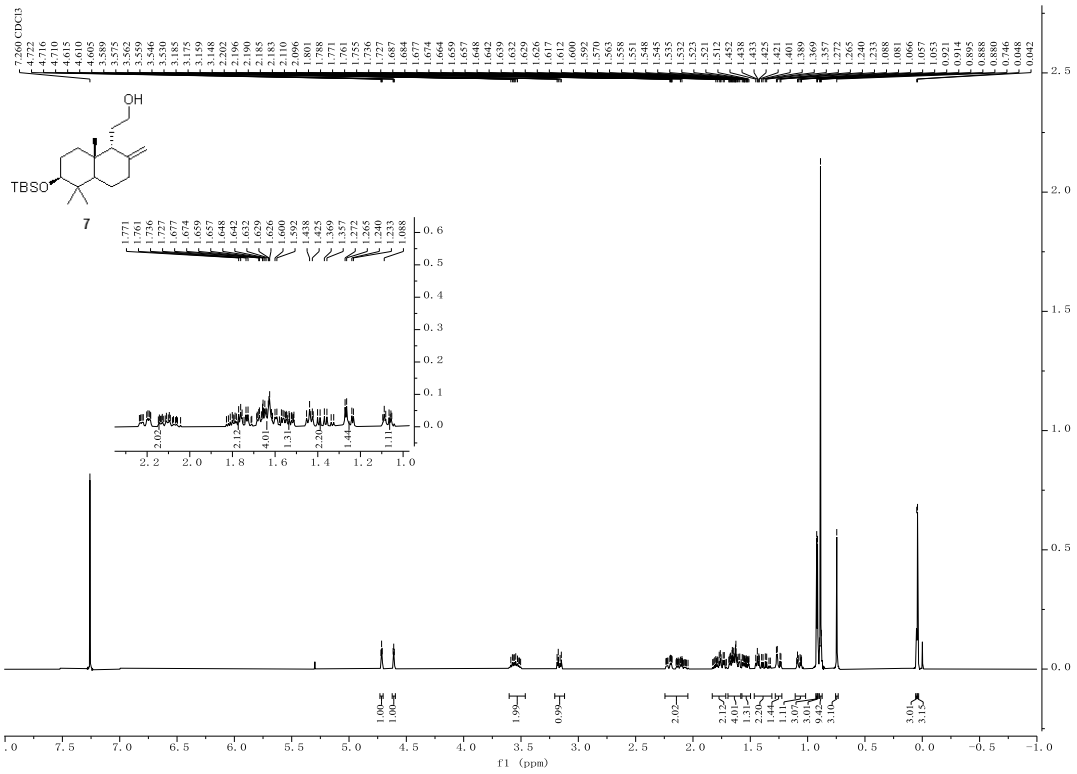
^{1}H NMR spectrum of compound **6**



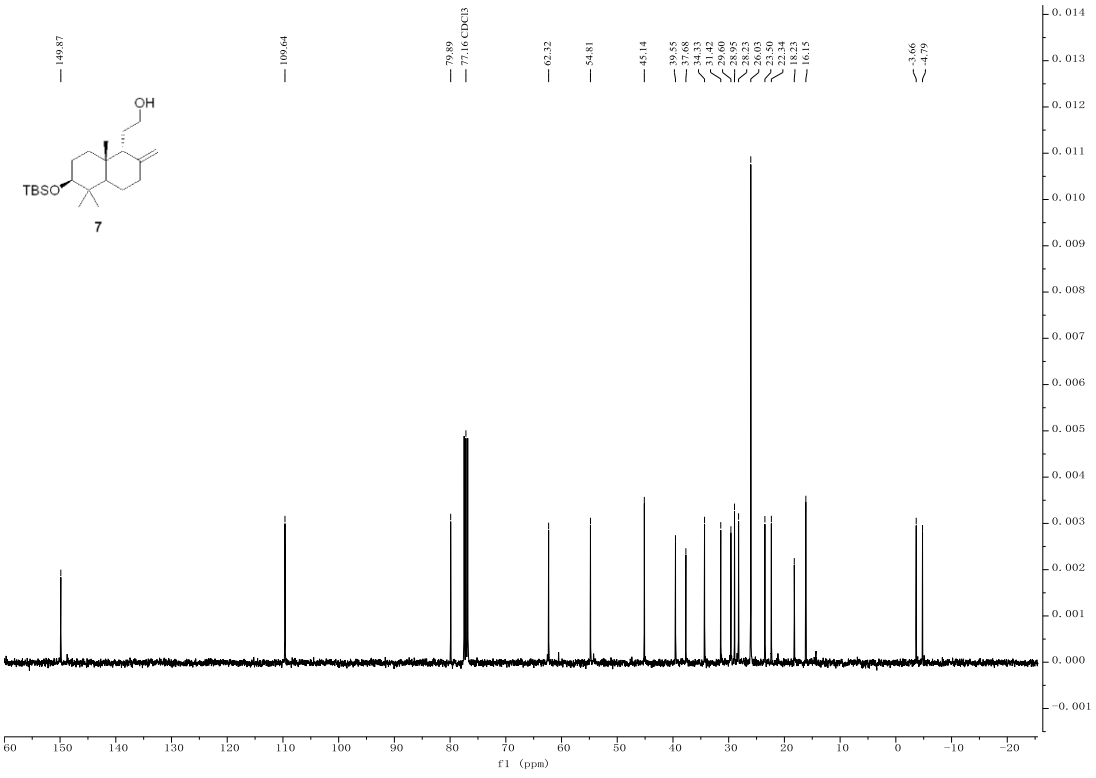
^{13}C NMR spectrum of compound **6**



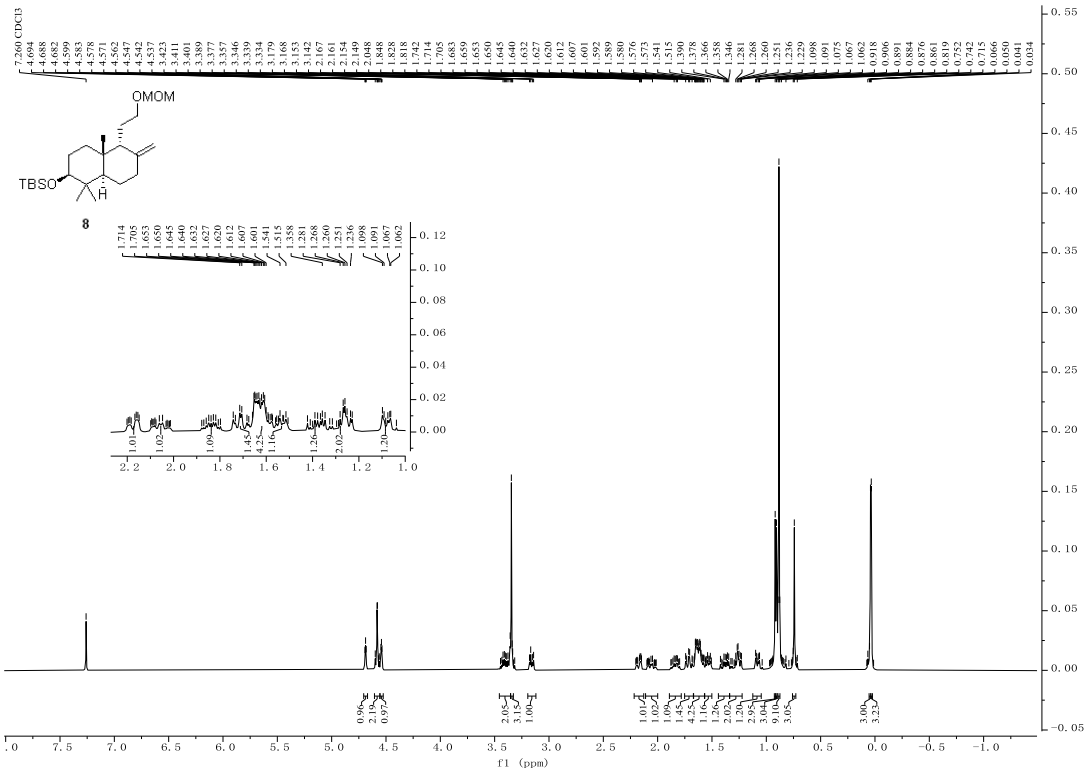
^{1}H NMR spectrum of compound **7**



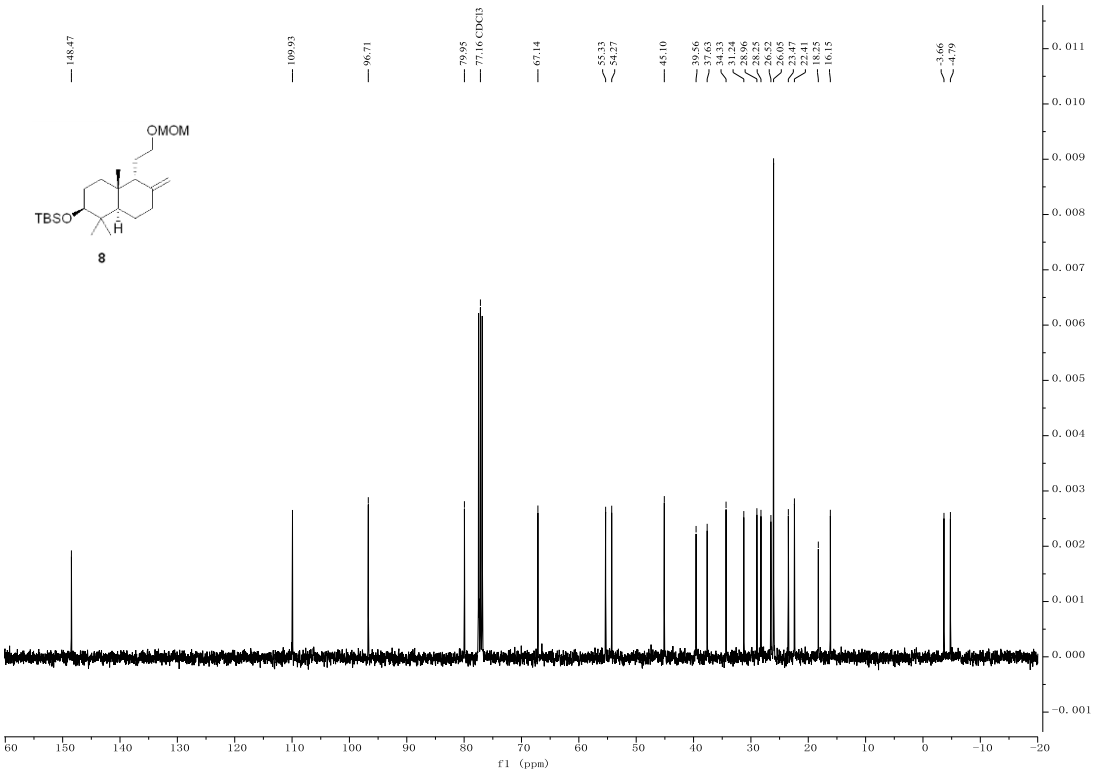
^{13}C NMR spectrum of compound **7**



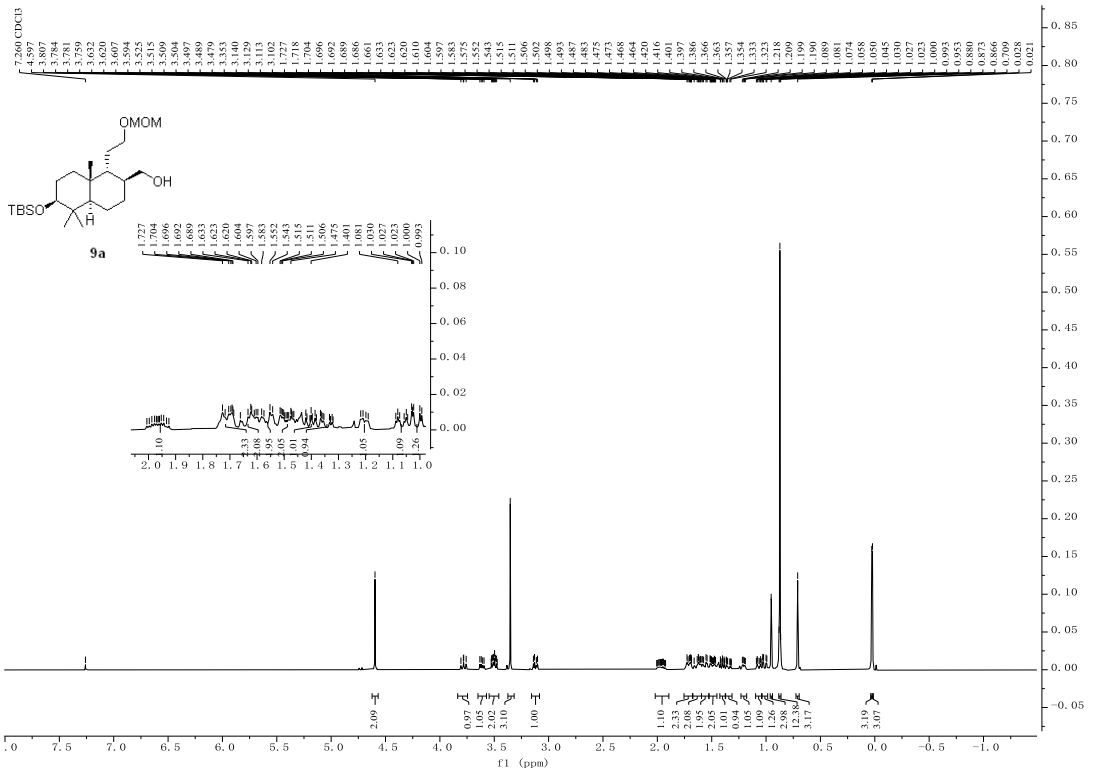
^{1}H NMR spectrum of compound **8**



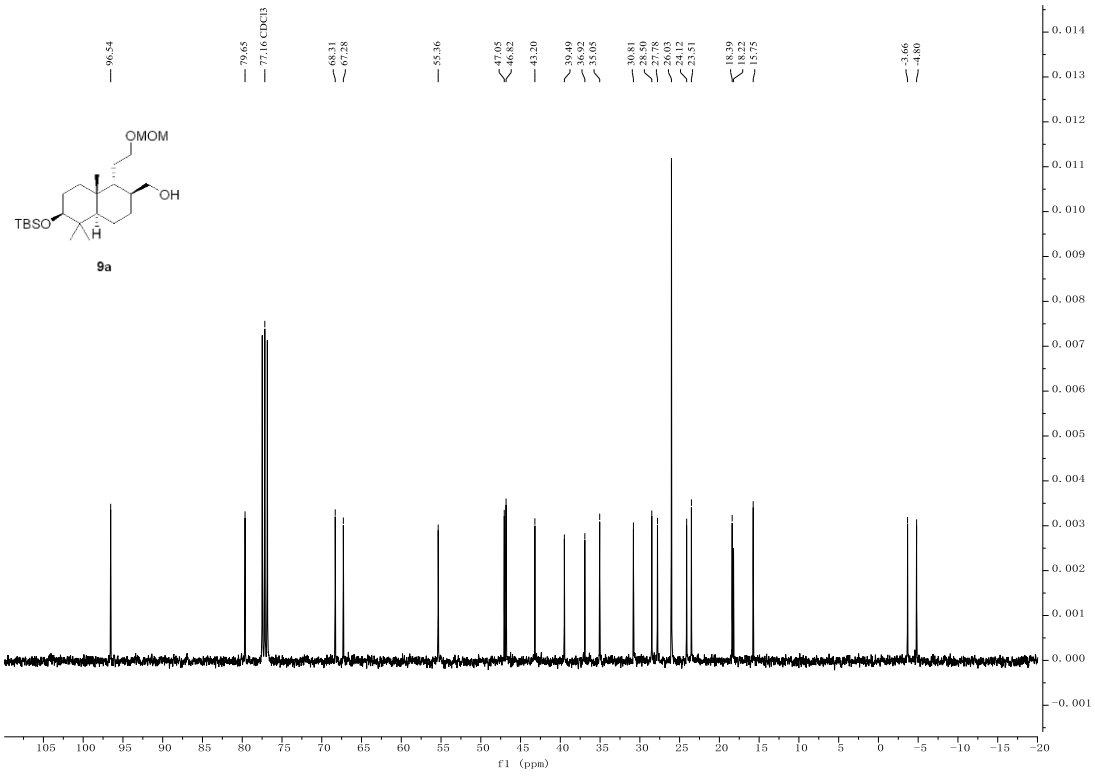
^{13}C NMR spectrum of compound **8**



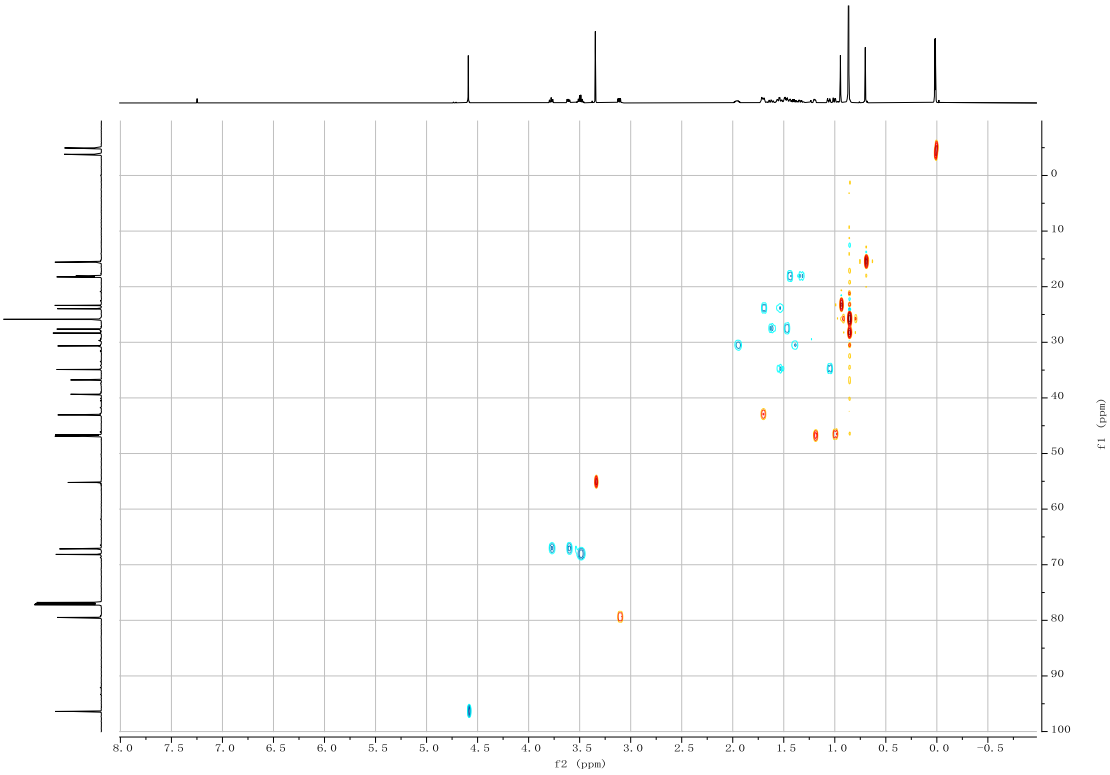
^{1}H NMR spectrum of compound **9a**

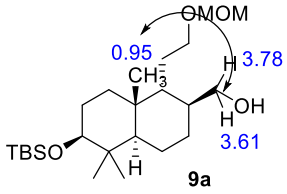


^{13}C NMR spectrum of compound **9a**

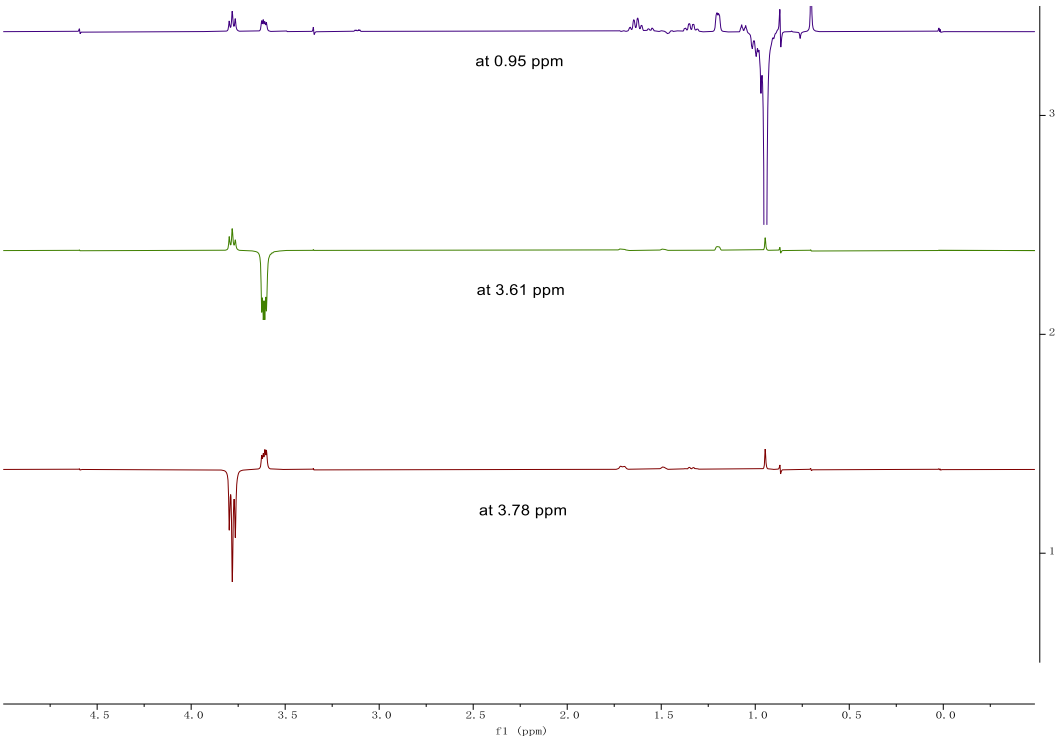


HMQC spectrum of compound **9a**

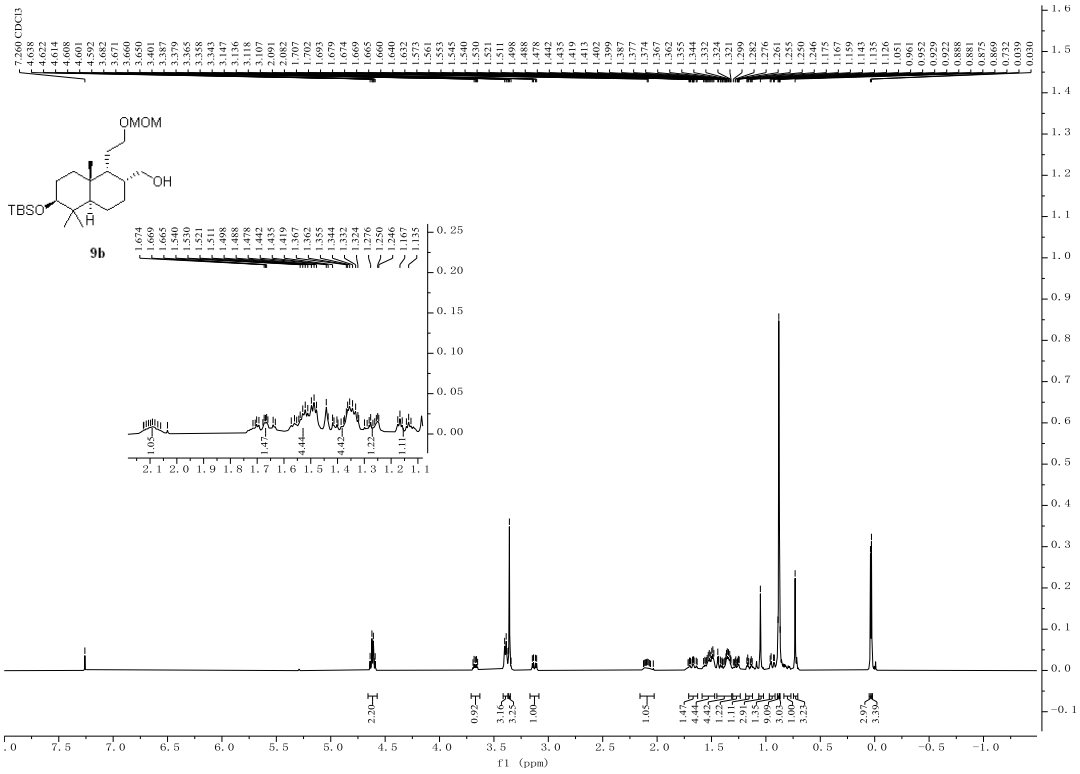




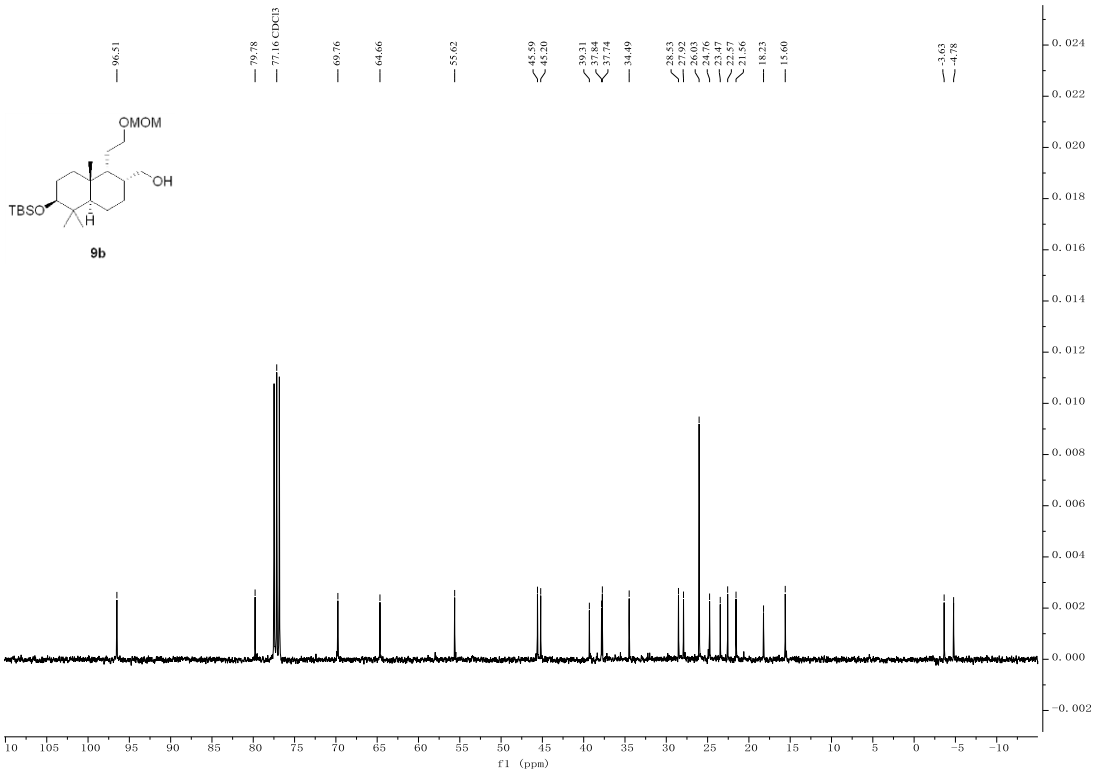
NOE spectrum of compound **9a**



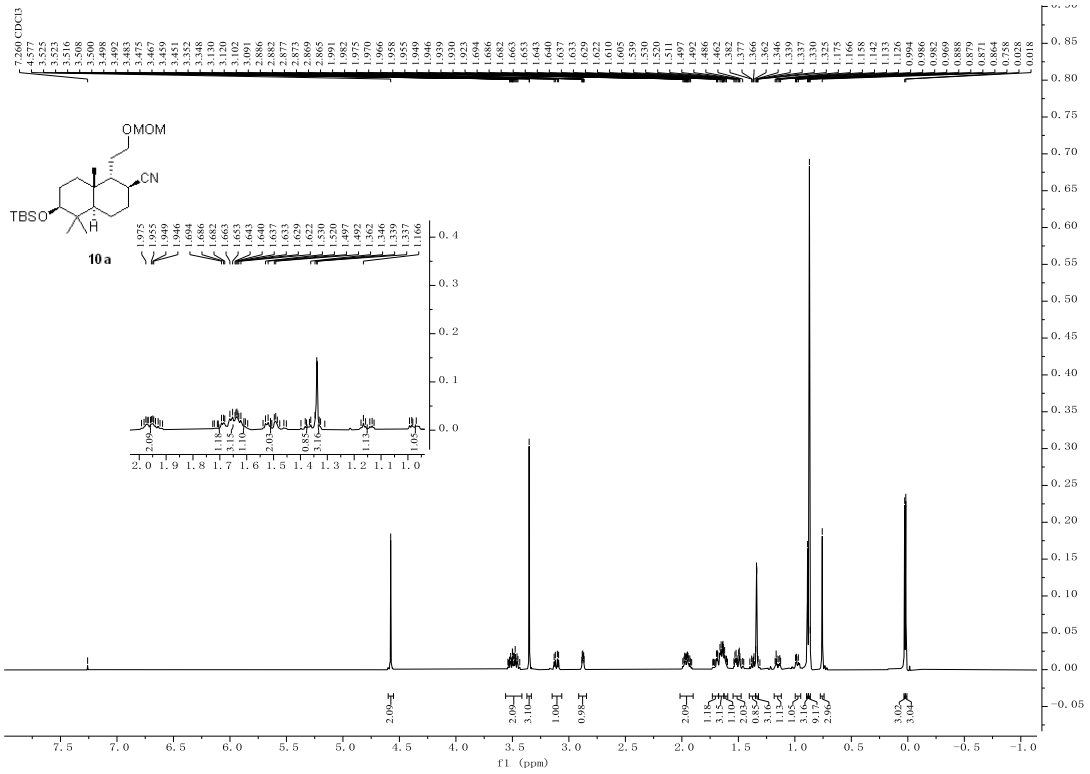
^{1}H NMR spectrum of compound **9b**



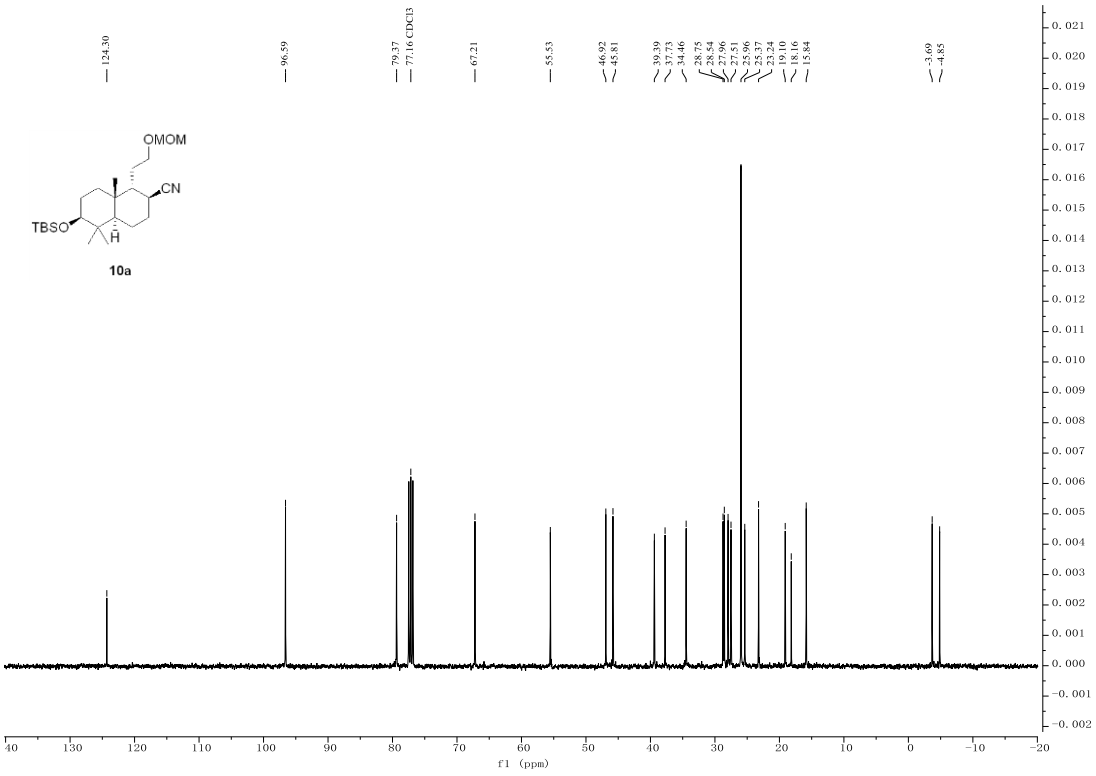
^{13}C NMR spectrum of compound **9b**



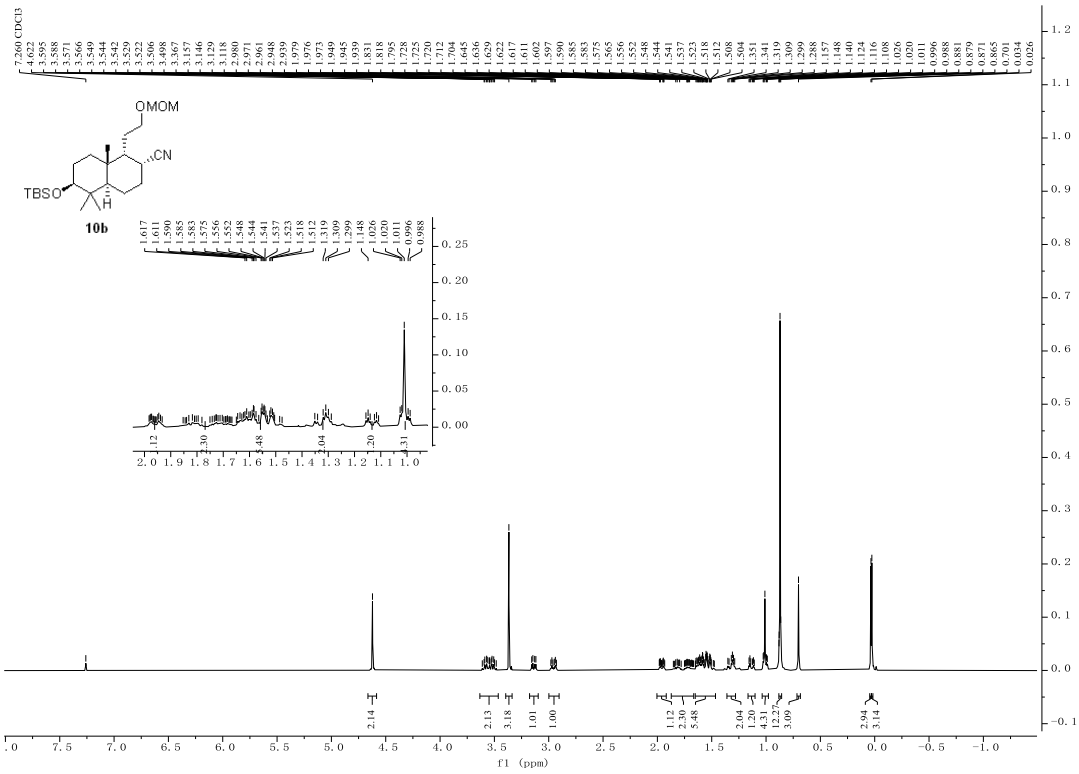
^{1}H NMR spectrum of compound **10a**



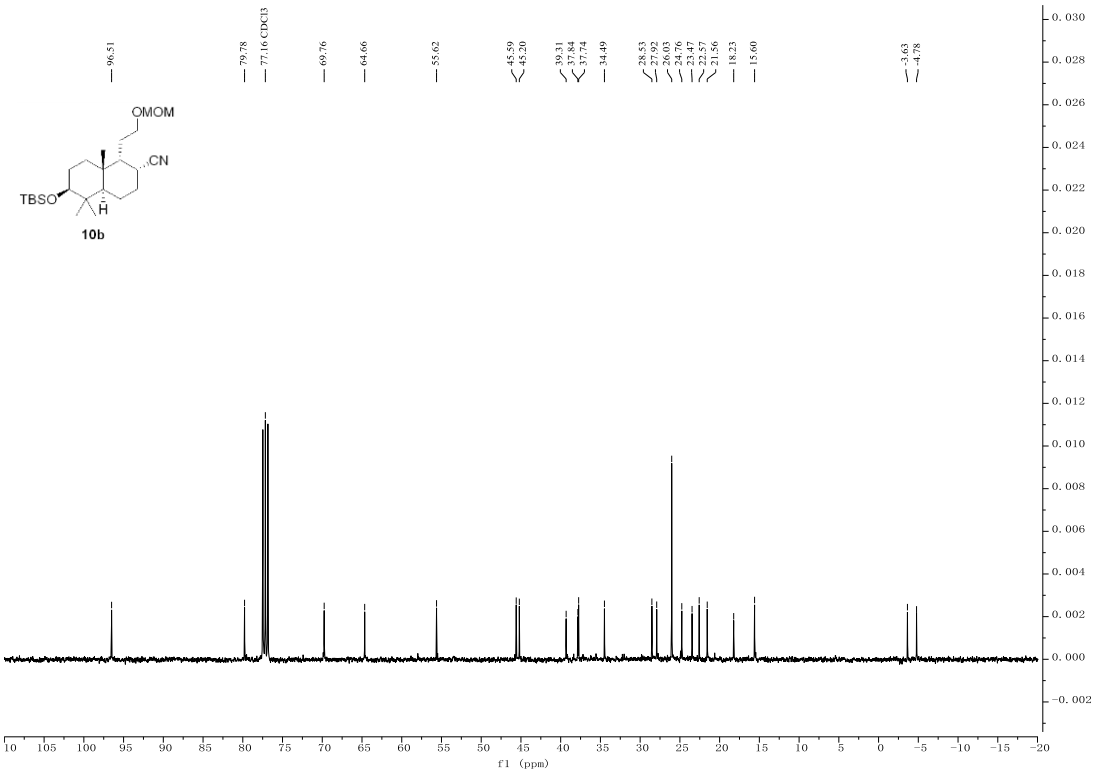
^{13}C NMR spectrum of compound **10a**



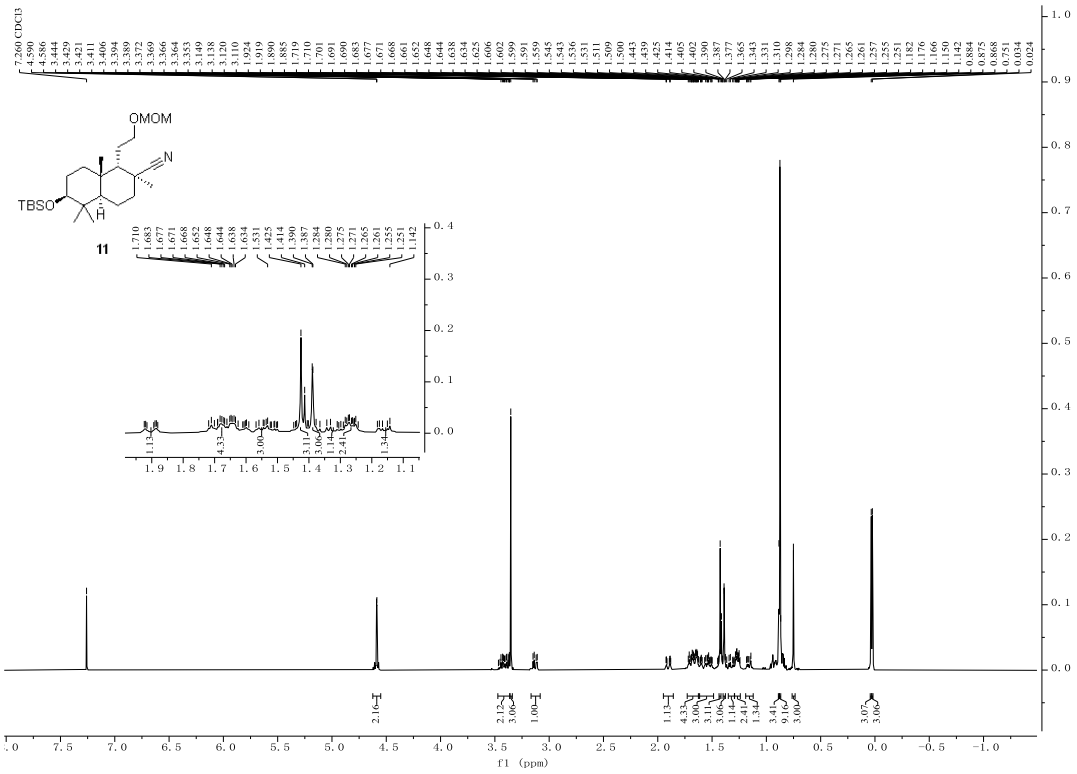
^{1}H NMR spectrum of compound **10b**



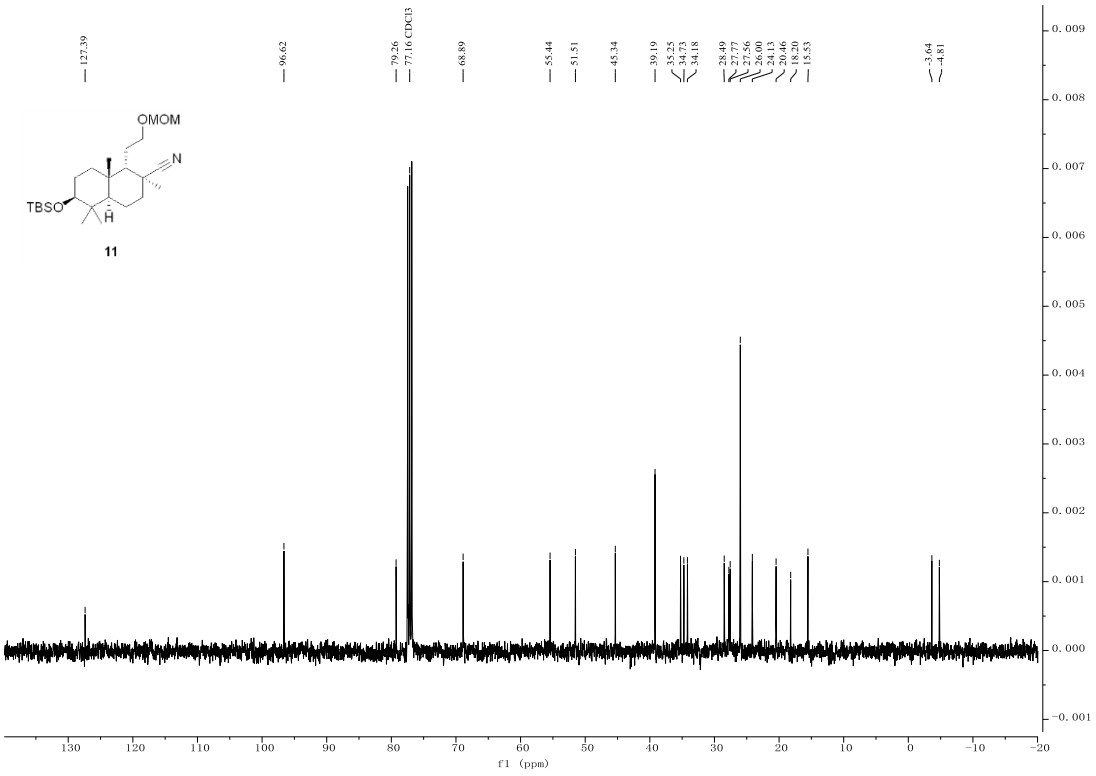
^{13}C NMR spectrum of compound **10b**



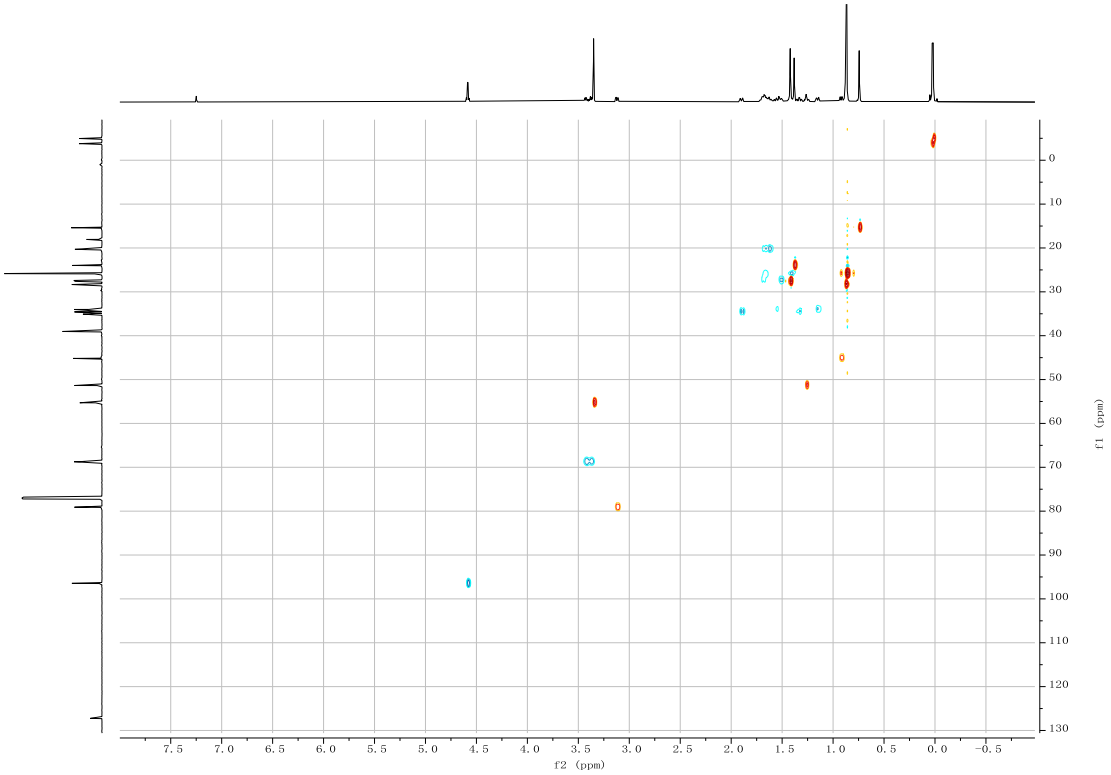
^{1}H NMR spectrum of compound **11**



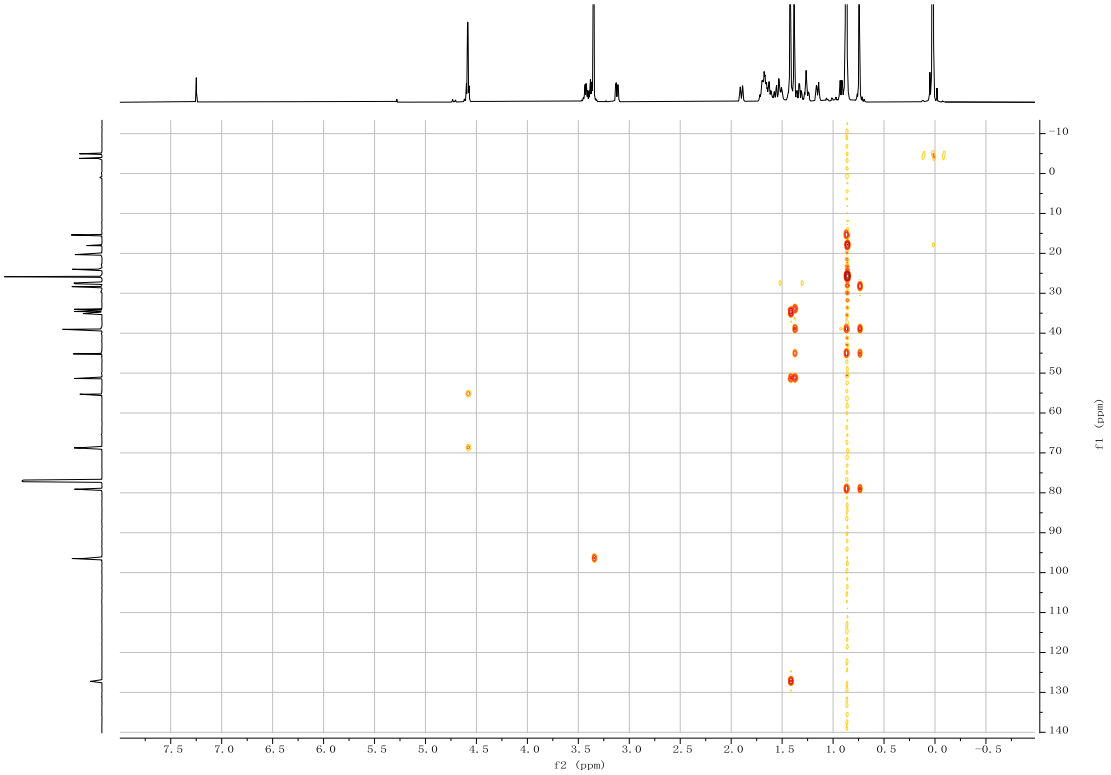
^{13}C NMR spectrum of compound **11**



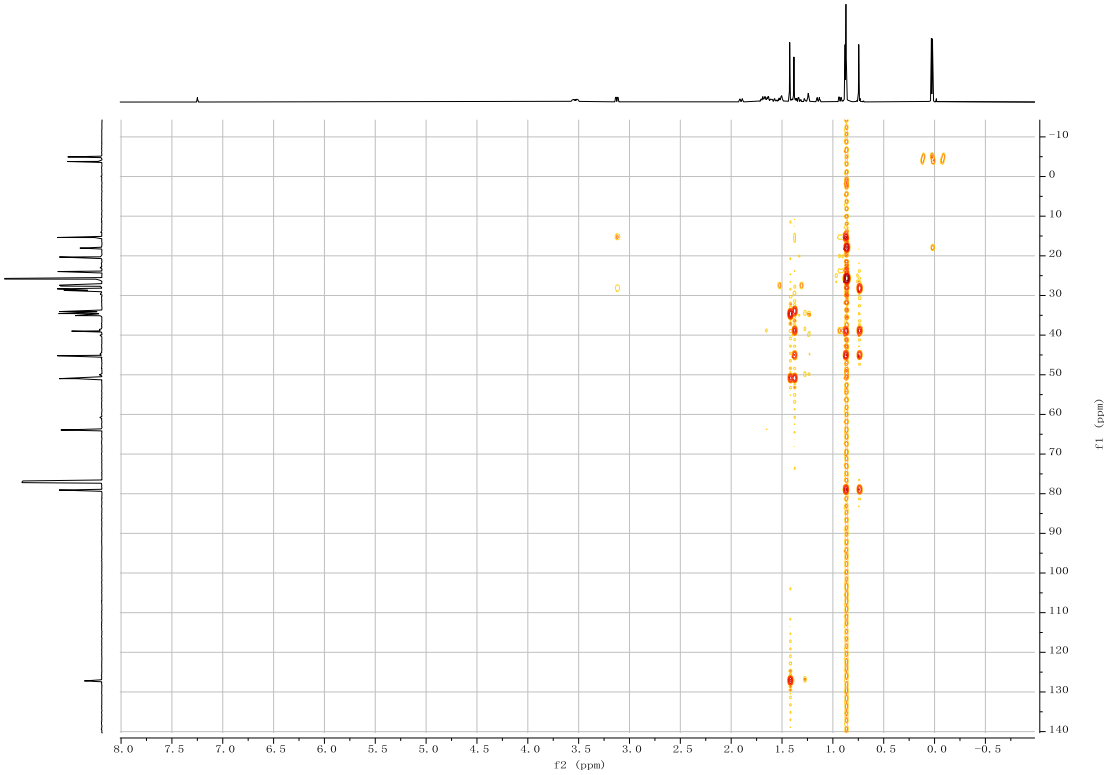
HMQC spectrum of compound **11**

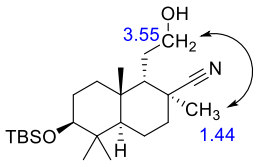


HMBC spectrum of compound **11**



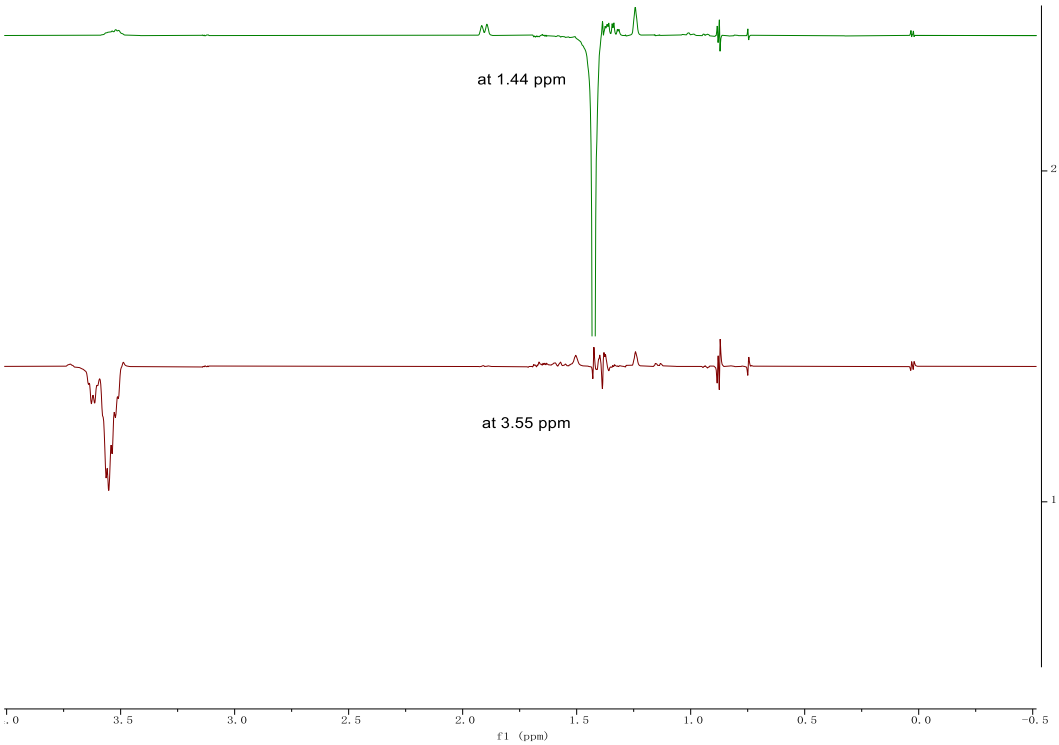
HMBC spectrum of compound **11'** (deprotection)



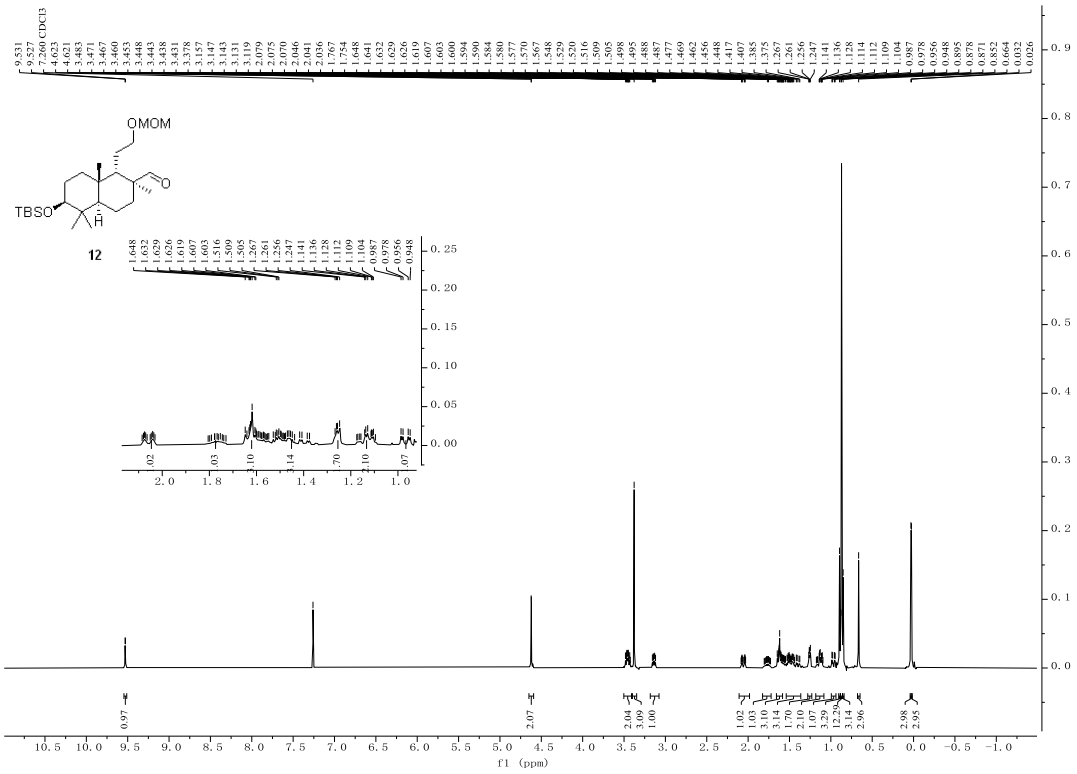


11'(deprotection)

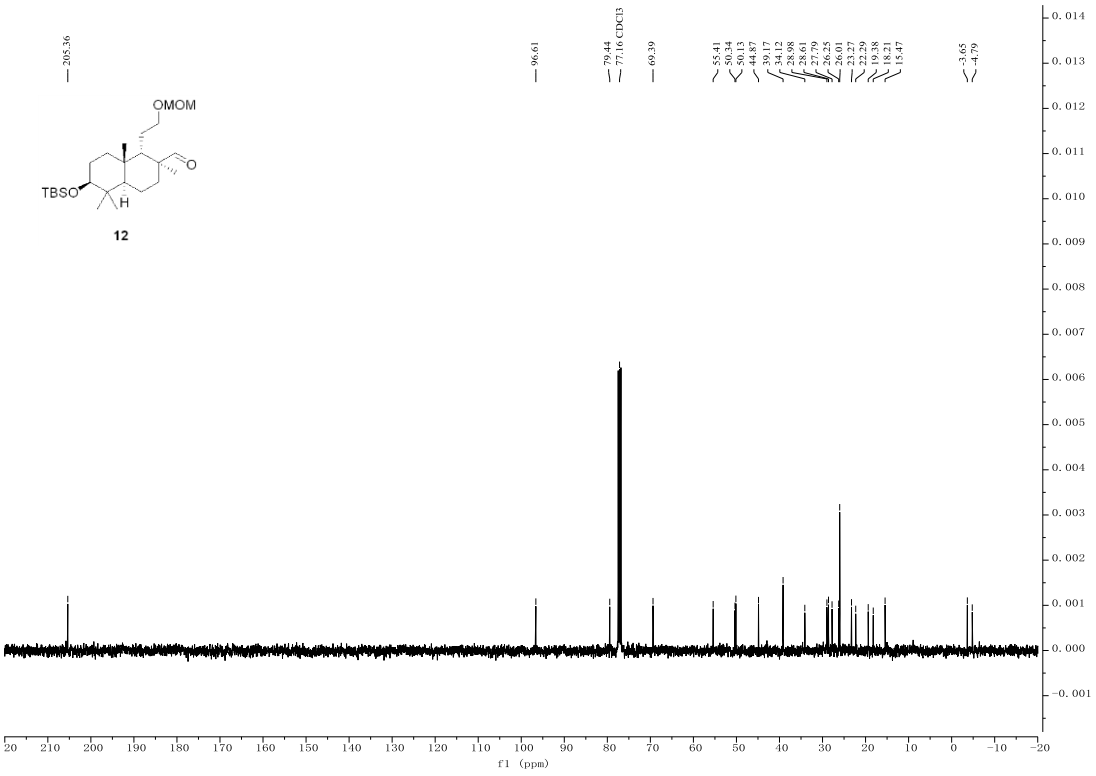
NOE spectrum of compound **11'** (deprotection)



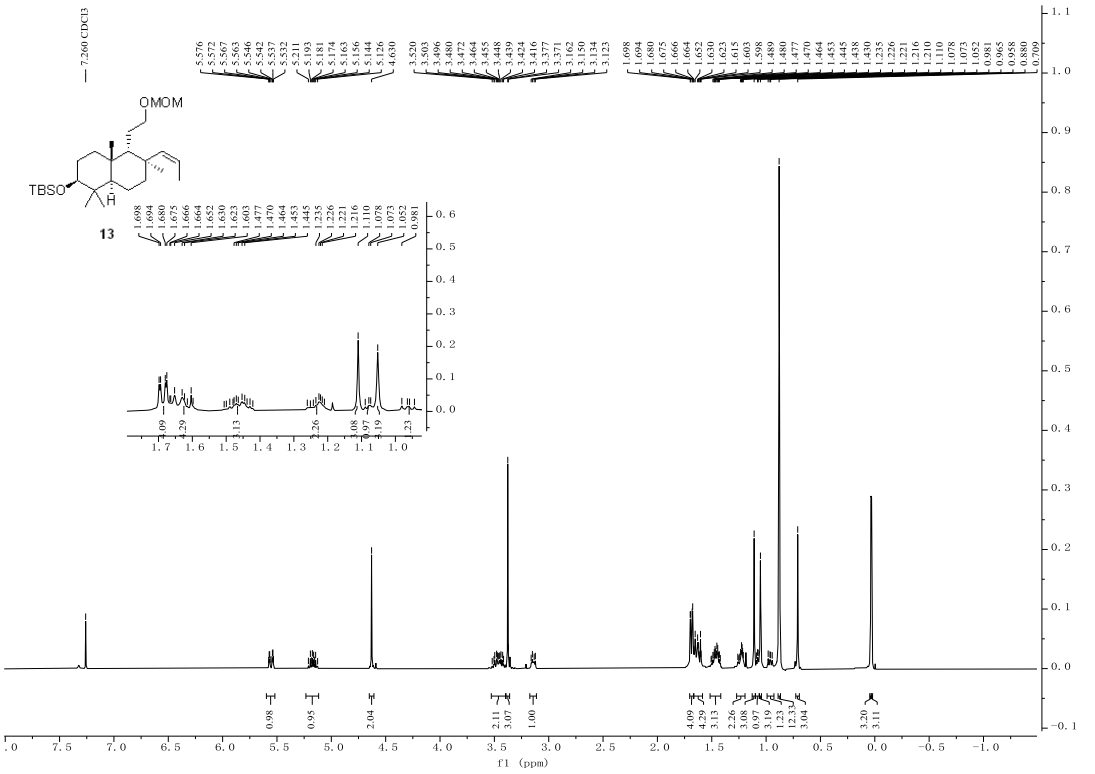
^{1}H NMR spectrum of compound **12**



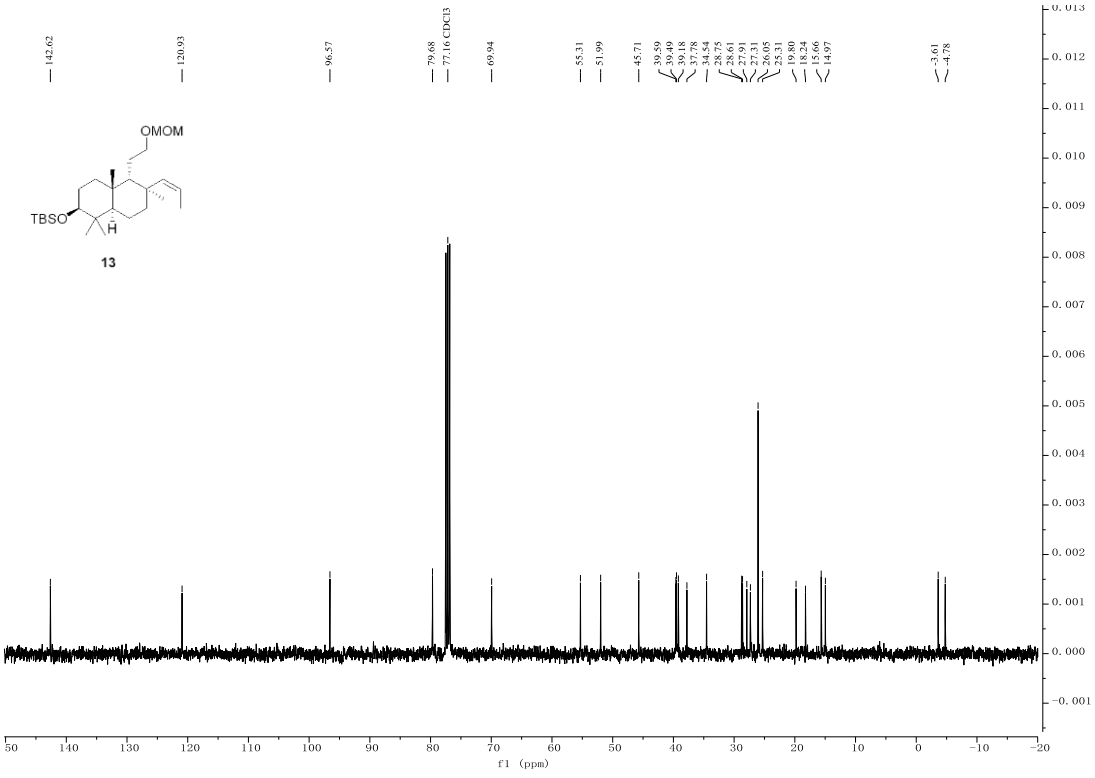
^{13}C NMR spectrum of compound **12**



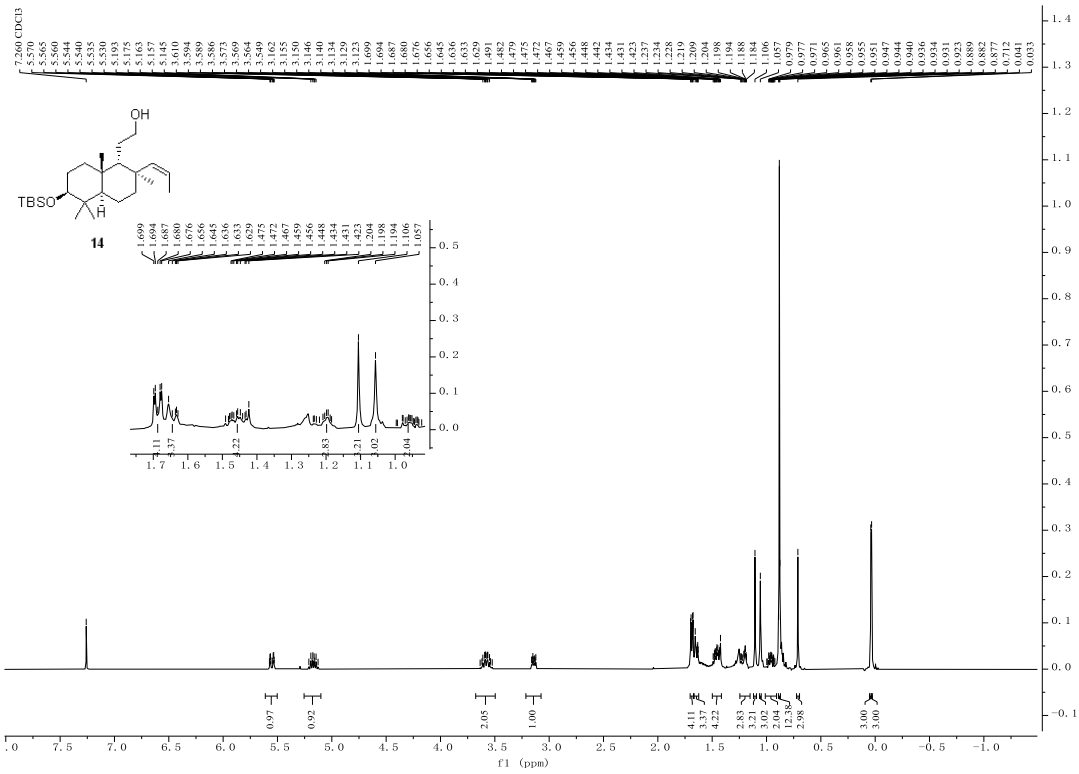
^{1}H NMR spectrum of compound **13**



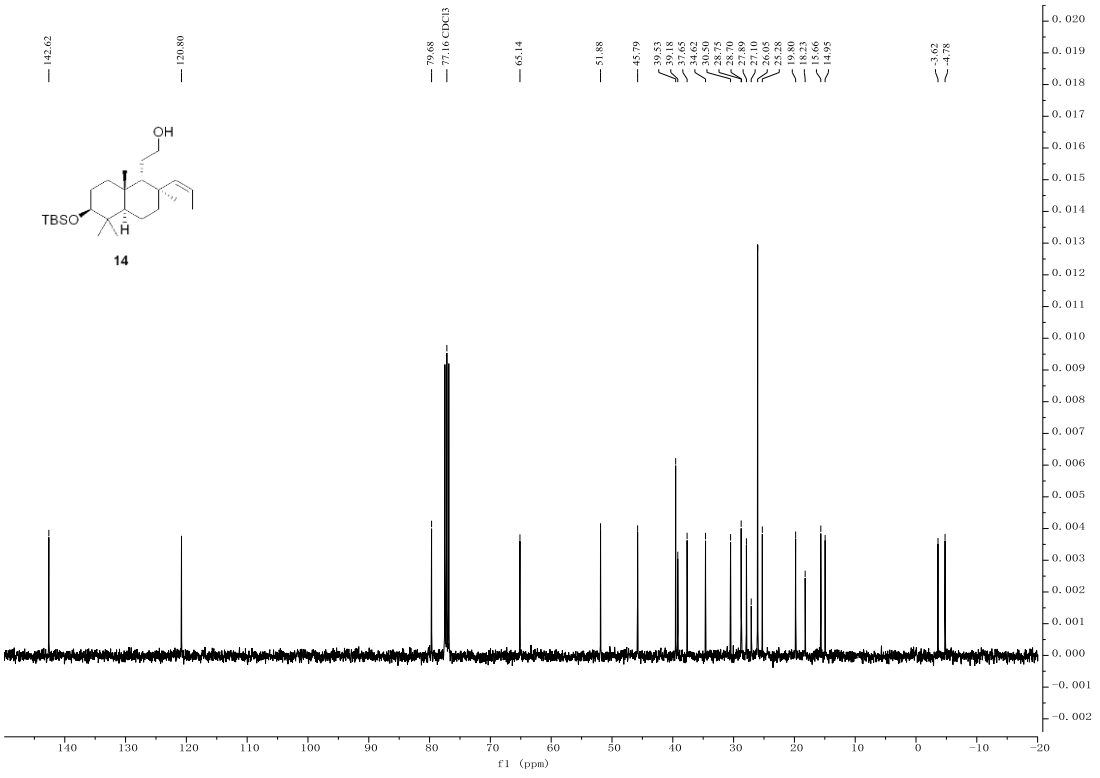
^{13}C NMR spectrum of compound **13**



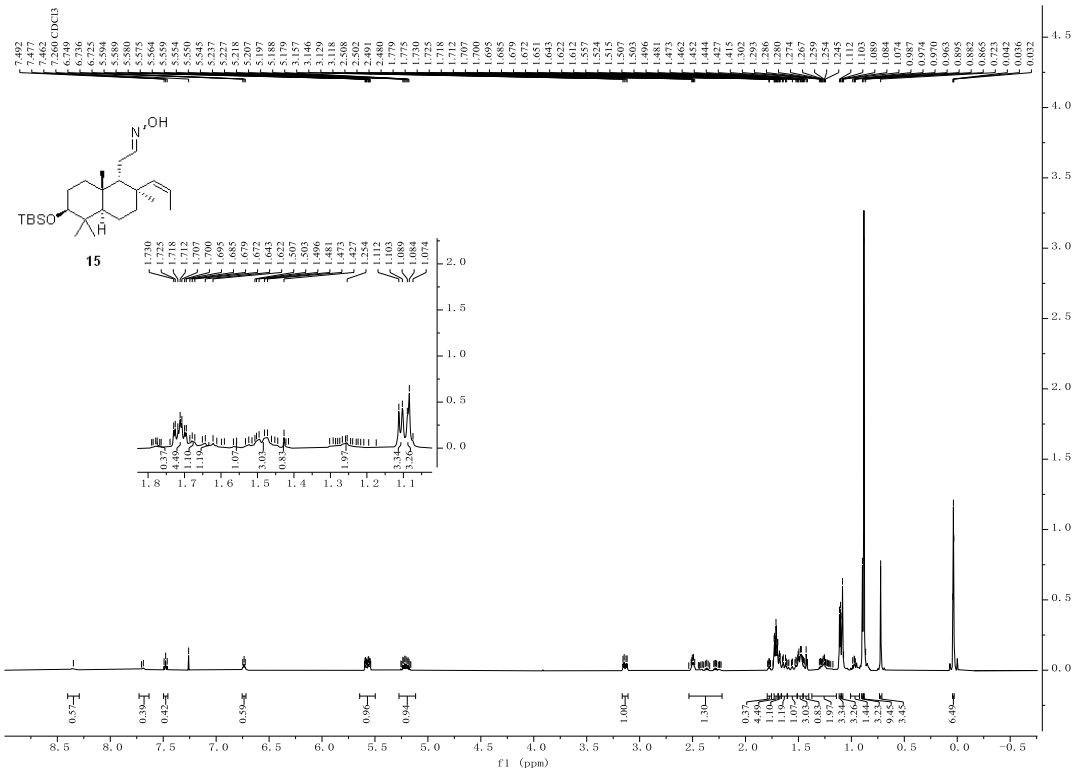
^{1}H NMR spectrum of compound **14**



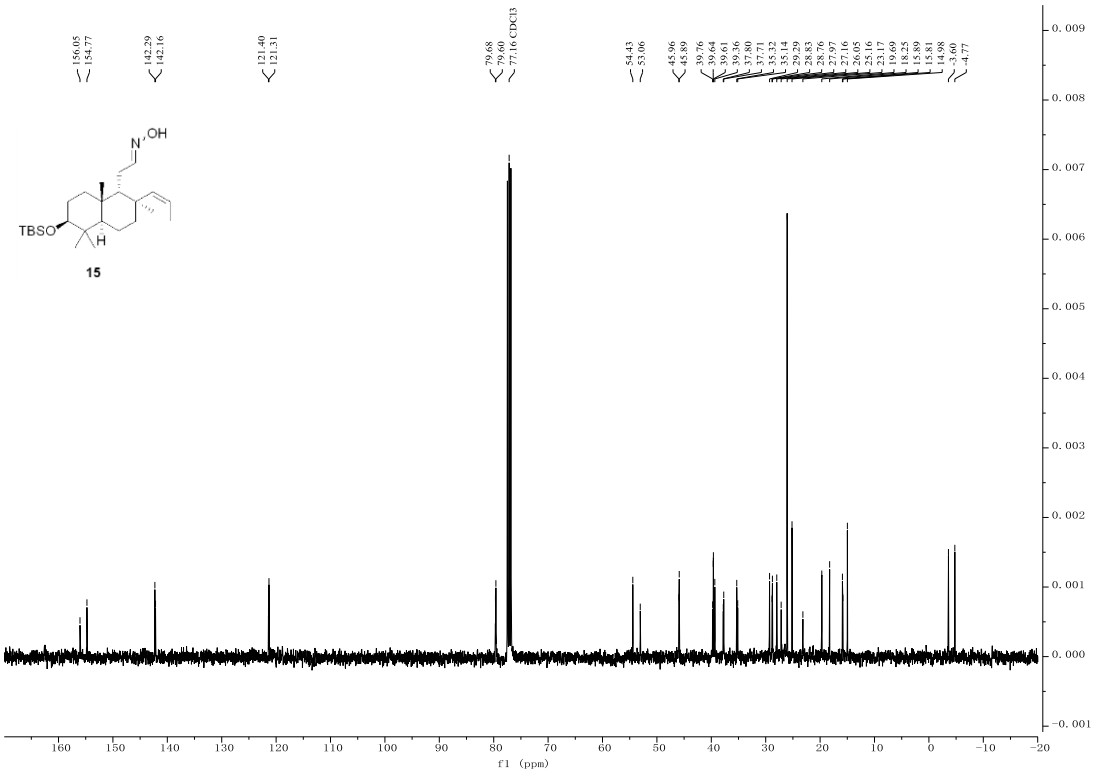
^{13}C NMR spectrum of compound **14**



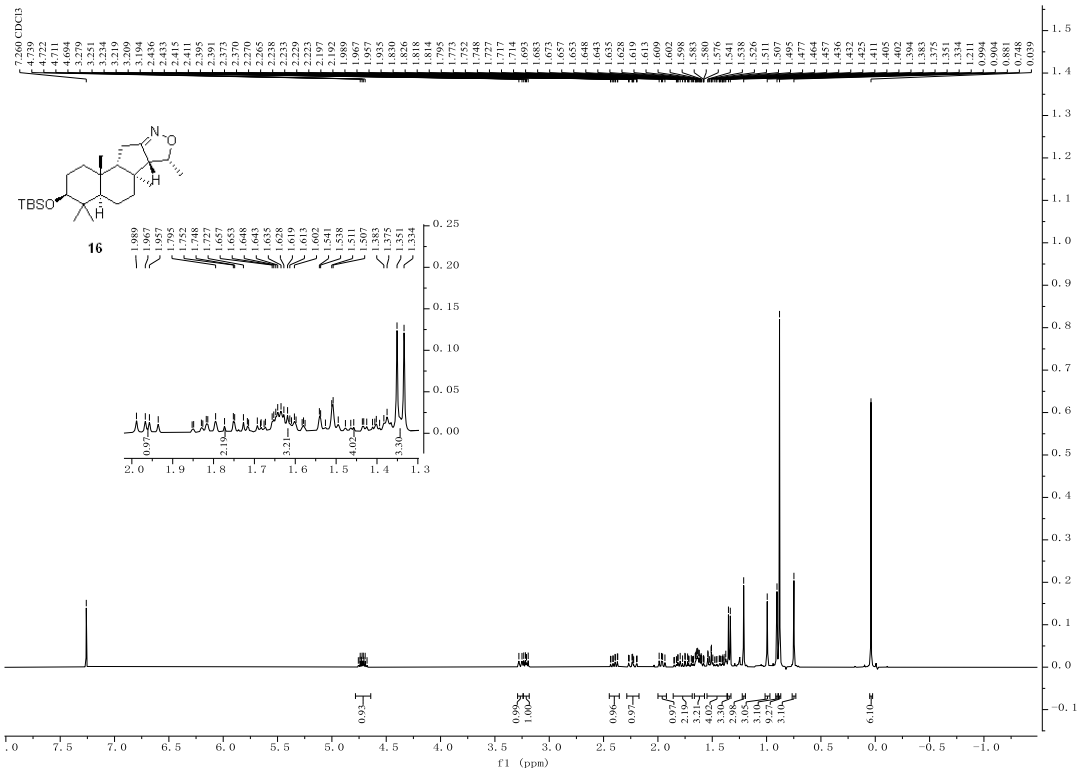
^{1}H NMR spectrum of compound **15**



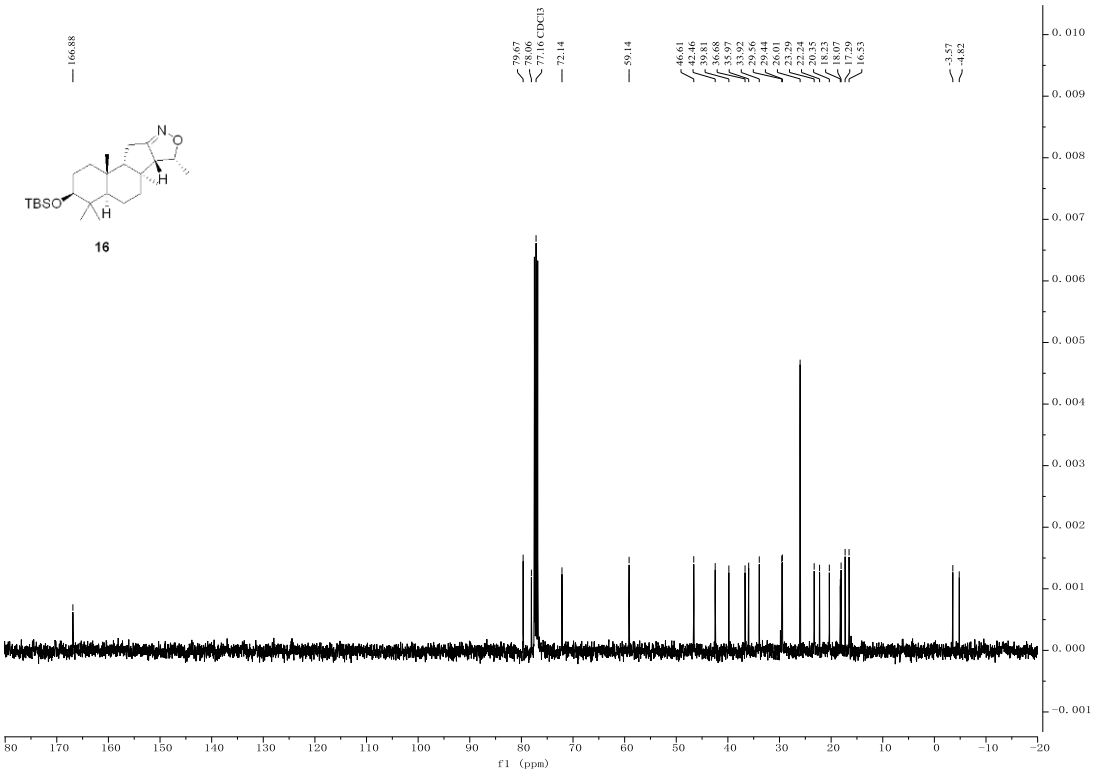
^{13}C NMR spectrum of compound **15**



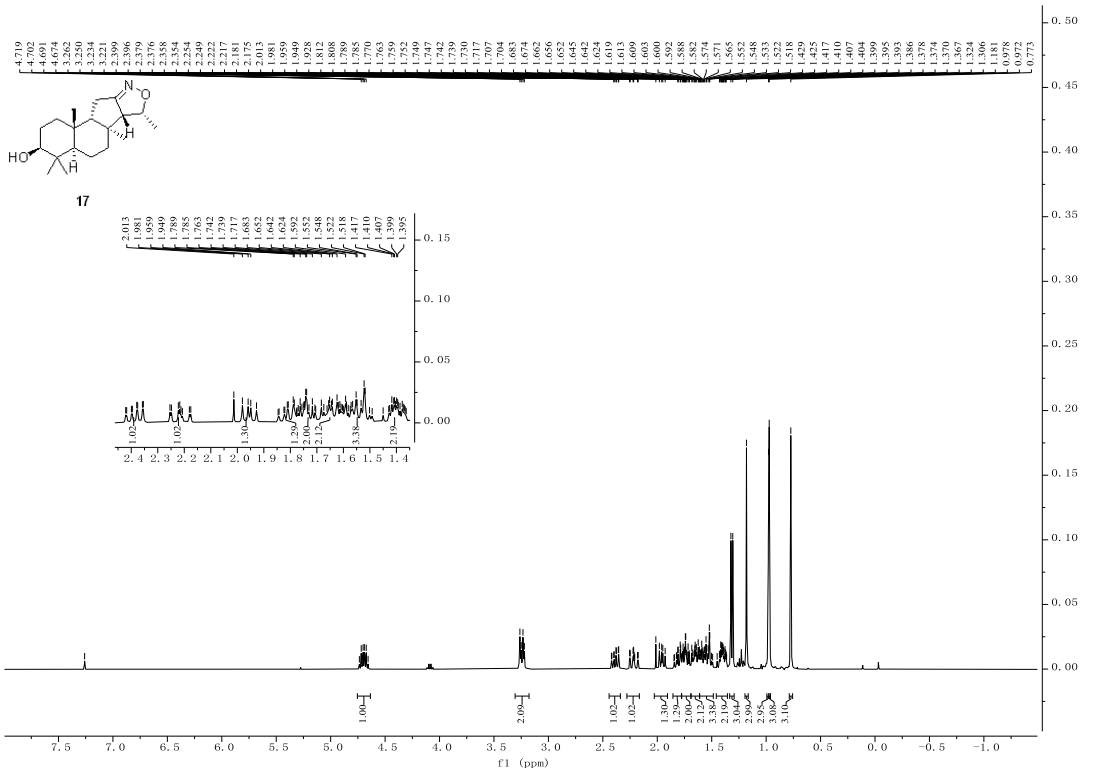
^{1}H NMR spectrum of compound **16**



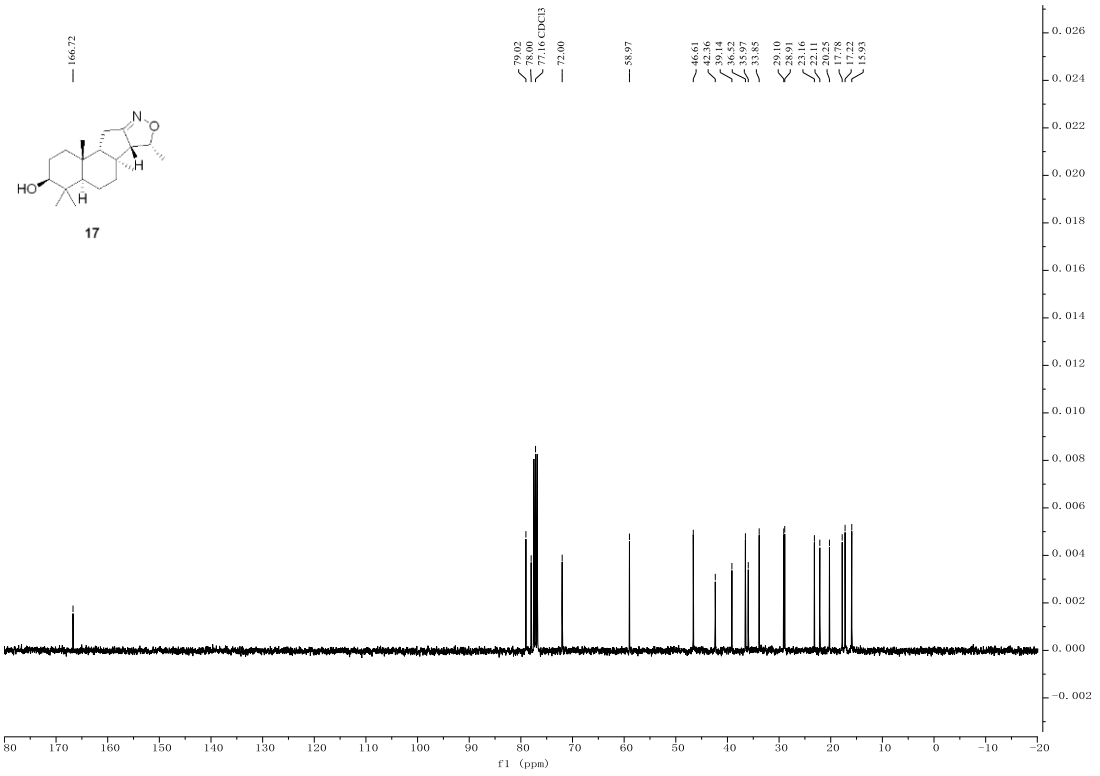
^{13}C NMR spectrum of compound **16**



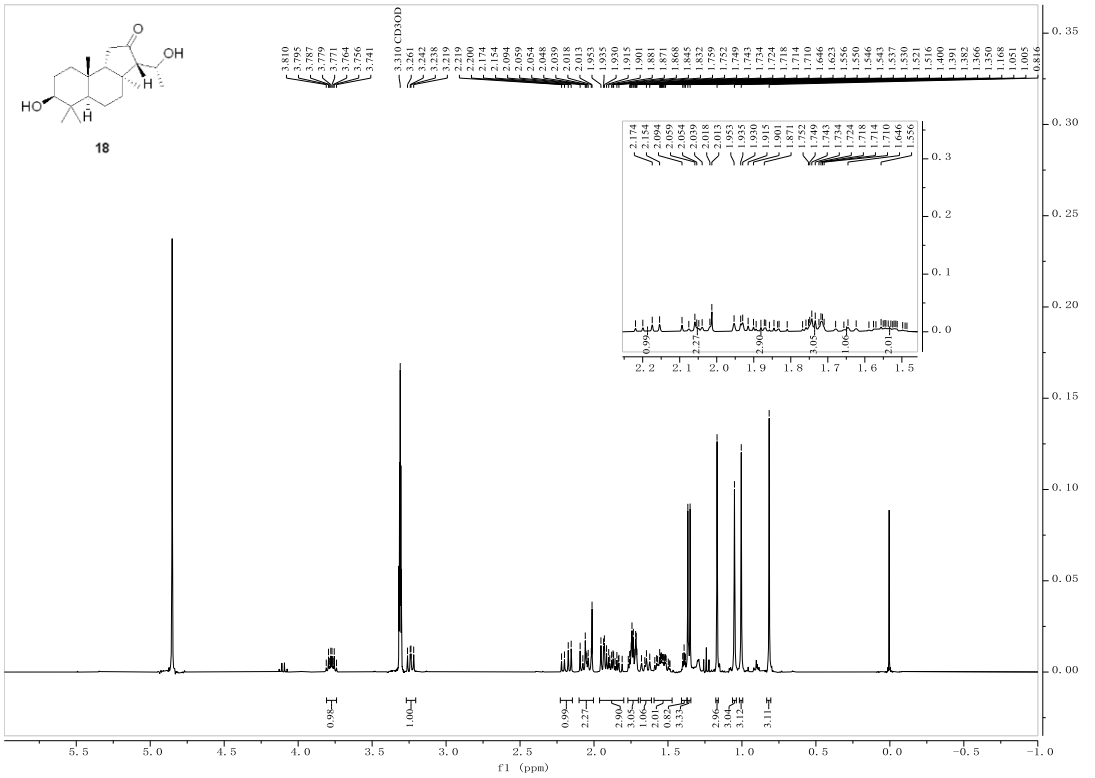
^{1}H NMR spectrum of compound **17**



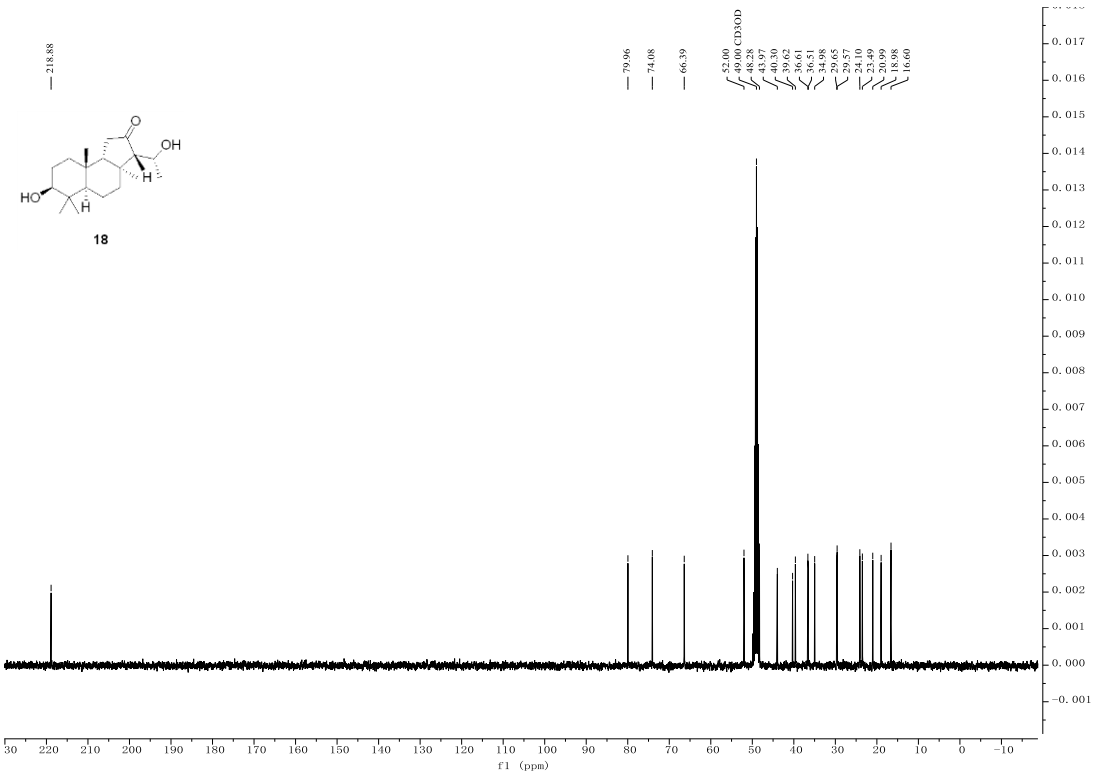
^{13}C NMR spectrum of compound **17**



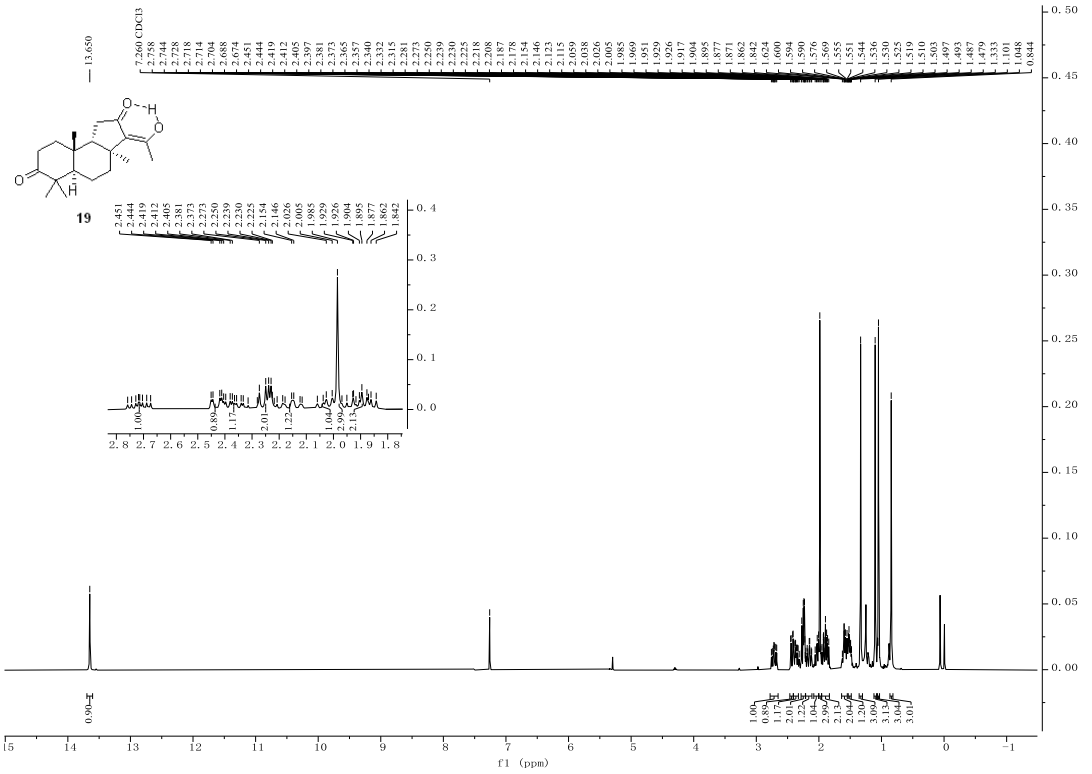
^{1}H NMR spectrum of compound **18**



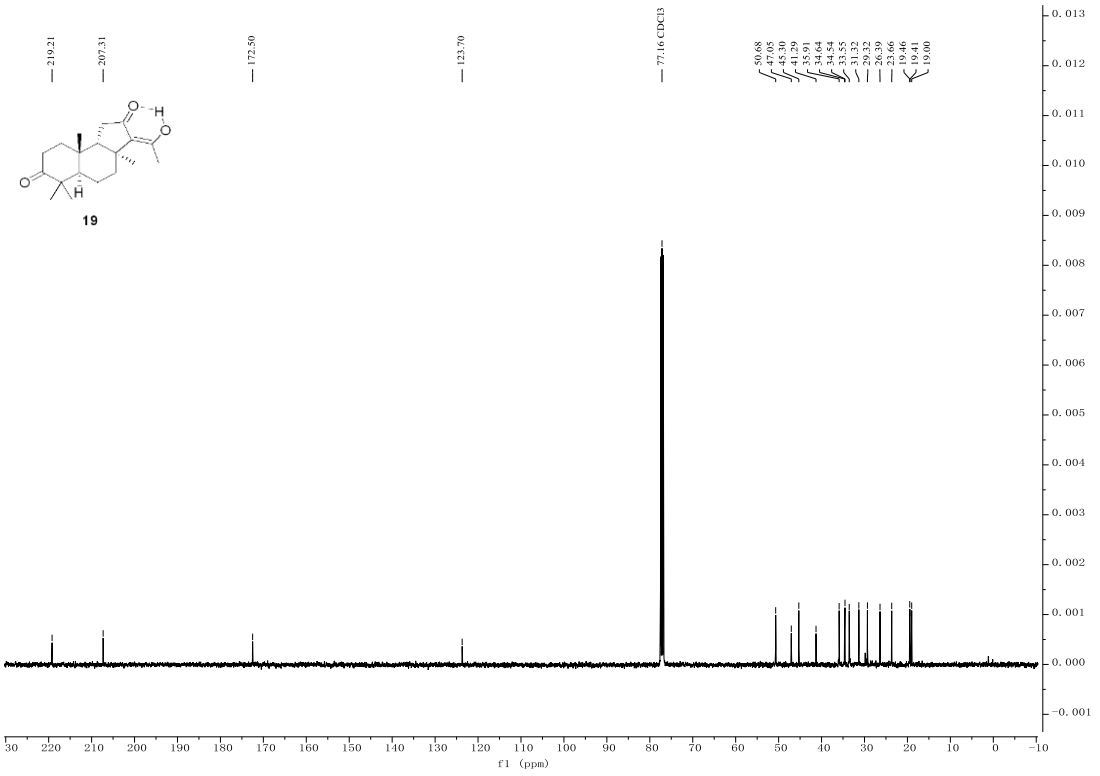
^{13}C NMR spectrum of compound **18**



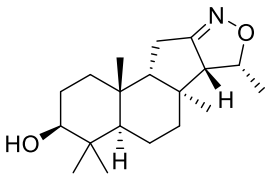
^{1}H NMR spectrum of compound **19**



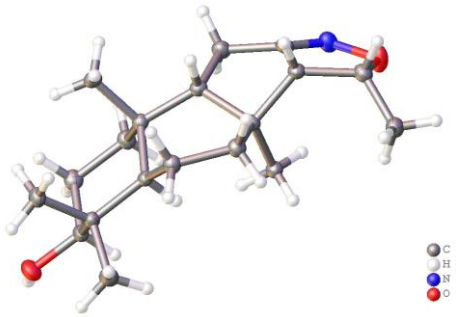
^{13}C NMR spectrum of compound **19**



X-ray diffraction data of compound **17** (CCDC 2244331)



17



Crystal data and structure refinement compound 17

Identification code	exp_8288
Empirical formula	$C_{19}H_{31}NO_2$
Formula weight	305.45
Temperature / K	113.70(14)
Crystal system	monoclinic
Space group	$P2_1/n$
a / Å, b / Å, c / Å	7.3053(3), 12.1351(4), 18.2588(9)
α/°, β/°, γ/°	90.00, 92.115(4), 90.00
Volume / Å^3	1617.56(12)
Z	4
ρ_{calc} / mg mm^{-3}	1.254
μ / mm^{-1}	0.080
F(000)	672
Crystal size / mm^3	0.30 × 0.27 × 0.15
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection	5.94 to 52°
Index ranges	$-8 \leq h \leq 7$, $-14 \leq k \leq 14$, $-17 \leq l \leq 22$
Reflections collected	12610
Independent reflections	3144[R(int) = 0.0428 (inf-0.9Å)]
Data/restraints/parameters	3144/0/205
Goodness-of-fit on F^2	1.037
Final R indexes [I>2σ (I) i.e. F_o>4σ (F_o)]	R_1 = 0.0465, wR_2 = 0.1033
Final R indexes [all data]	R_1 = 0.0612, wR_2 = 0.1129
Largest diff. peak/hole / e Å^{-3}	0.263/-0.208
Flack Parameters	N
Completeness	0.9980