

Supporting Information
for
A concise and practical stereoselective
synthesis of ipragliflozin L-proline

Shuai Ma, Zhenren Liu, Jing Pan, Shunli, Zhang, Weicheng Zhou*

Address: State Key Lab of New Drug & Pharmaceutical Process, Shanghai
Key Lab of Anti-Infectives, Shanghai Institute of Pharmaceutical Industry,
China State Institute of Pharmaceutical Industry, No. 285, Gebaini Rd.,
Shanghai 201203, P. R. of China

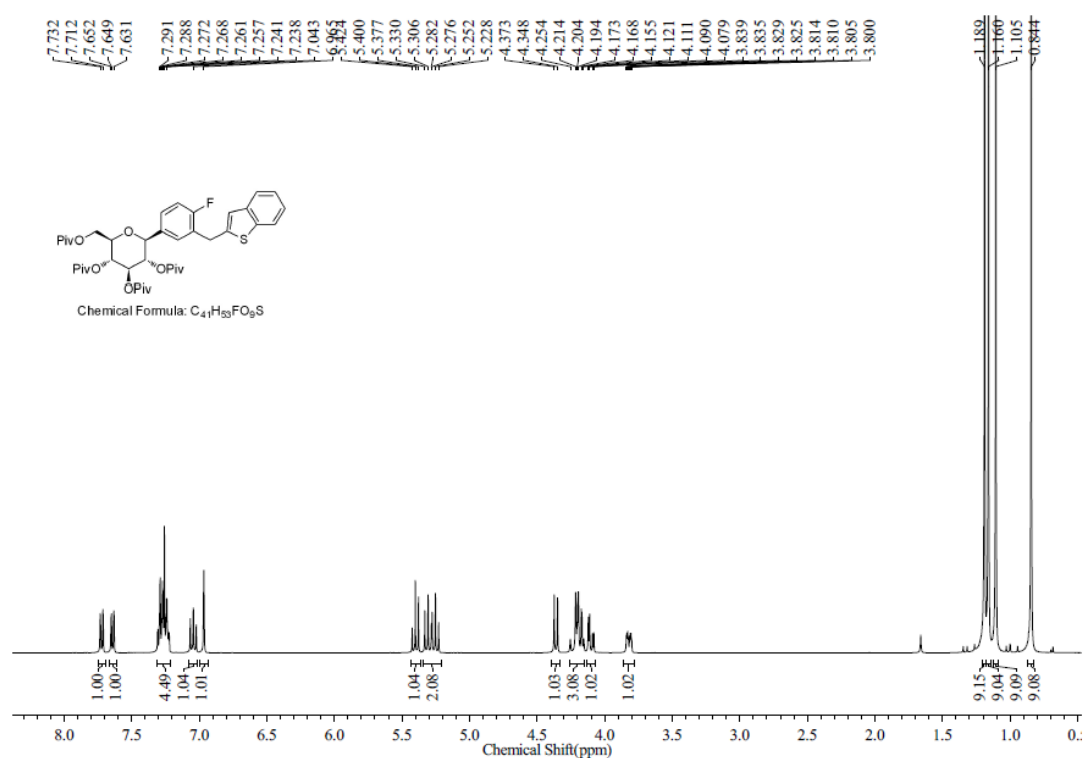
Email: Weicheng Zhou*- zhouweicheng58@163.com

*Corresponding author

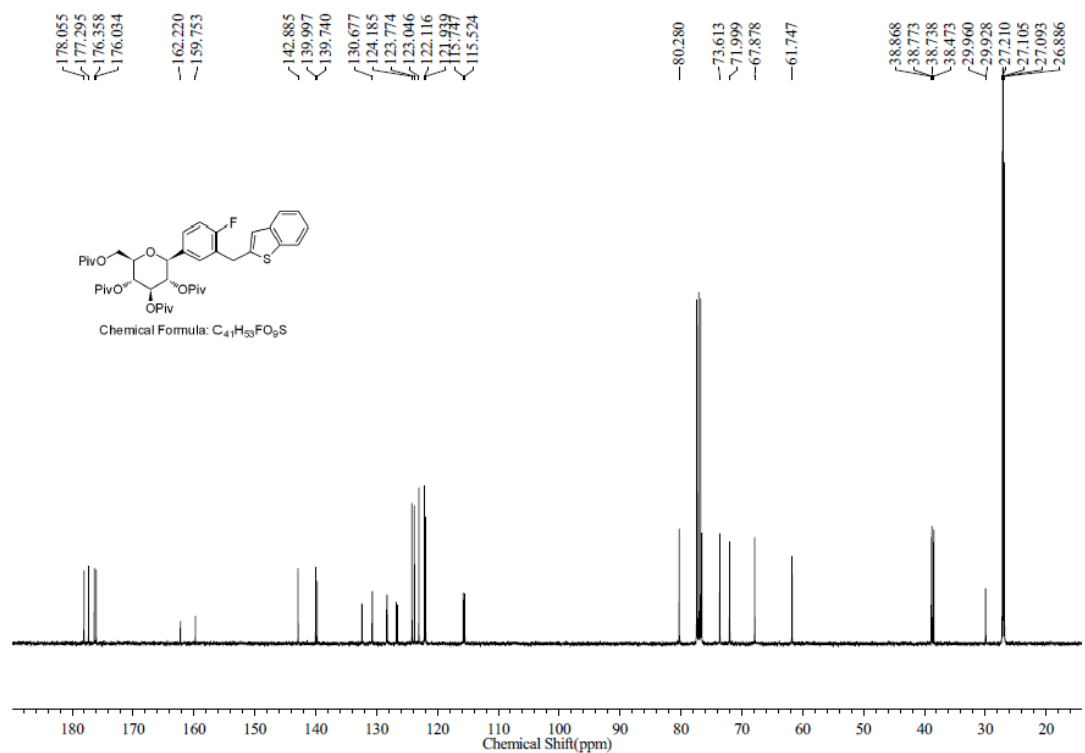
**^1H NMR, ^{13}C NMR and HRMS spectra of compounds 1, 5, 6, 5',
6' and 8, and HPLC diagram of 5**

Table of contents

¹ H NMR and ¹³ C NMR spectrum of compound 5	S3
HRMS spectrum of compound 5	S4
HPLC spectrum of compound 5	S5
¹ H NMR and ¹³ C NMR spectrum of compound 6	S6
HRMS spectrum of compound 6	S7
¹ H NMR and ¹³ C NMR spectrum of compound 1	S8
¹ H NMR and ¹³ C NMR spectrum of compound 8	S9
¹ H NMR and ¹³ C NMR spectrum of compound 6'	S10
¹ H NMR and ¹³ C NMR spectrum of compound 5'	S11



1H NMR spectrum of compound 5



^{13}C NMR spectrum of compound 5

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

170 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 5-55 H: 5-65 O: 1-9 Na: 1-1 S: 0-1 F: 0-1

SIPI

I5

Q-Tof micro

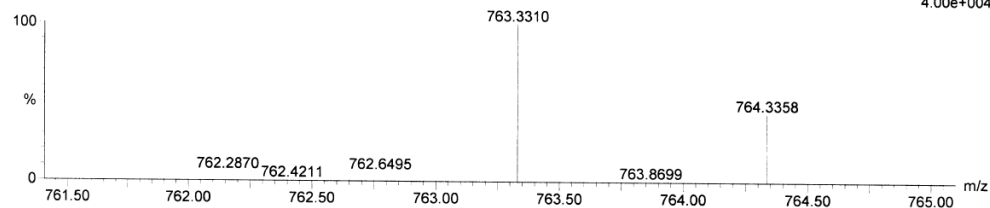
YA019

08:25:33,23-Nov-2016

Q16-1771HR 14 (0.260) AM (Cen,4, 80.00, Ar,5000.0,767.35,1.00); Sm (Mn, 2x3.00); Sb (1,40.00); Cm (4,25)

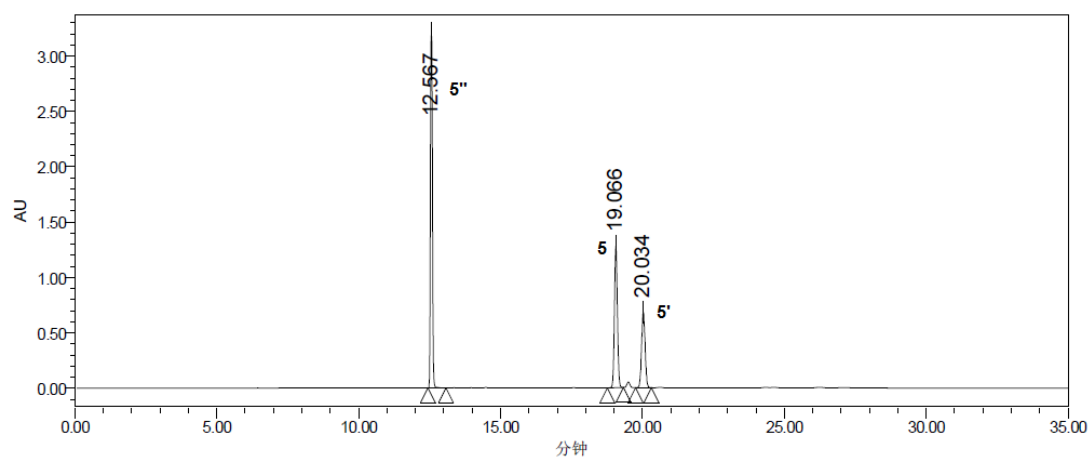
TOF MS ES+

4.00e+004



Minimum:				-1.5		
Maximum:	5.0	5.0		50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
763.3310	763.3292	1.8	2.4	14.5	n/a	C41 H53 O9 Na S F

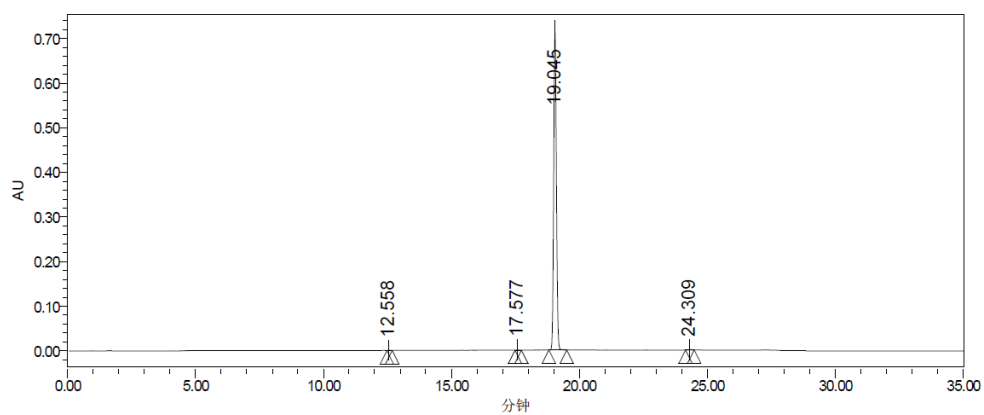
HRMS spectrum of compound 5



峰结果

	保留时间 (分钟)	名称	面积 (微伏*秒)	高度 (微伏)	% 面积
1	12.567		16130039	3205166	51.47
2	19.066		9336482	1277501	29.79
3	20.034		5873495	681279	18.74

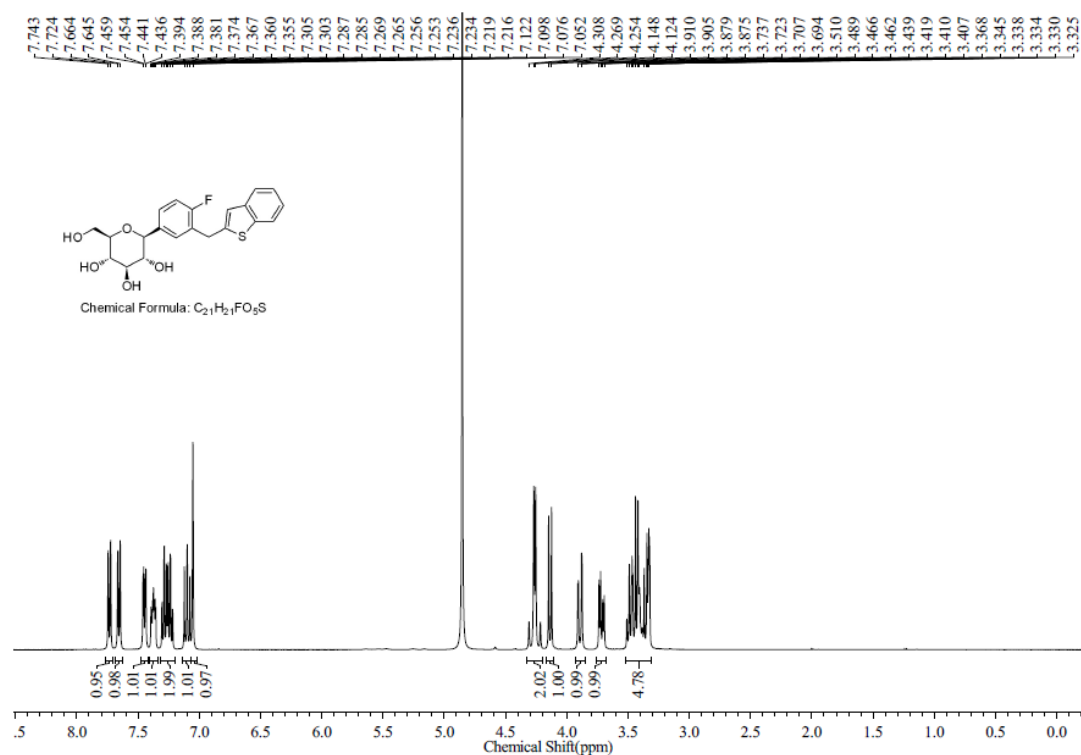
HPLC spectrum of compounds 5, 5' and 5''



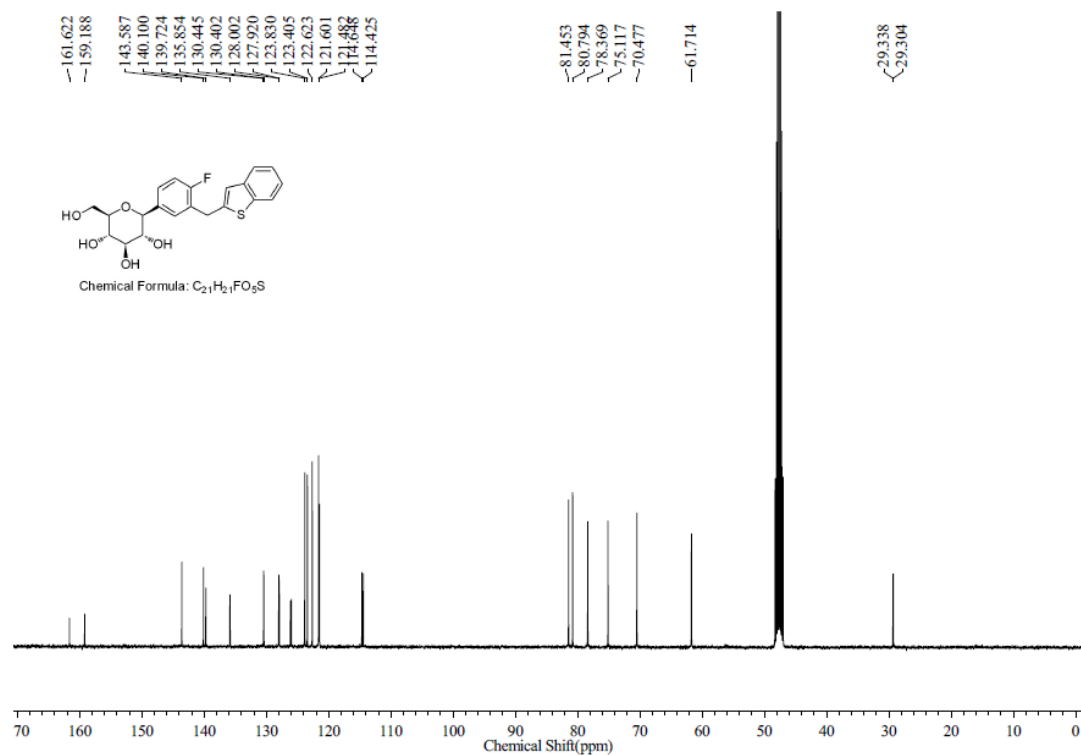
峰结果

	保留时间 (分钟)	面积 (微伏*秒)	高度 (微伏)	% 面积
1	12.558	2239	558	0.04
2	17.577	3983	744	0.08
3	19.045	5247427	715860	99.79
4	24.309	4739	454	0.09

HPLC spectrum of compound 5



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



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

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

50 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

Elements Used:
C: 5-35 H: 5-35 O: 1-5 F: 0-1 Na: 1-1 S: 0-1

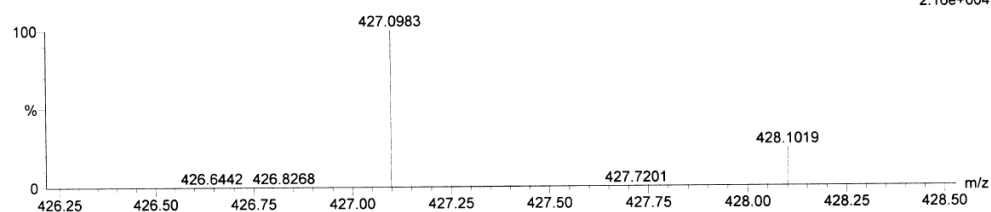
Q-Tof micro

07:32:59,23-Nov-2016

YA019

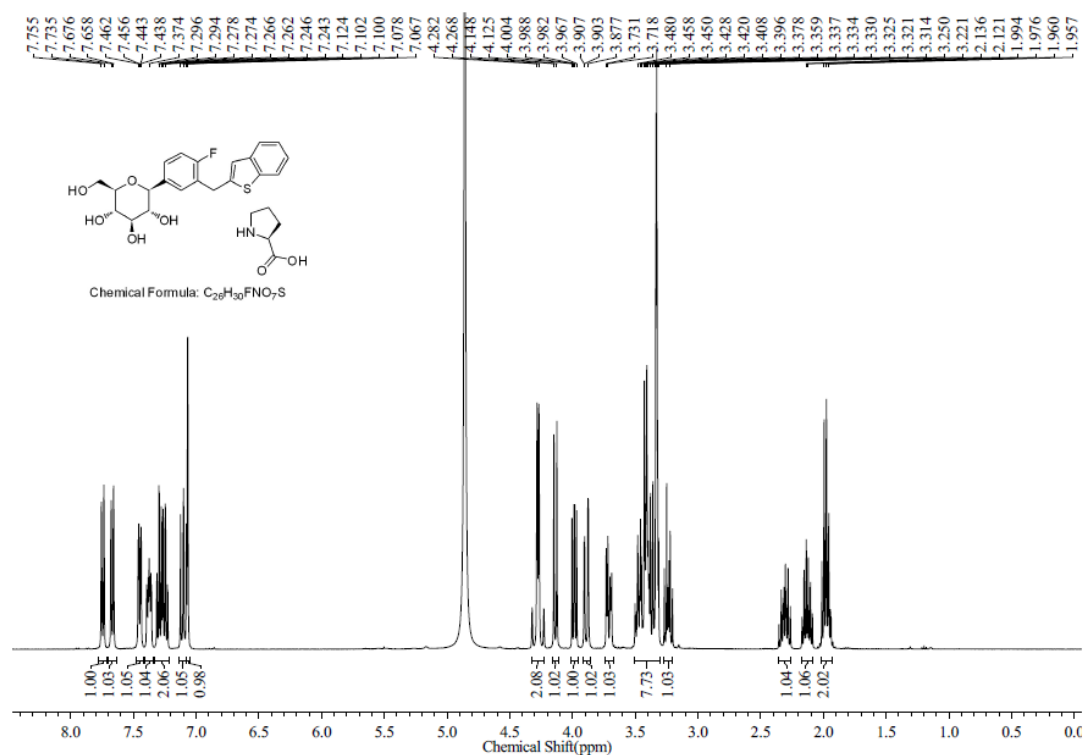
Q16-1870HR 66 (1.224) AM (Cen.4, 80.00, Ar.5000.0.431.12,1.00); Sm (Mn, 2x3.00); Sb (1,40.00); Cm (53:66)

TOF MS ES+
2.16e+004

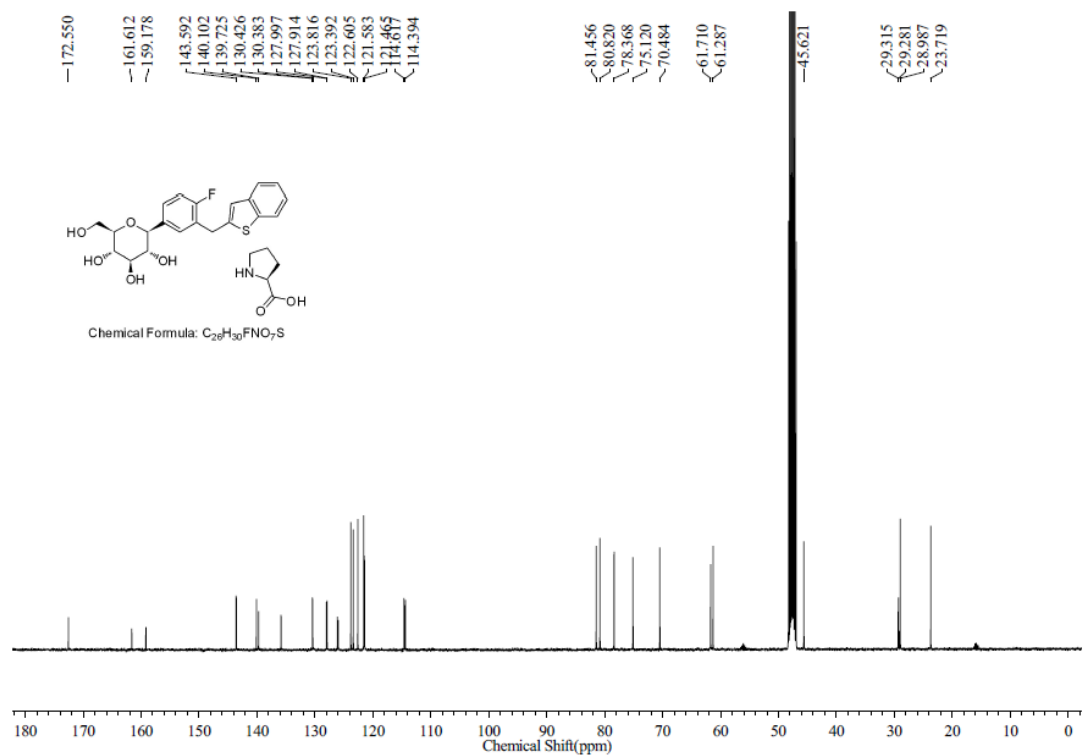


Minimum:				-1.5					
Maximum:		5.0	5.0	50.0					
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula			
427.0983	427.0980	0.3	0.7	14.5	n/a	C24	H20	O4	Na S
	427.0991	-0.8	-1.9	10.5	n/a	C21	H21	O5	F Na S

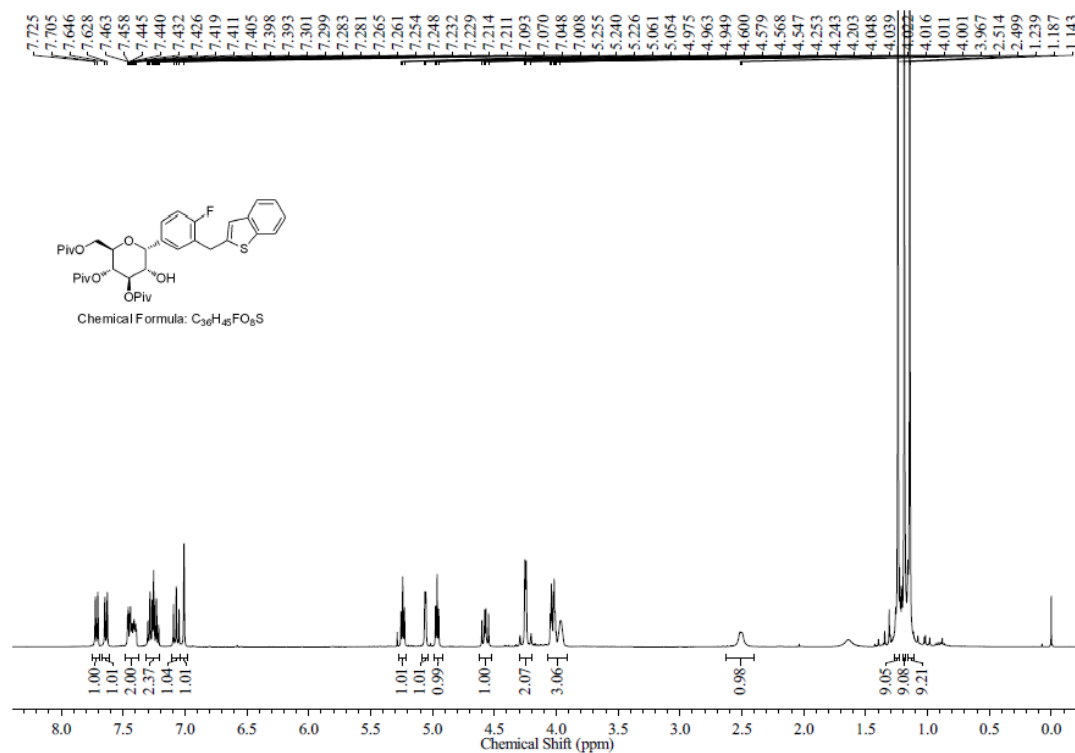
HRMS spectrum of compound **6**



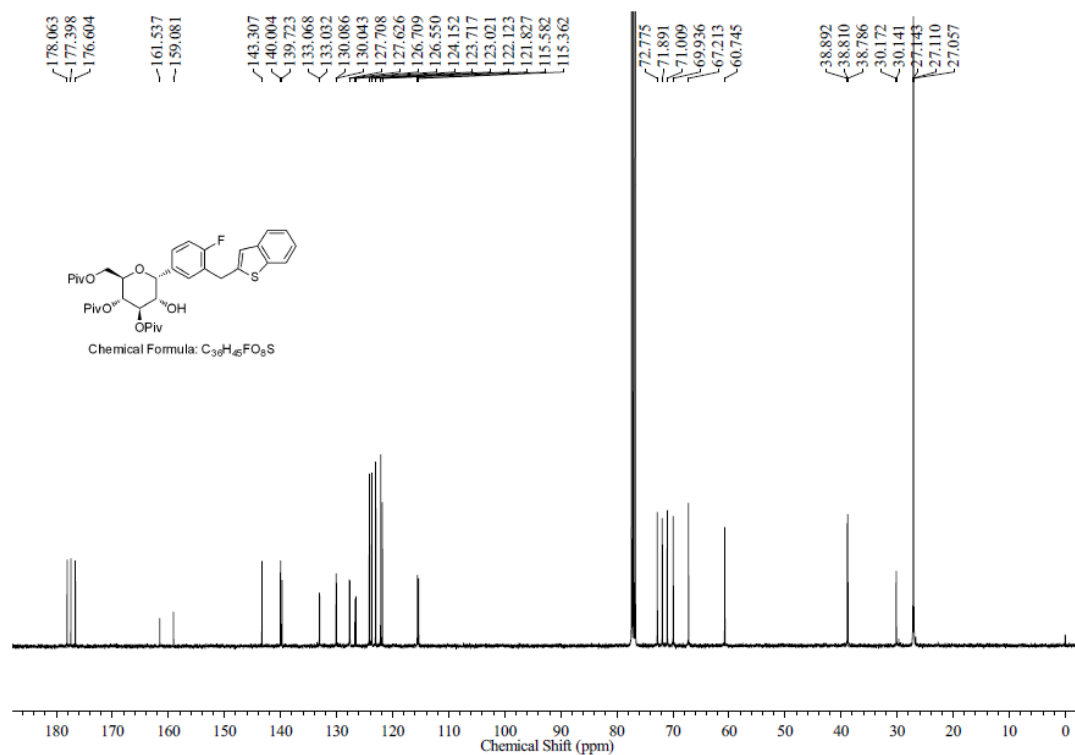
^1H NMR spectrum of compound **1**



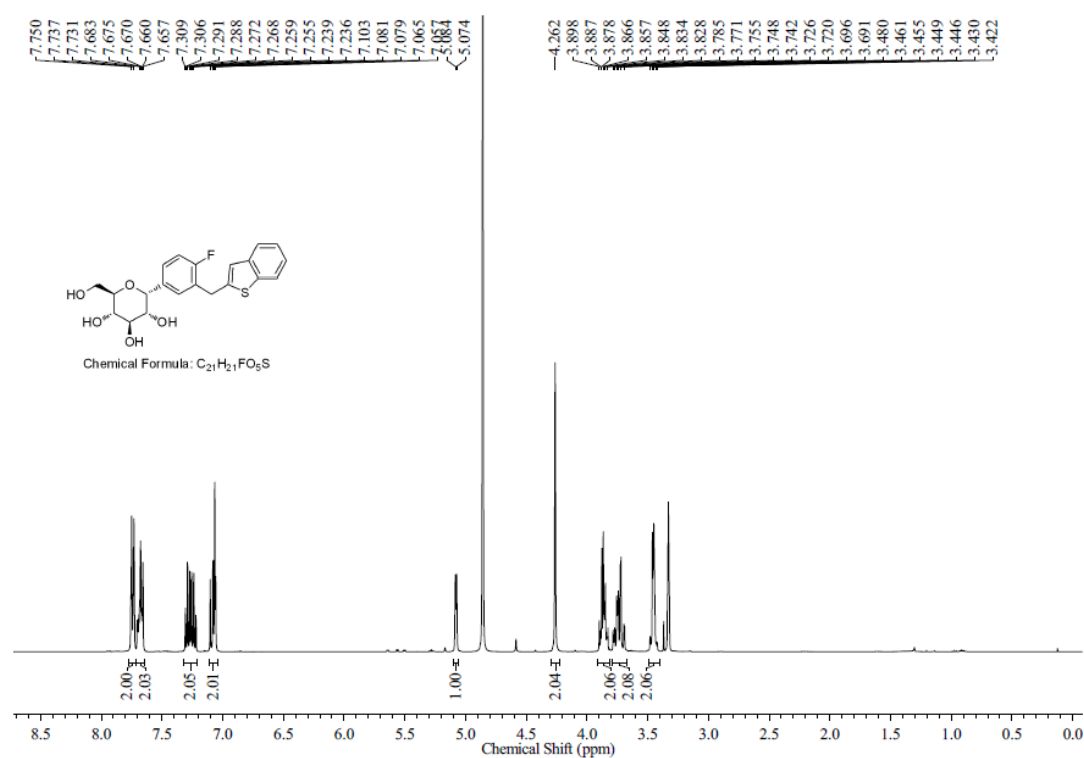
^{13}C NMR spectrum of compound **1**



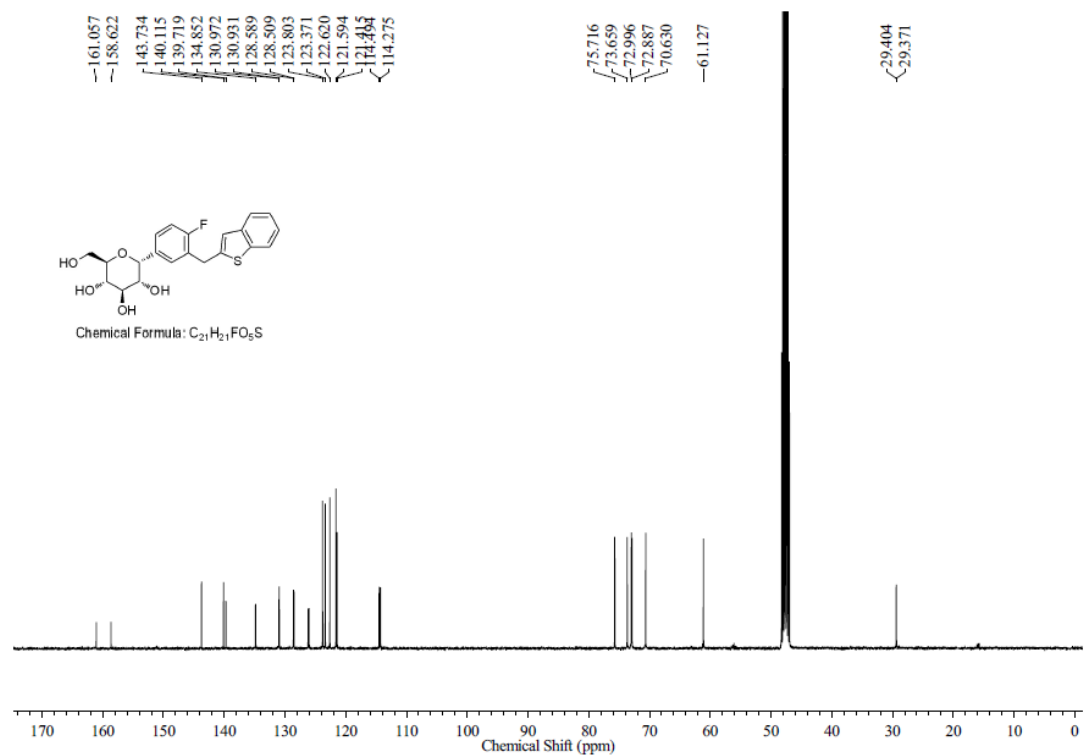
1H NMR spectrum of compound 8



^{13}C NMR spectrum of compound 8



^1H NMR spectrum of compound **6'**



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

