Supplementary Material

Bioactive Phytochemicals: Efficient Synthesis of Optically Active Substituted Flav-3-enes and Flav-3-en-3-*O*-derivatives

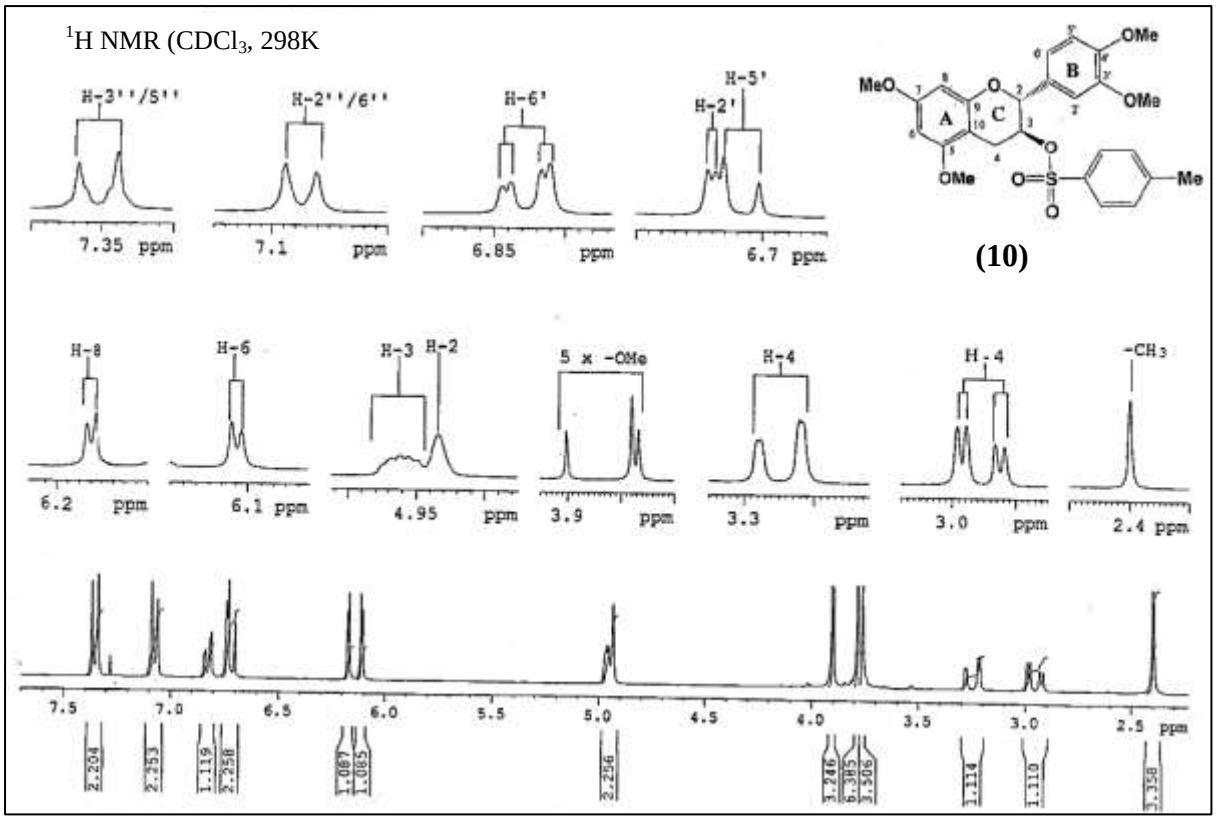
Matthew Chilaka Achilonu,[1,2] Moosa Mahmood Sedibe,[2] and Karabo Shale[1]

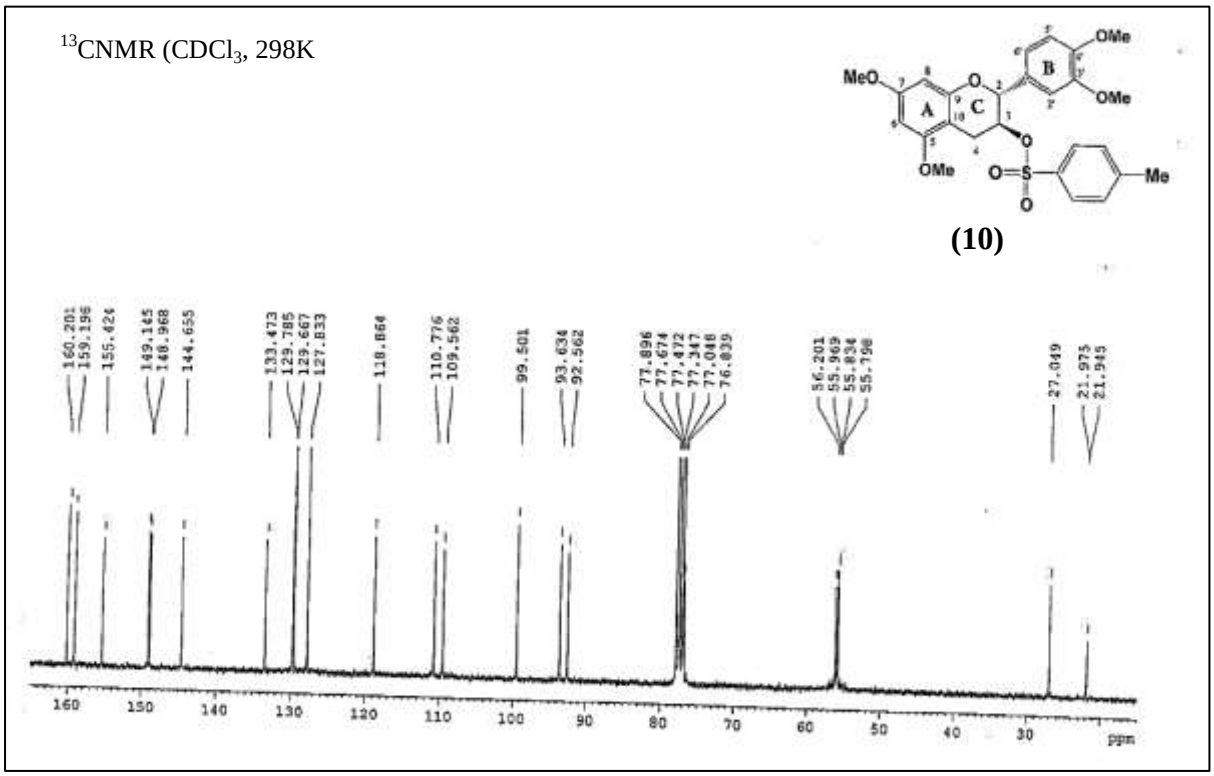
[1]Faculty of Natural Sciences, Mangosuthu University of Technology, Umlazi, Durban, KwaZulu Natal, South Africa

[2]Department of Agriculture, Faculty of Health and Environmental Sciences, Central University of Technology, Free State, 1 Park Road, Bloemfontein 9301, South Africa

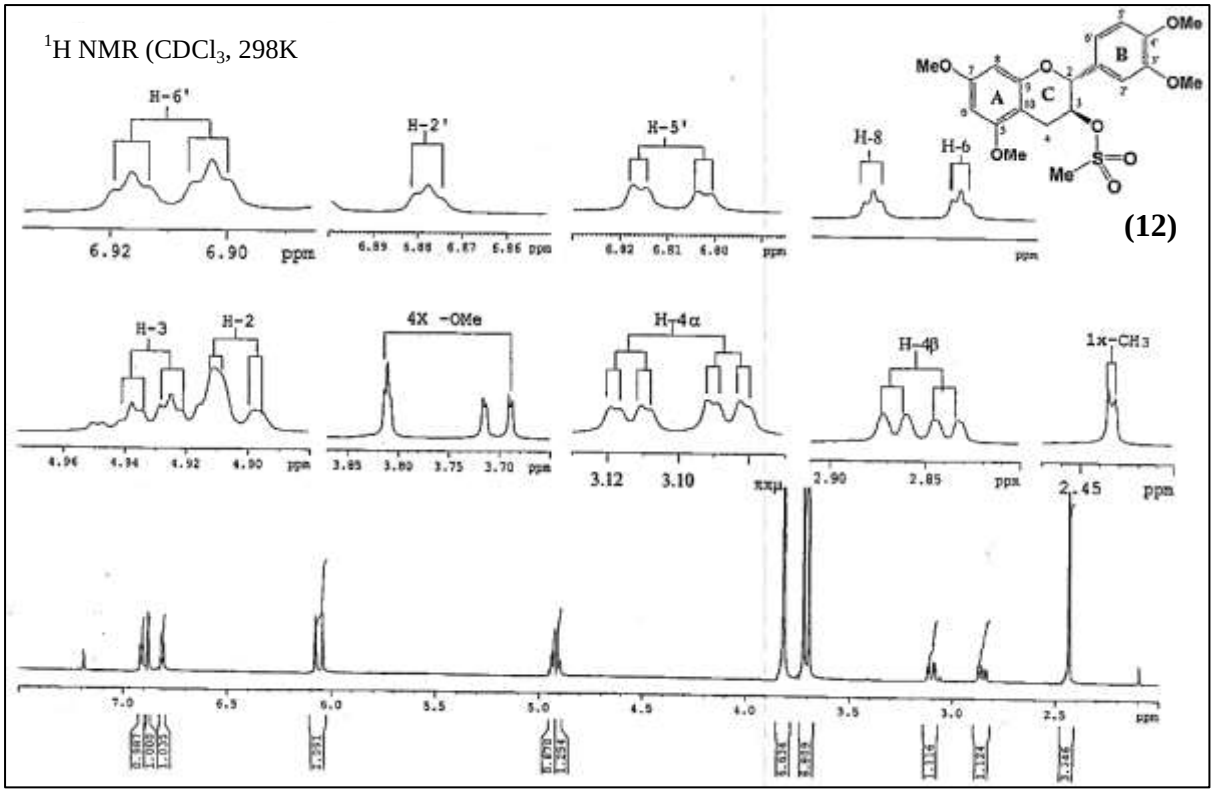
Author to whom correspondence should be addressed; E-Mail: mcachilonu@yahoo.co.uk; machilonu@cut.ac.za

Representative ^{1}H and ^{13}C NMR Spectra of Substituted Flav-3-enes and Flav-3-O-derivatives



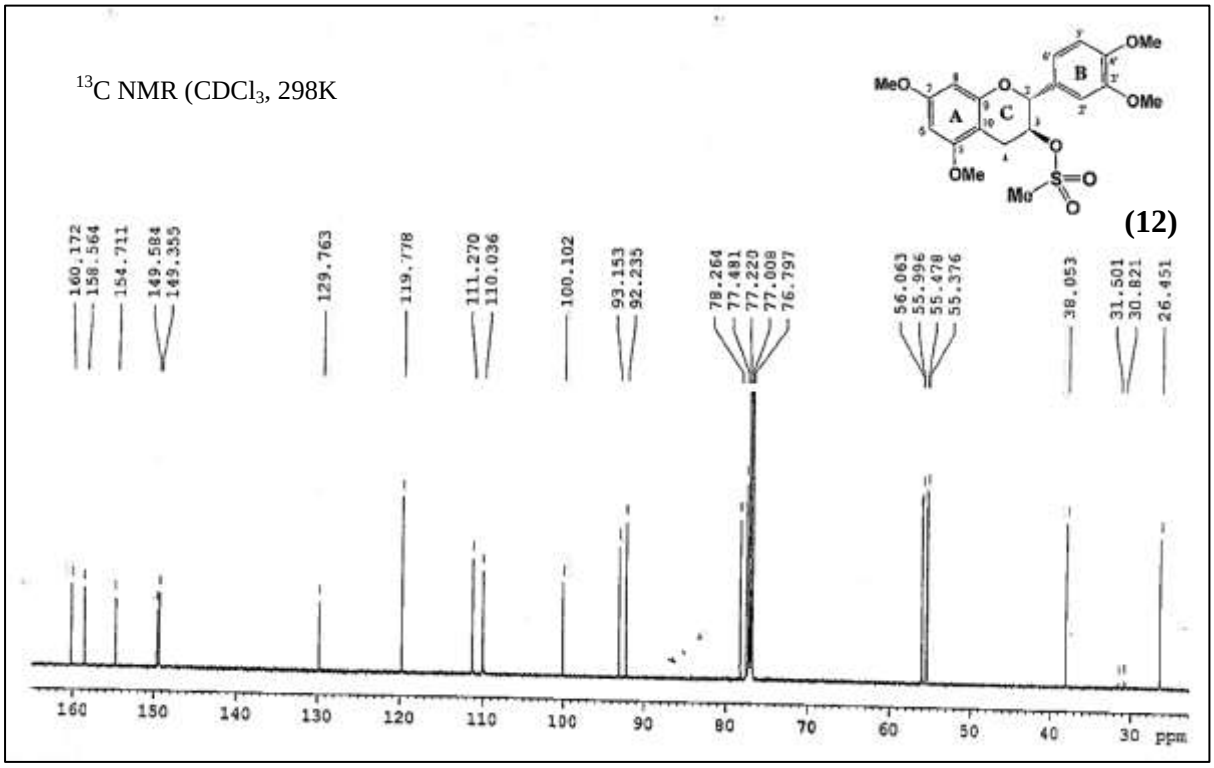


^{1}H NMR ($CDCl_3$, 298K



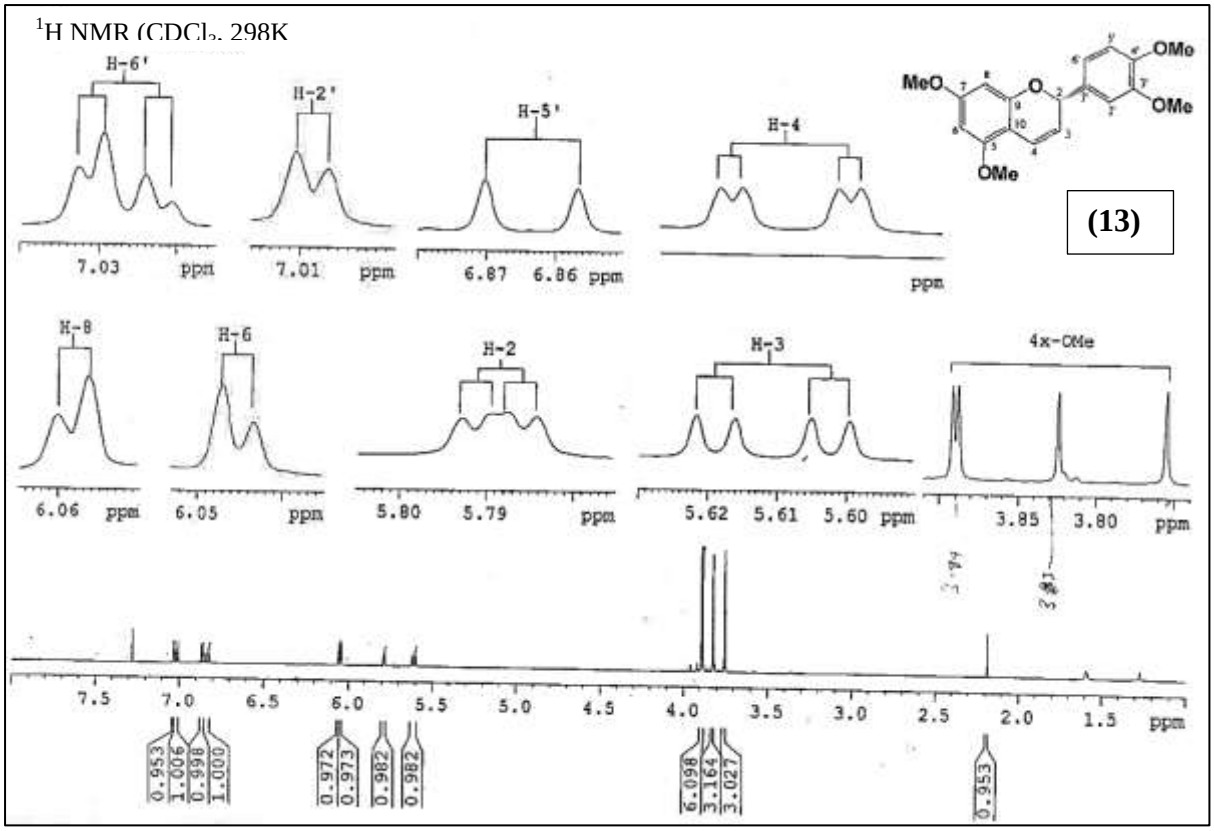
(12)

^{13}C NMR ($CDCl_3$, 298K

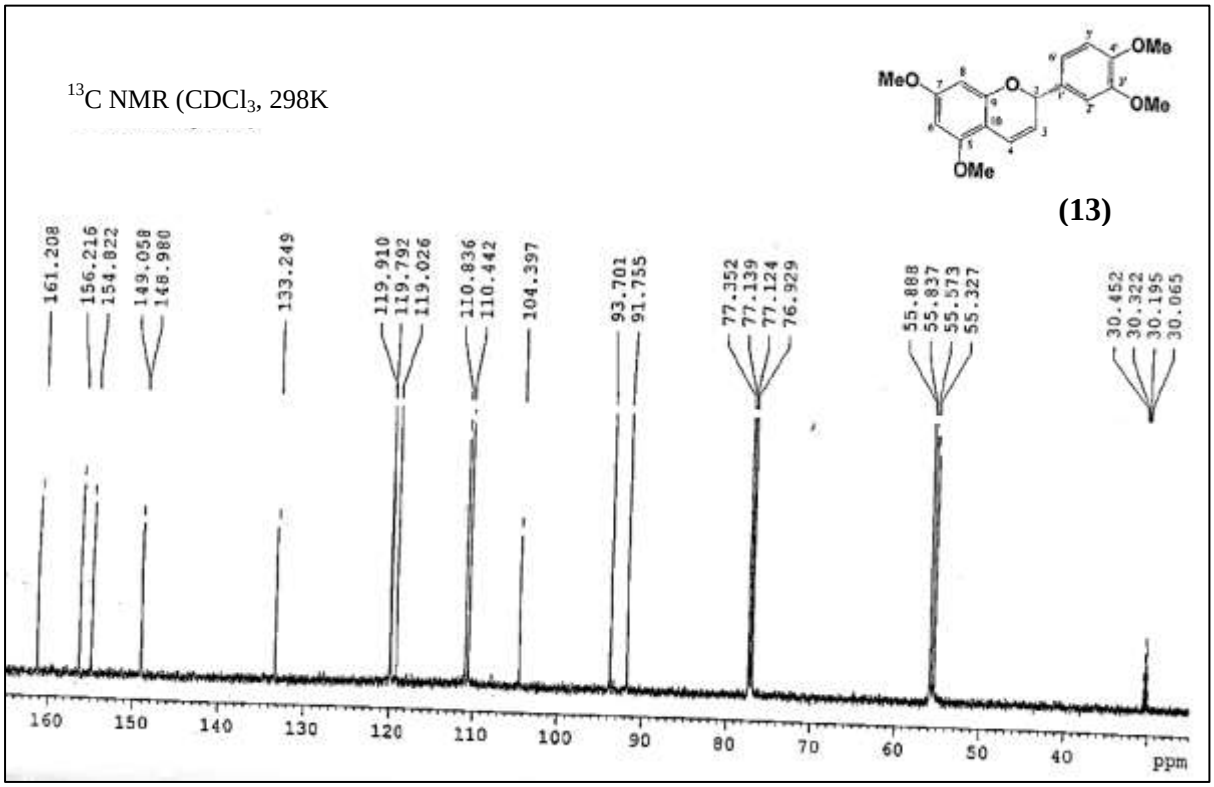


(12)

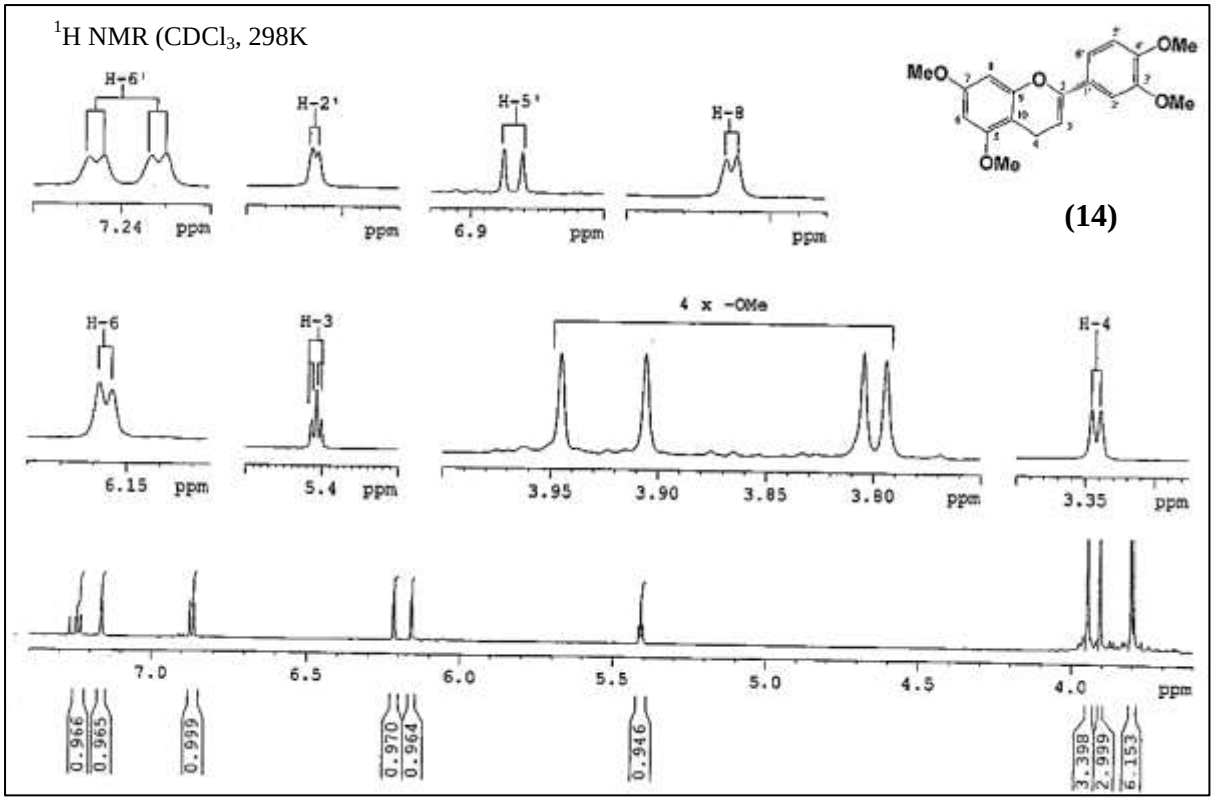
^{1}H NMR (CDCl$_3$, 298K



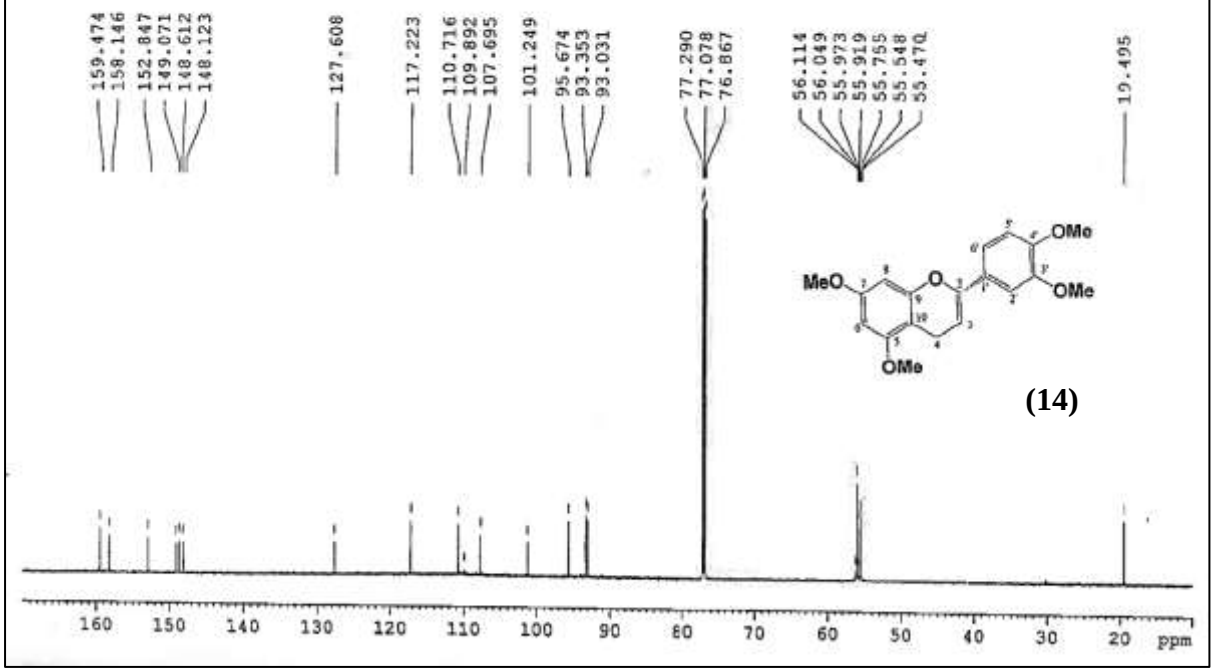
^{13}C NMR (CDCl$_3$, 298K

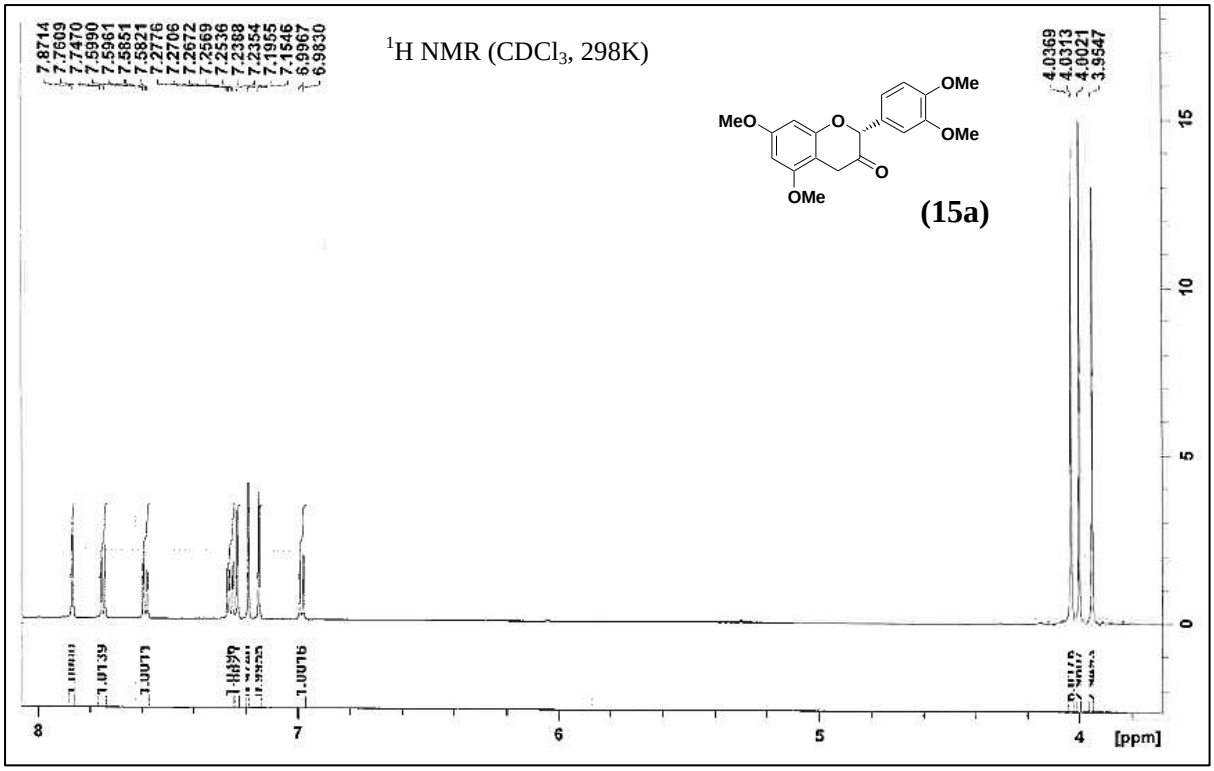


^{1}H NMR ($CDCl_3$, 298K

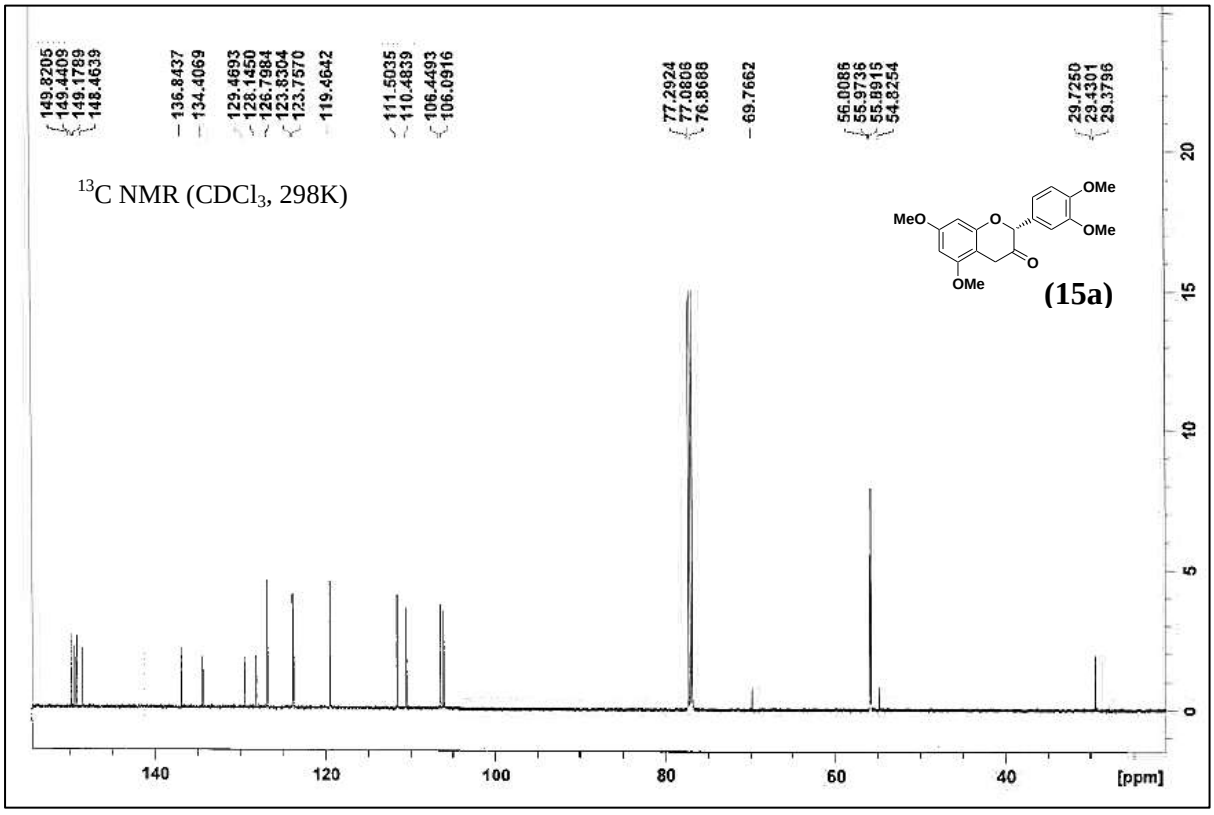


^{13}C NMR ($CDCl_3$, 298K

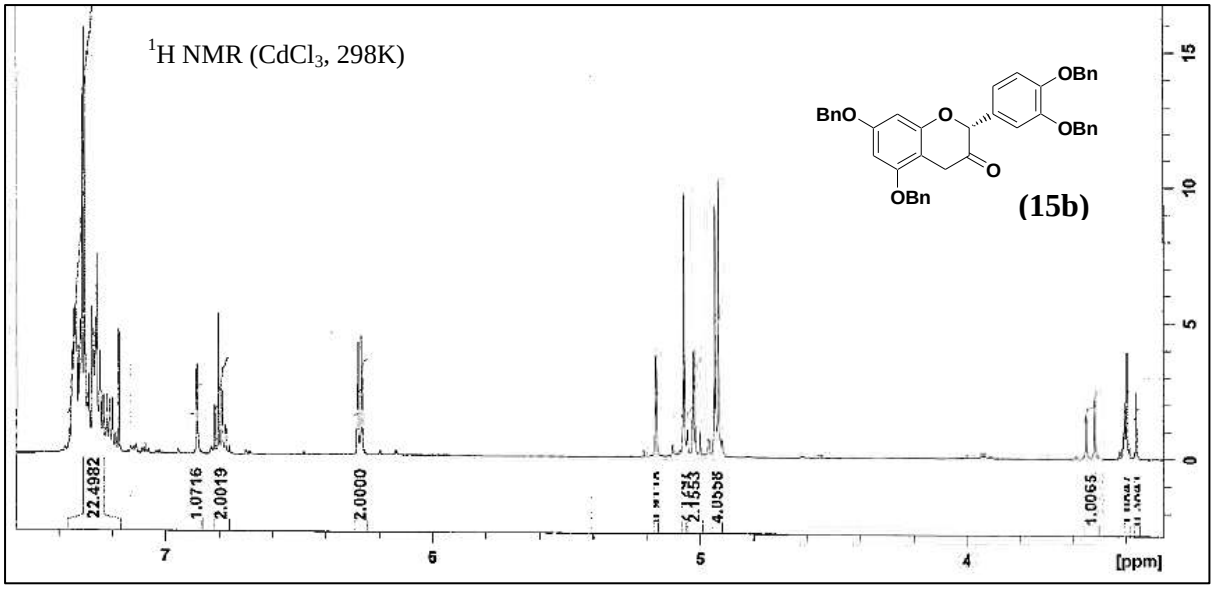


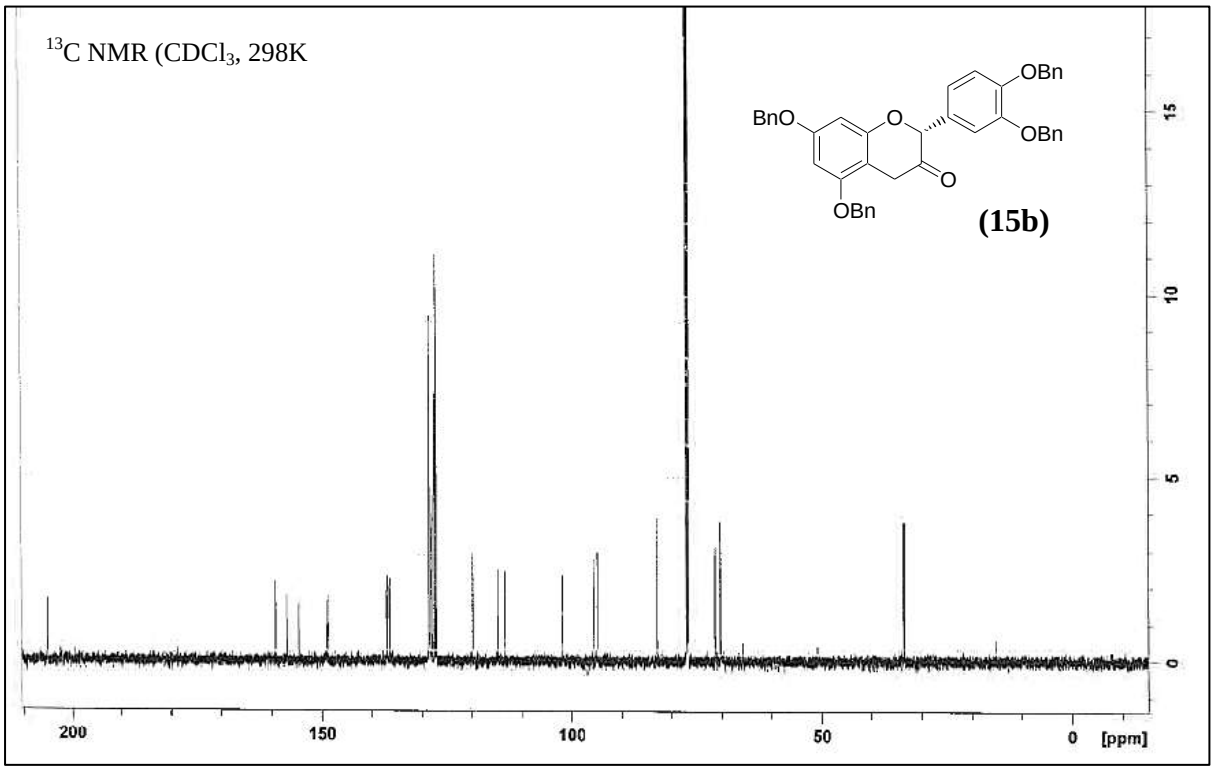


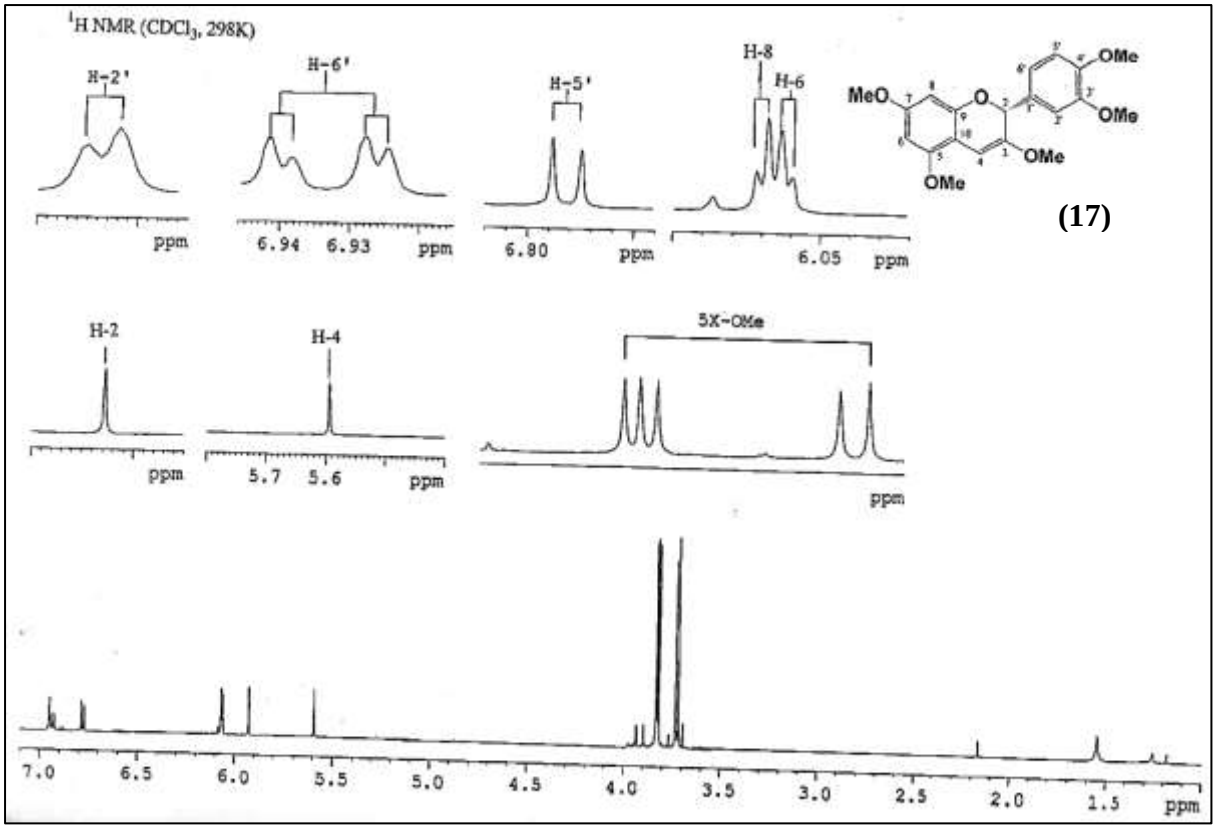
^{1}H NMR ($CDCl_3$, 298K)

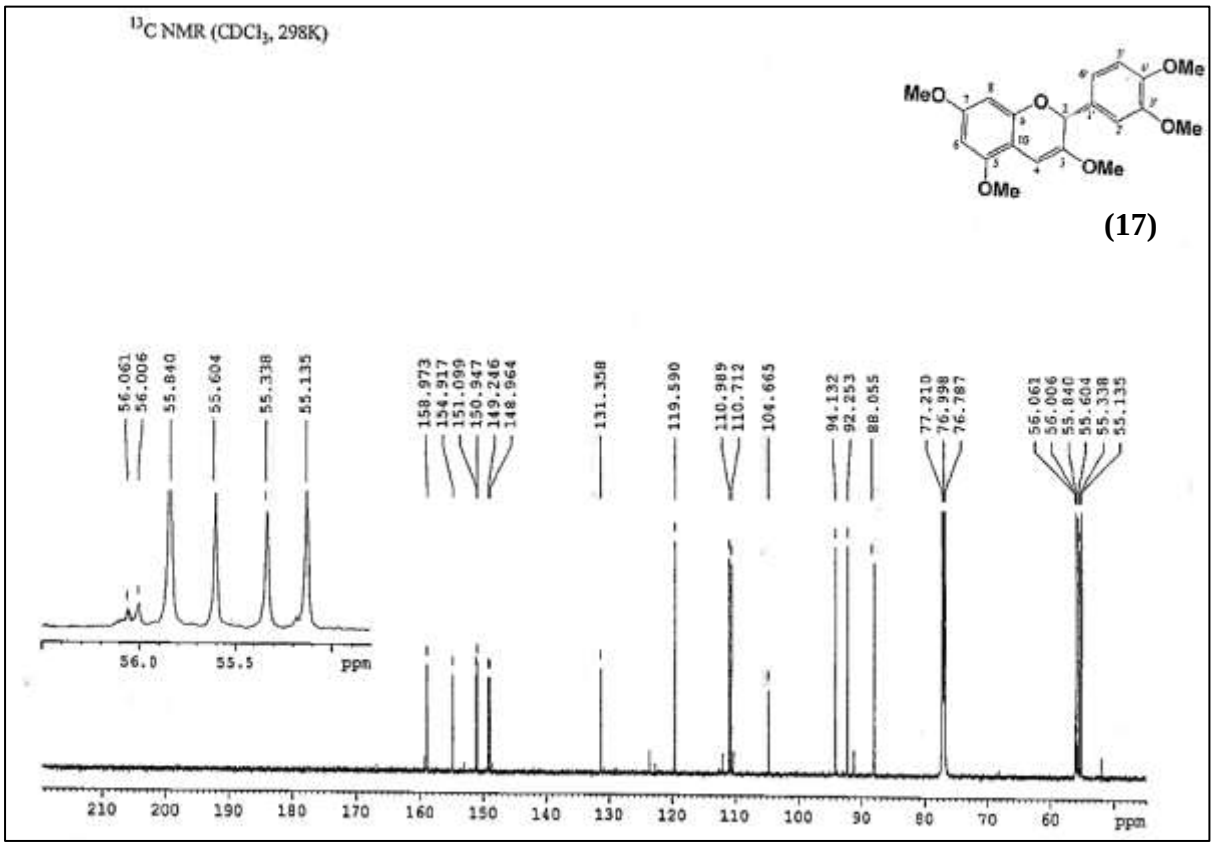


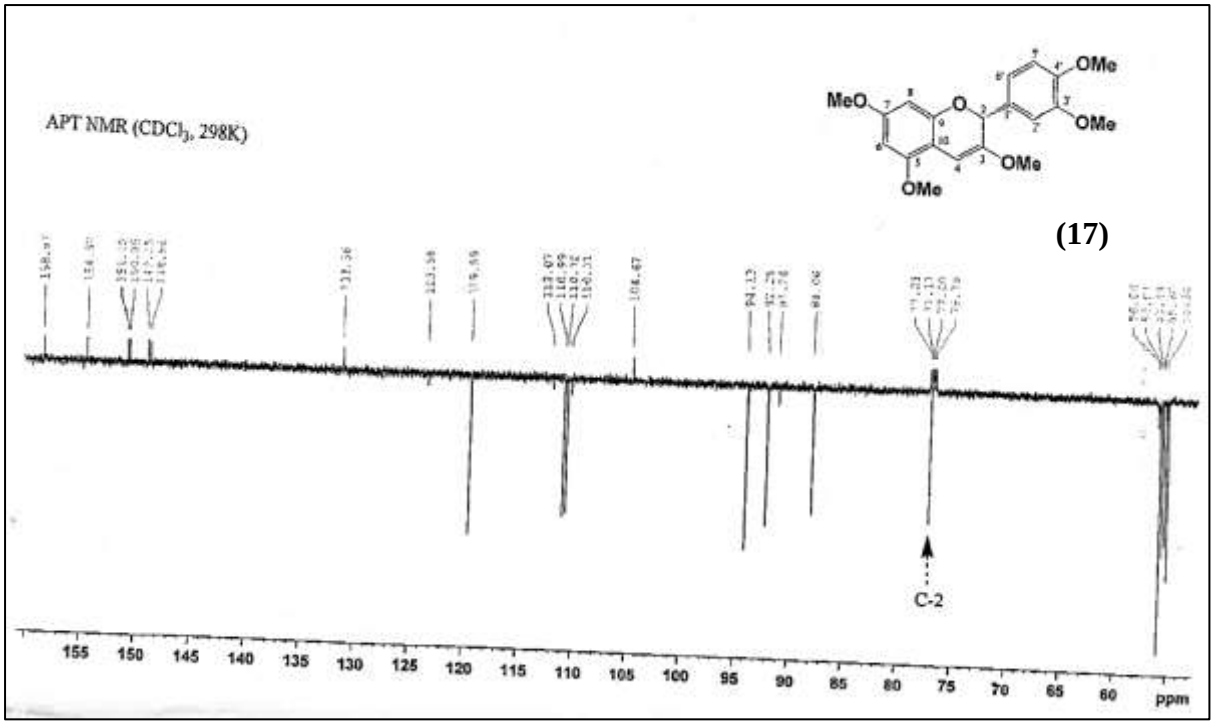
^{13}C NMR ($CDCl_3$, 298K)

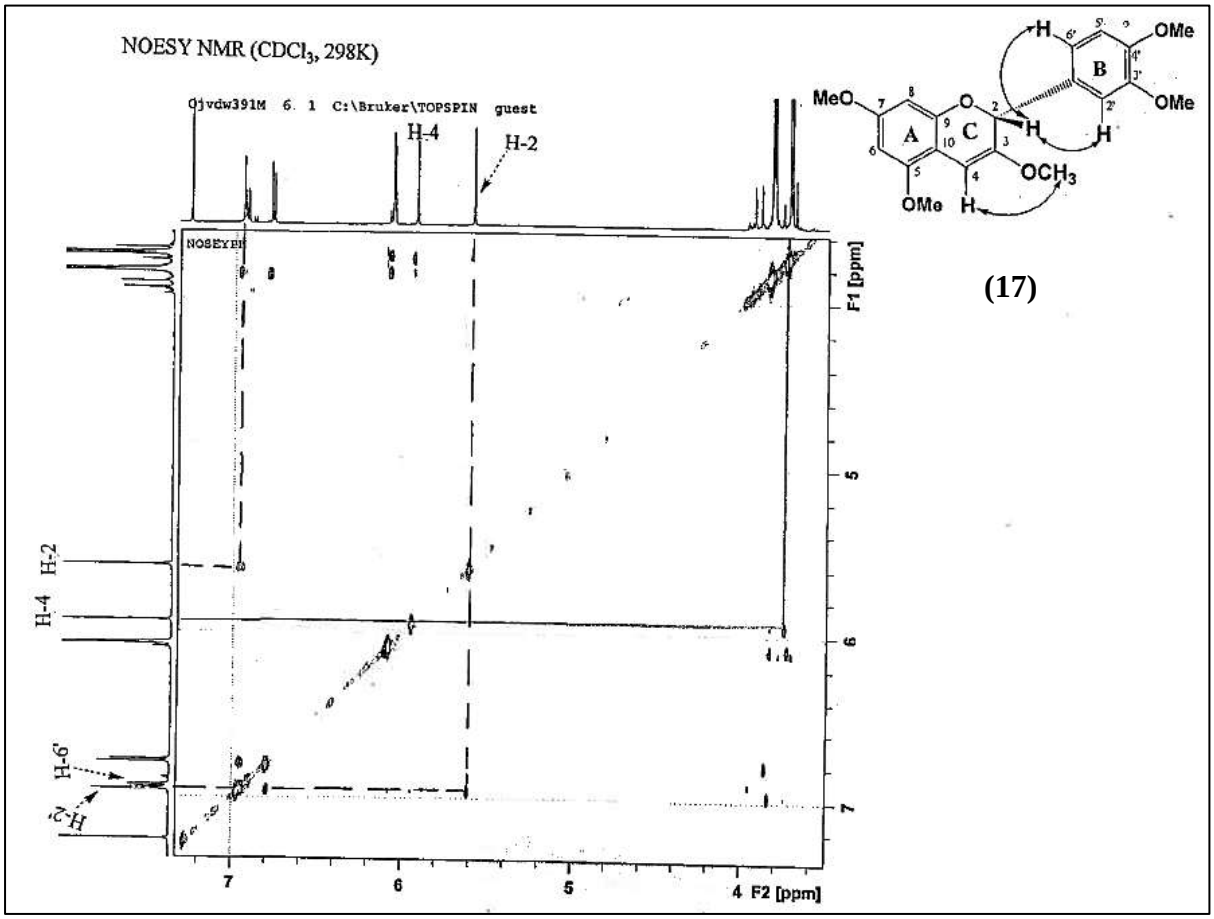

^{1}H NMR ($CdCl_3$, 298K)
BnO
OBn
OBn
OBn
O
O
(15b)
22.4982
1.0716
2.0019
2.0000
2.1553
4.0588
1.0065
7
6
5
4
[ppm]

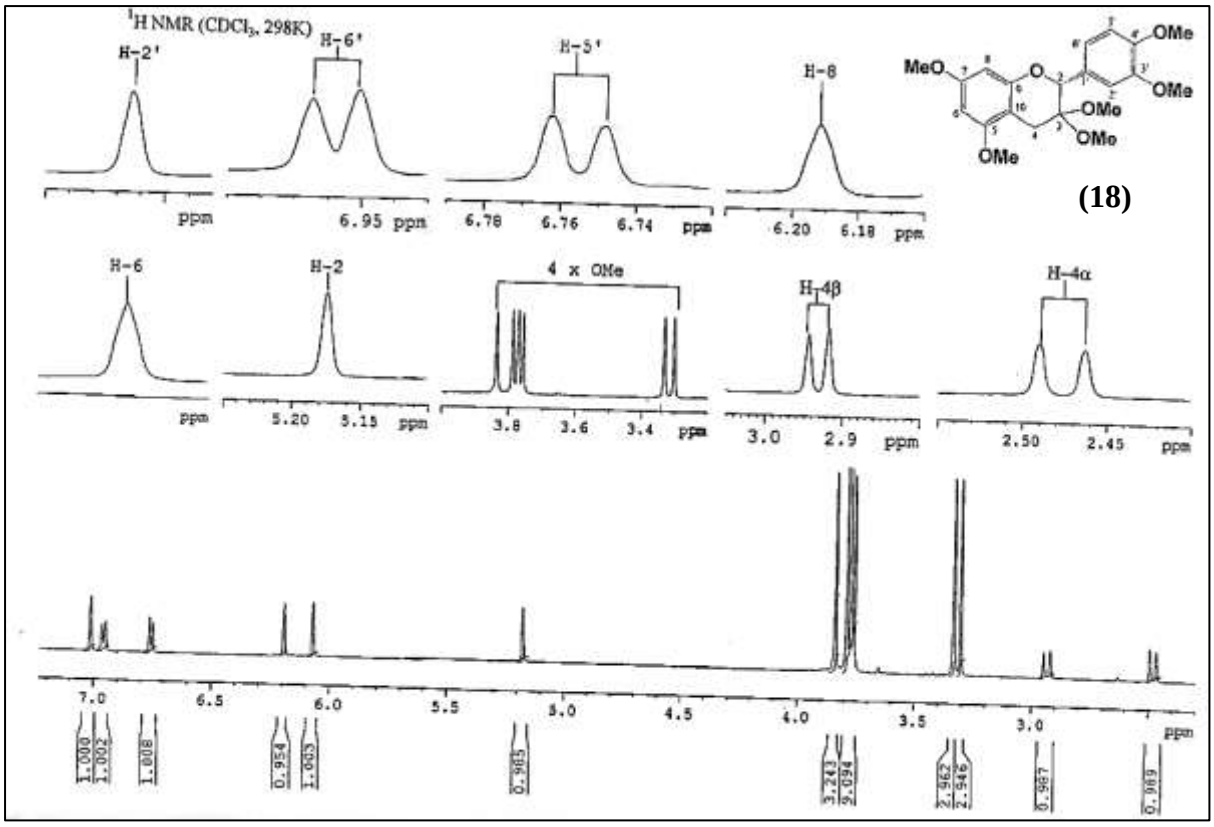

^{13}C NMR ($CDCl_3$, 298K
BnO
OBn
OBn
OBn
O
O
(15b)
200
150
100
50
0
[ppm]

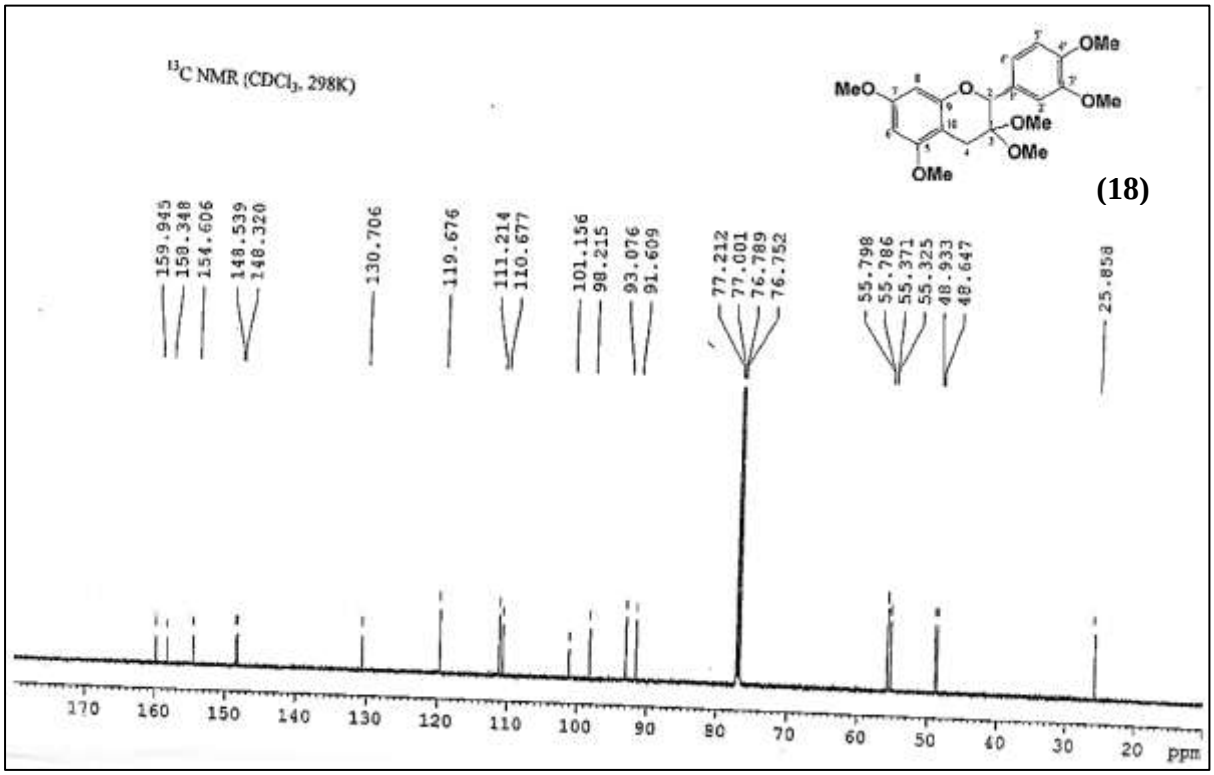

^{1}H NMR (CDCl$_3$, 298K)
H-2'
H-6'
H-5'
H-8
H-6
MeO
OMe
OMe
OMe
OMe
(17)
ppm
6.94
6.93
6.80
6.05
H-2
H-4
5X-OMe
5.7
5.6
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5

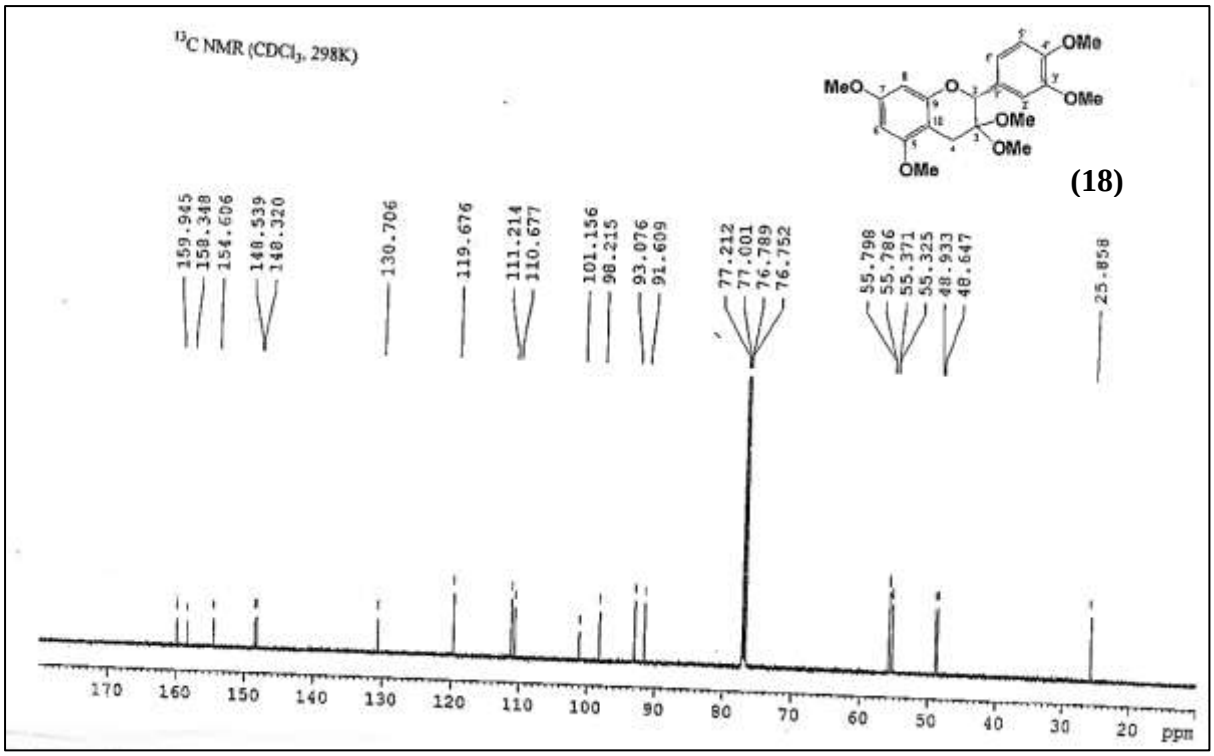

^{13}C NMR (CDCl$_3$, 298K)
MeO
OMe
OMe
OMe
OMe
(17)
56.061
56.006
55.840
55.604
55.338
55.135
158.973
154.917
151.099
150.947
149.246
148.964
131.358
119.590
110.989
110.712
104.665
94.132
92.253
88.055
77.210
76.998
76.787
56.0
55.5
ppm
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60

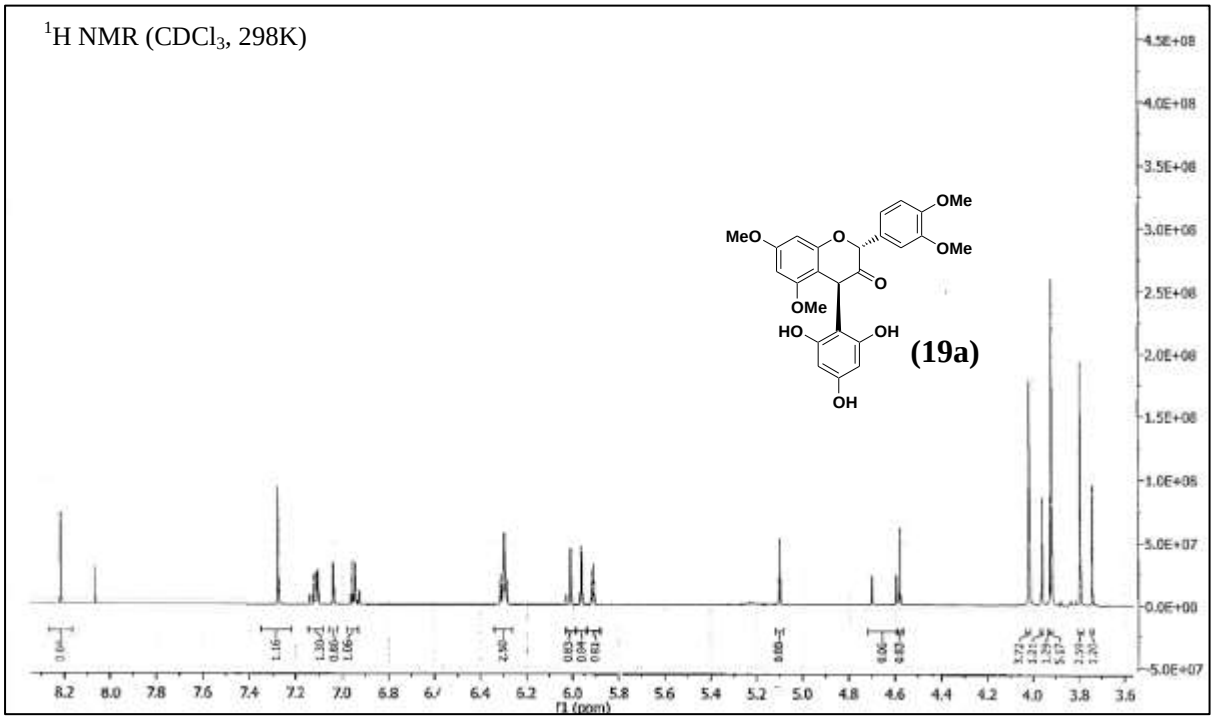

APT NMR (CDCl3, 298K)
MeO
OMe
OMe
OMe
OMe
(17)
C-2
155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 ppm


NOESY NMR (CDCl3, 298K)
Ojvdw391M 6. 1 C:\Bruker\TOPSPIN guest
H-4
H-2
NOESYPH
F1 [ppm]
H-2
H-4
H-6'
C-H
7
6
5
4 F2 [ppm]
MeO
OMe
OMe
OMe
OCH3
H
A
B
C
(17)

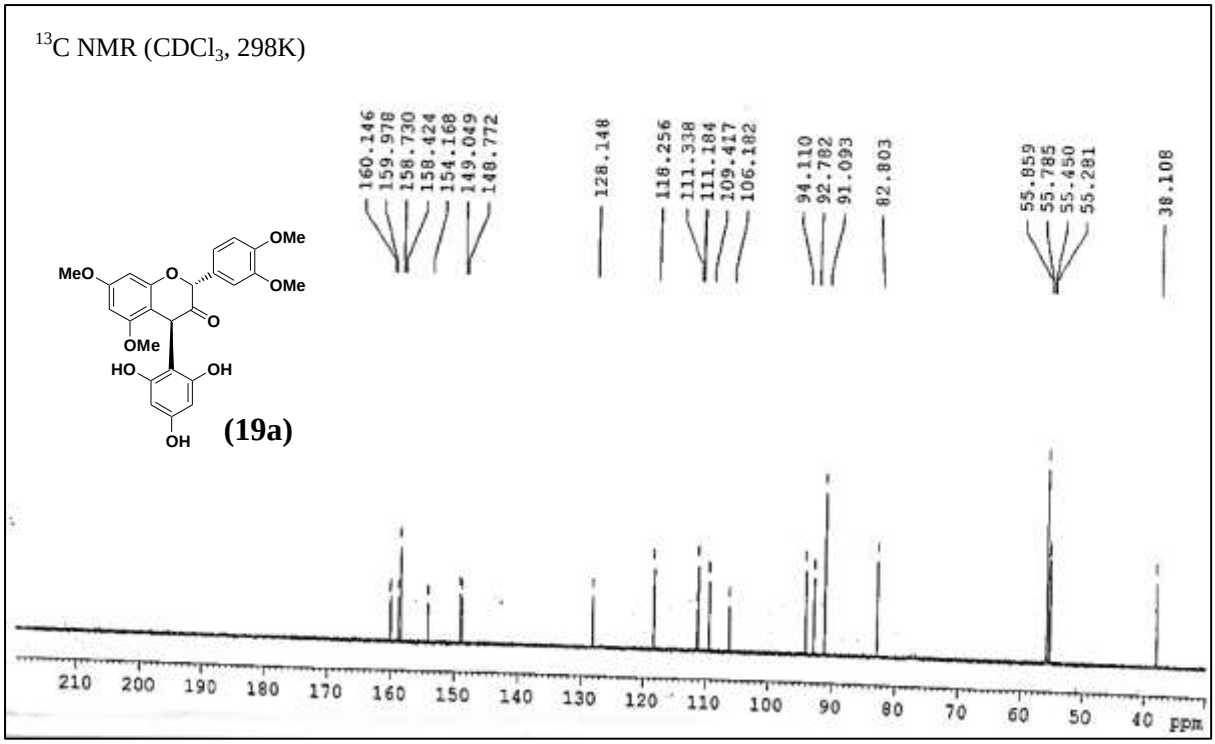

^{1}H NMR (CDCl$_3$, 298K)
H-2'
H-6'
H-5'
H-8
MeO
OMe
OMe
OMe
OMe
OMe
(18)
H-6
H-2
4 x OMe
H-4β
H-4α
ppm
6.95 ppm
6.78
6.76
6.74
6.20
6.18
5.20
5.15
3.8
3.6
3.4
3.0
2.9
2.50
2.45
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
1.000
1.002
1.008
0.954
1.003
0.985
3.241
9.094
2.962
2.946
0.967
0.989


^{13}C NMR (CDCl$_3$, 298K)
MeO
OMe
OMe
OMe
OMe
OMe
(18)
159.945
158.348
154.606
148.539
148.320
130.706
119.676
111.214
110.677
101.156
98.215
93.076
91.609
77.212
77.001
76.789
76.752
55.798
55.786
55.371
55.325
48.933
48.647
25.858
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


13C NMR (CDCl3, 298K)
MeO
OMe
OMe
OMe
OMe
(18)
159.945
158.348
154.606
140.539
140.320
130.706
119.676
111.214
110.677
101.156
98.215
93.076
91.609
77.212
77.001
76.789
76.752
55.798
55.786
55.371
55.325
48.933
48.647
25.858
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

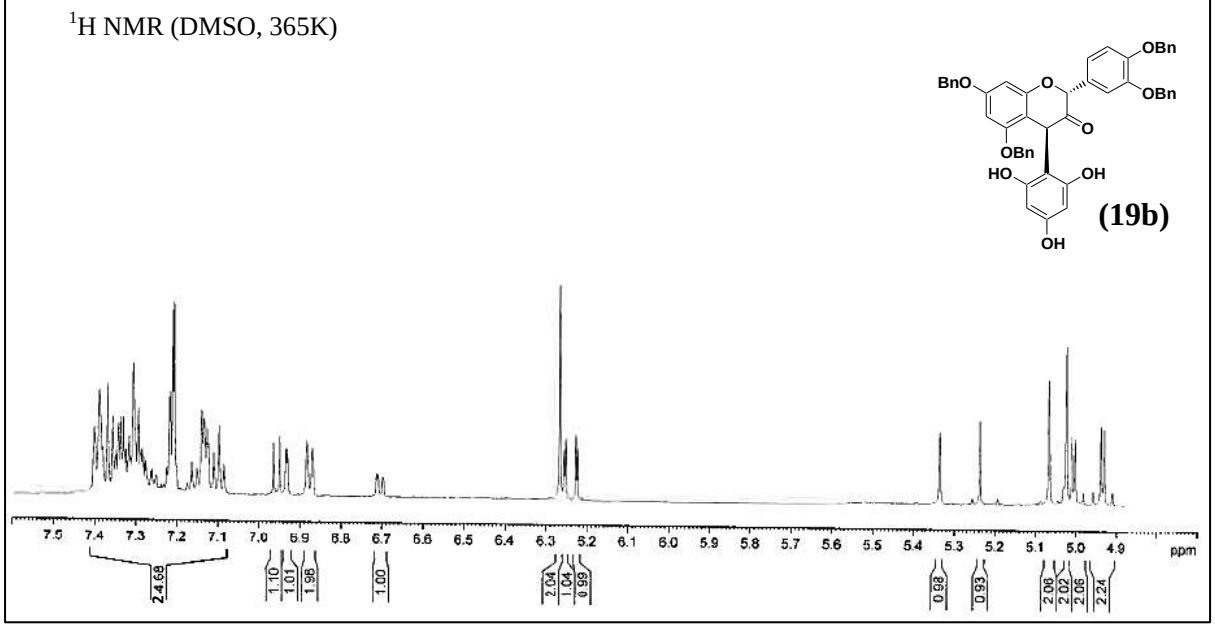

1H NMR (CDCl3, 298K)
MeO
OMe
OMe
OMe
O
HO
OH
OH
(19a)
8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6

^{13}C NMR ($CDCl_3$, 298K)



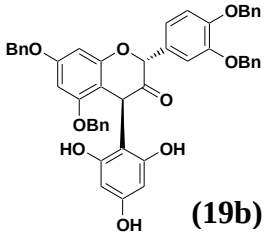
(19a)

^{1}H NMR (DMSO, 365K)

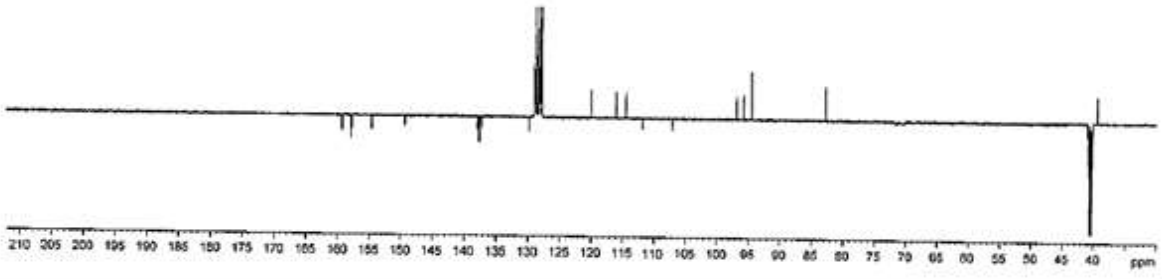


(19b)

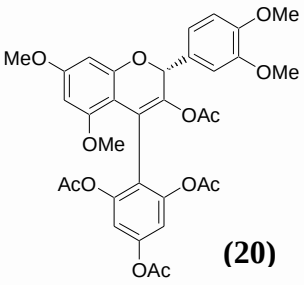
^{13}C APT-NMR (DMSO, 365K)



(19b)

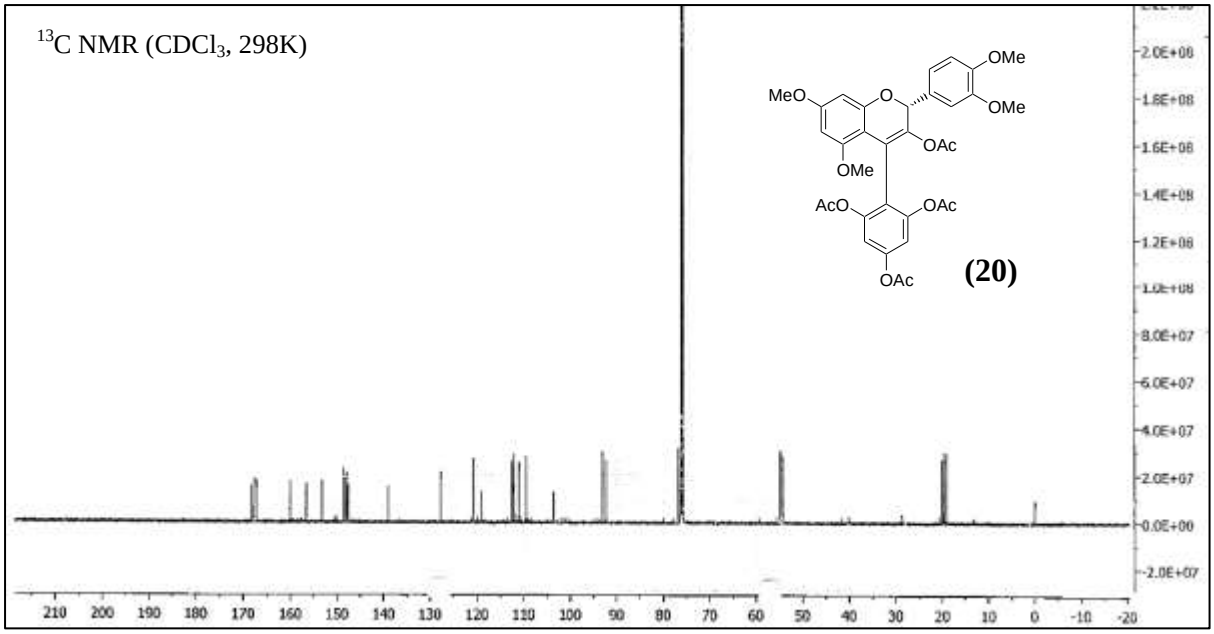


^{1}H NMR (acetone, 298K)

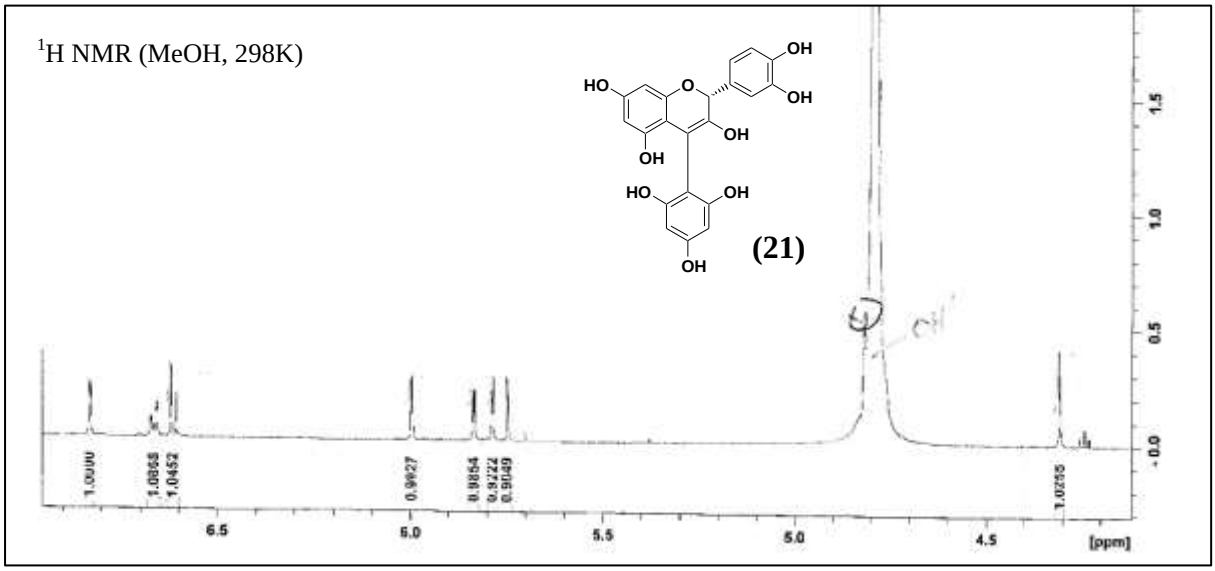


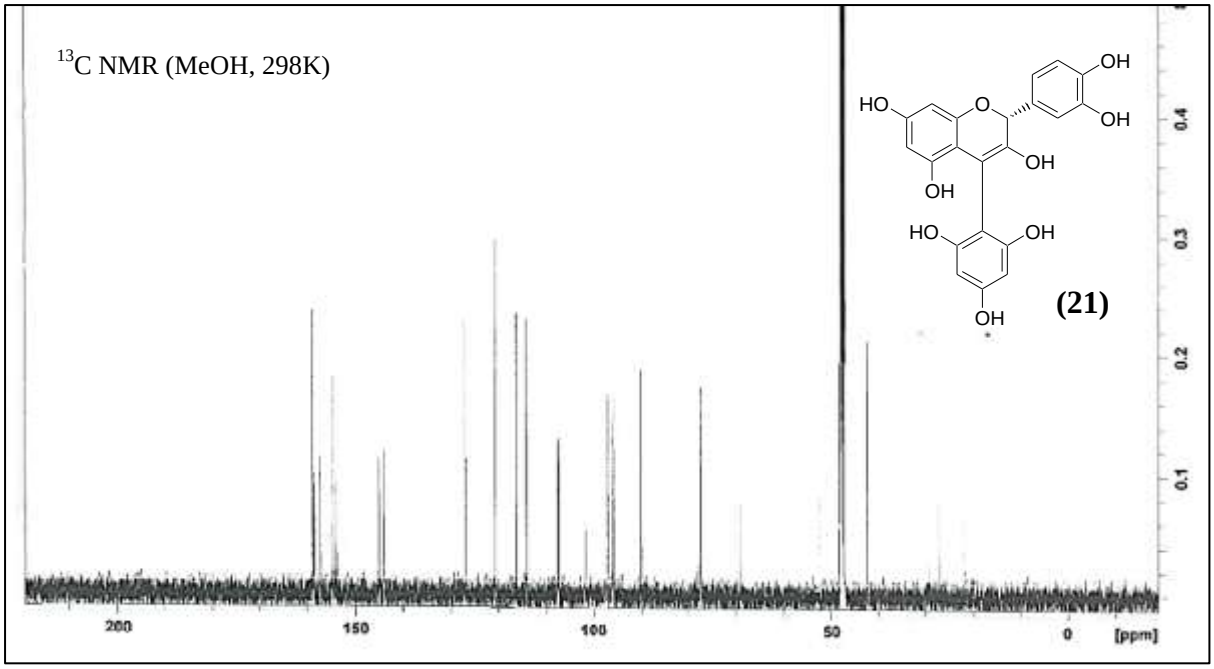
(20)

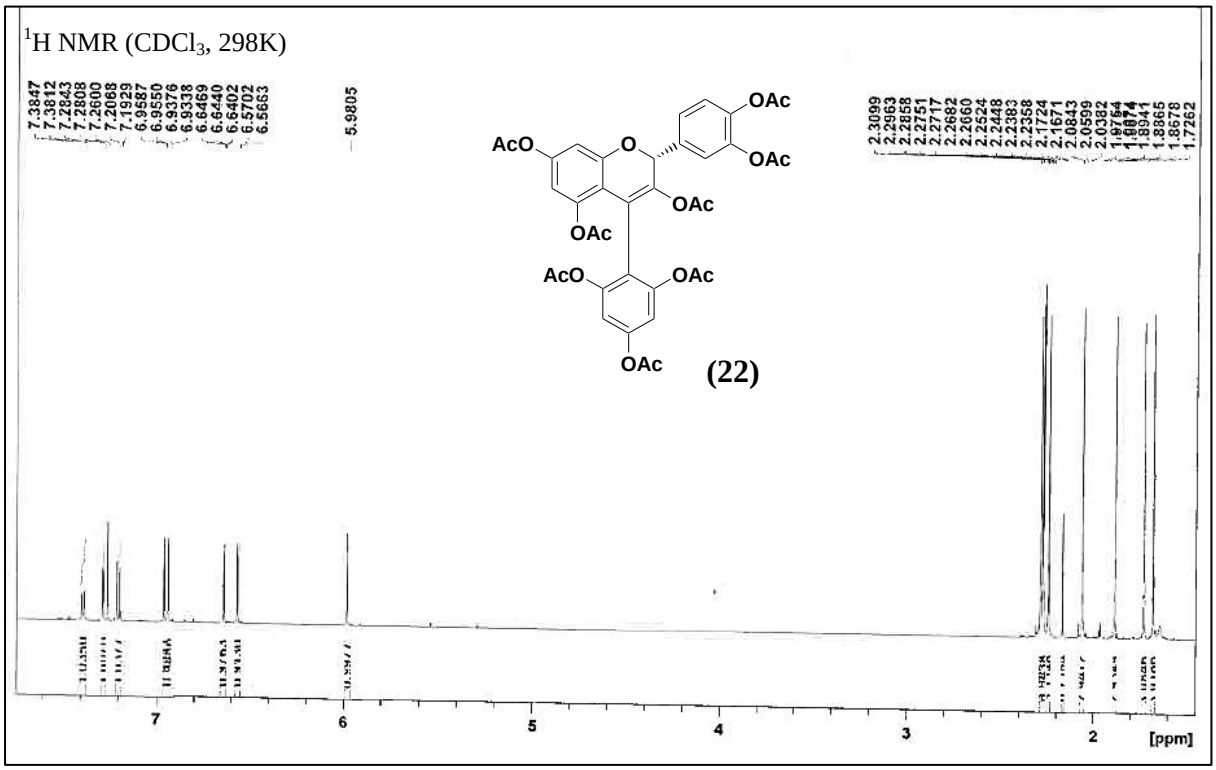
^{13}C NMR ($CDCl_3$, 298K)



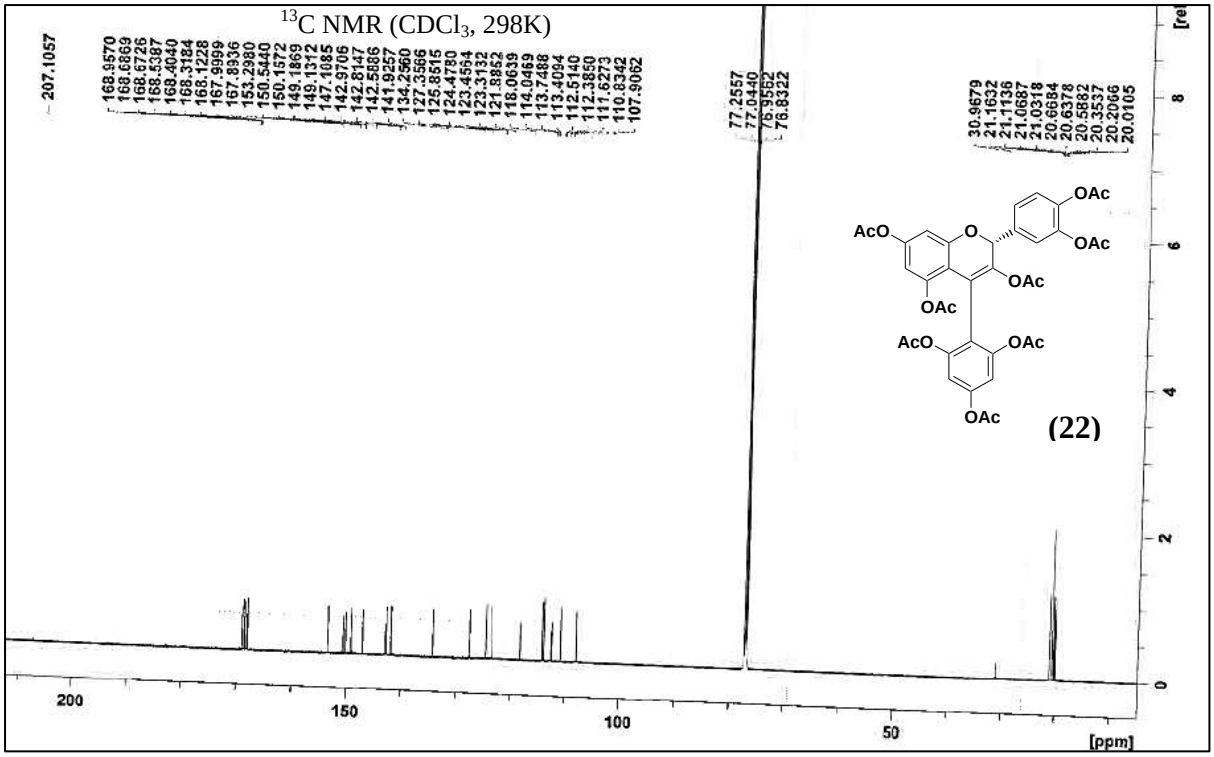
^{1}H NMR (MeOH, 298K)



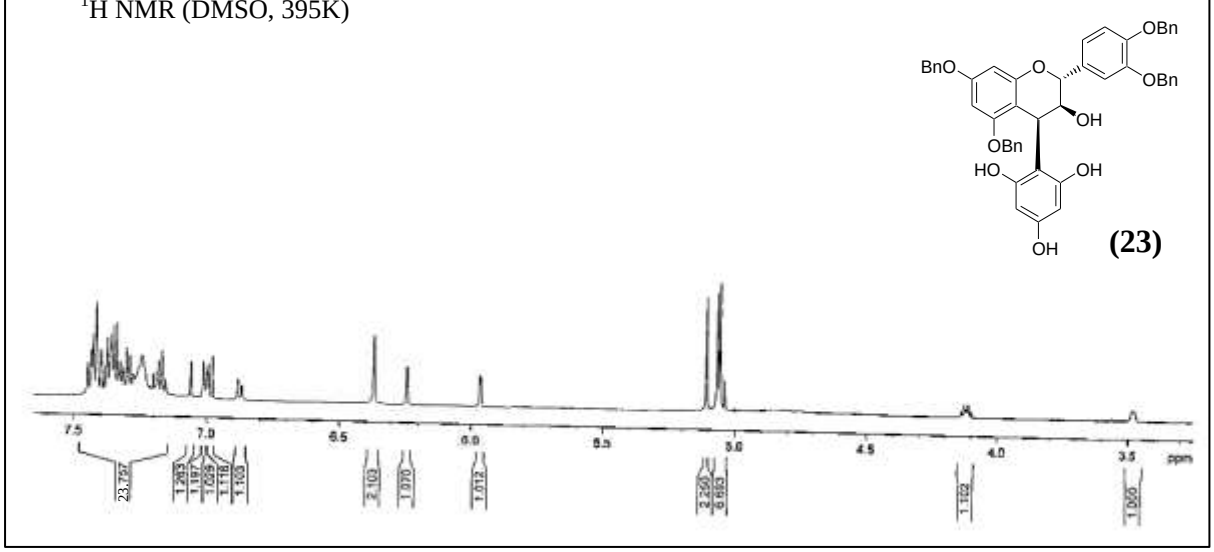

13C NMR (MeOH, 298K)
HO
O
OH
OH
OH
OH
HO
OH
OH
(21)
200
150
100
50
0
[ppm]
0.1
0.2
0.3
0.4


1H NMR (CDCl3, 298K)
7.3847
7.3612
7.2843
7.2808
7.2600
7.2068
7.1929
6.9587
6.9550
6.9376
6.9338
6.6469
6.6440
6.6402
6.5702
6.5663
5.9805
2.3099
2.2963
2.2858
2.2751
2.2717
2.2682
2.2660
2.2524
2.2448
2.2383
2.2358
2.1724
2.1671
2.0843
2.0599
2.0382
1.8941
1.8865
1.8678
1.7262
AcO
O
OAc
OAc
OAc
OAc
AcO
OAc
OAc
(22)
7
6
5
4
3
2
[ppm]

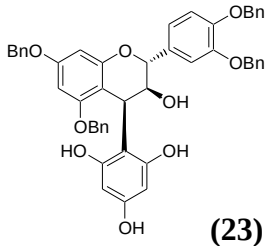
^{13}C NMR ($CDCl_3$, 298K)



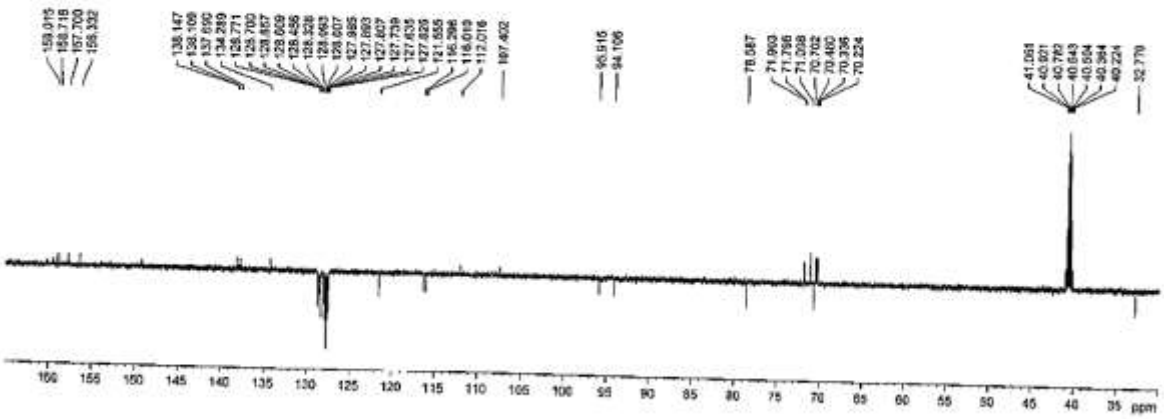
^{1}H NMR (DMSO, 395K)



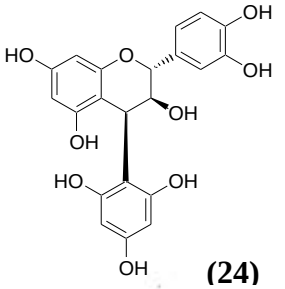
APT ^{13}C NMR (DMSO, 395K)



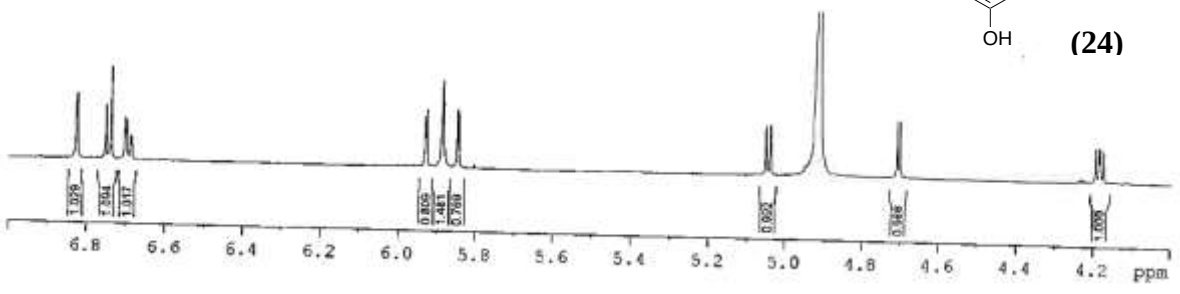
(23)



^{1}H NMR (MeOH, 295K)



(24)



^{13}C NMR (MeOH, 295K)