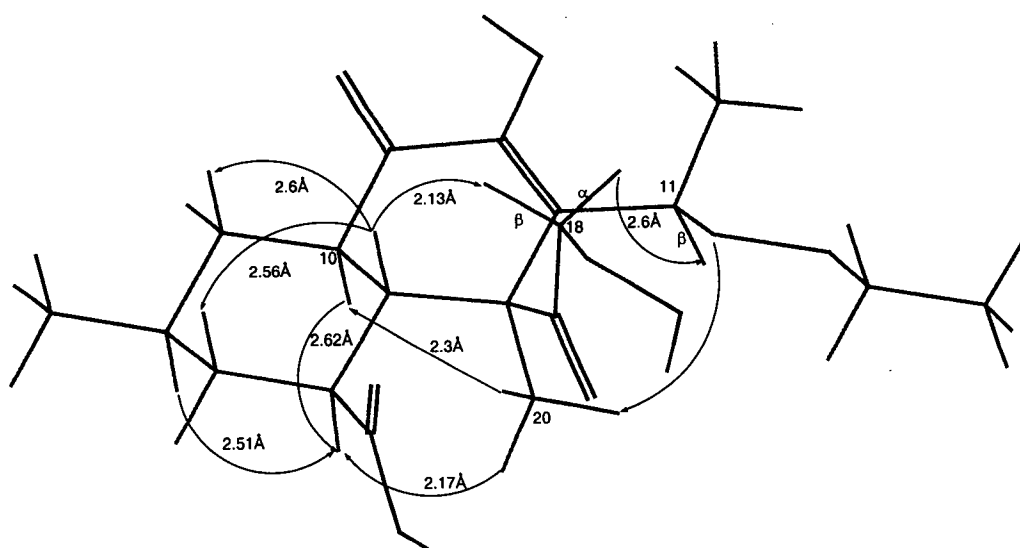


Table 1: ^1H (500 MHz) and ^{13}C (125 MHz) NMR assignments of cytosporic acid (1) in $\text{C}_5\text{D}_5\text{N}$

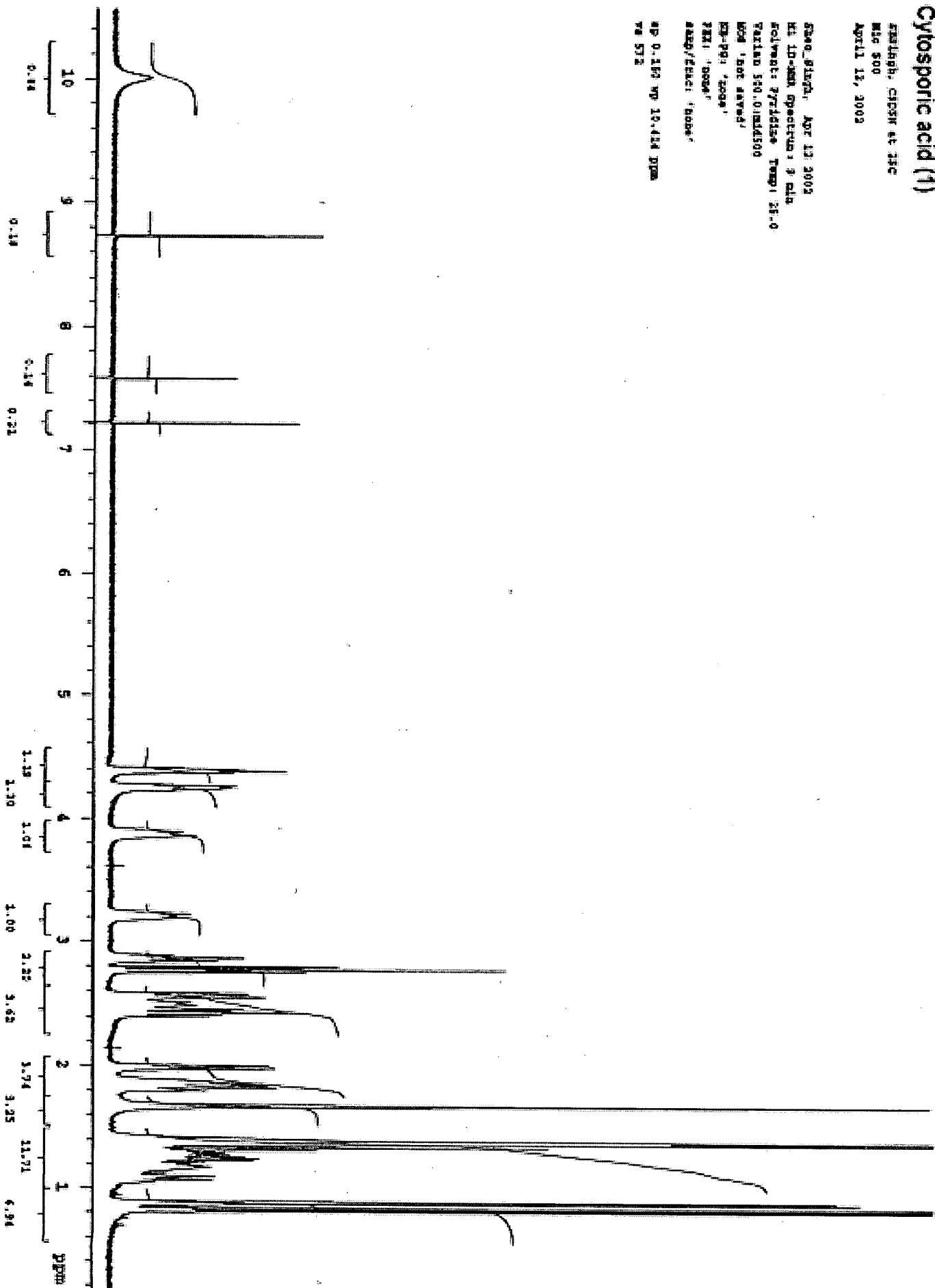
Position	δ_{C}	mult	δ_{H}	HMBC (C $\rightarrow$ H)
1	194.9	C°		H-10
2	146.4	C°		
3	137.9	C°		H-12, H-16, H-20
4	58.6	C°		H-5, H-20
5	42.8	CH	2.86, brt, $J = 11.5$	H-6, H-10, H-20
6	47.6	CH	2.78, dt, $J = 3.5, 11.5$	H-5
7	40.1	CH_2	H_{ax} : 1.99, brd, $J = 10$ H_{eq} : 1.37, m	H-5, H-6, H-21
8	30.9	CH	1.38, m	H-21
9	35.0	CH_2	H_{ax} : 2.56, brd, $J = 13.5$ H_{eq} : 1.06, m	H-21, H-10
10	43.3	CH	2.43, dt, $J = 4.0, 12.5$	H-9
11	36.5	CH	1.86, m	H-16
12	34.7	CH_2	1.83, m 2.50, m	H-11, H-16
13	31.4	CH_2	1.17, m	H-14, H-15
14	23.1	CH_2	1.26, m	H-15
15	14.3	CH_3	0.82, t, $J = 7.0$	H-13, H-14
16	18.1	CH_3	1.37, d, $J = 6.5$	H-11
17	211.3	C°		H-5, H_2 -18, H_2 -19, H-20
18	42.1	CH_2	H_{α} : 3.23, brm H_{β} : 3.86, brm	H_2 -19
19	58.2	CH_2	4.26, brm 4.40, brm	H_2 -18
20	14.7	CH_3	1.67, s	H-5
21	22.2	CH_3	0.88, d, $J = 6.0$	
22	177.5	C°		H-6

Figure 1: ChemDraw 3D model of cytosporic acid (1). Arrows denoting selected NOESY correlations in $\text{C}_5\text{D}_5\text{N}$. Hydrogens on C-12, C-13 and C-19 have been omitted for clarity.

Cytosporic acid (1)

Sample: C100H at 25C
MS: 500
April 15, 2003

Chem. Shift: Apr 13, 2003
H₁ 1D-NMR Spectrum: 300 MHz
Solvent: Pyridine-d₅ Temp: 25.0
Pulse: zgpg30-01m14500
NS: 1600 scans
PC: 100%
RG: 100%
AQ: 0.163 s
FID: 10.000 V
WDW: EM
GB: 0.163 s
TE: 300.2 K
AQ: 0.163 s
WDW: EM
GB: 0.163 s
TE: 300.2 K



Cytosporic acid (1)

Carbon-13 NMR Spectrum
Varian Unity500
Solvent: Pyridine Temp: 25.0
Reference: Jayasuriya, Jan 16 99

