

ANEXO I

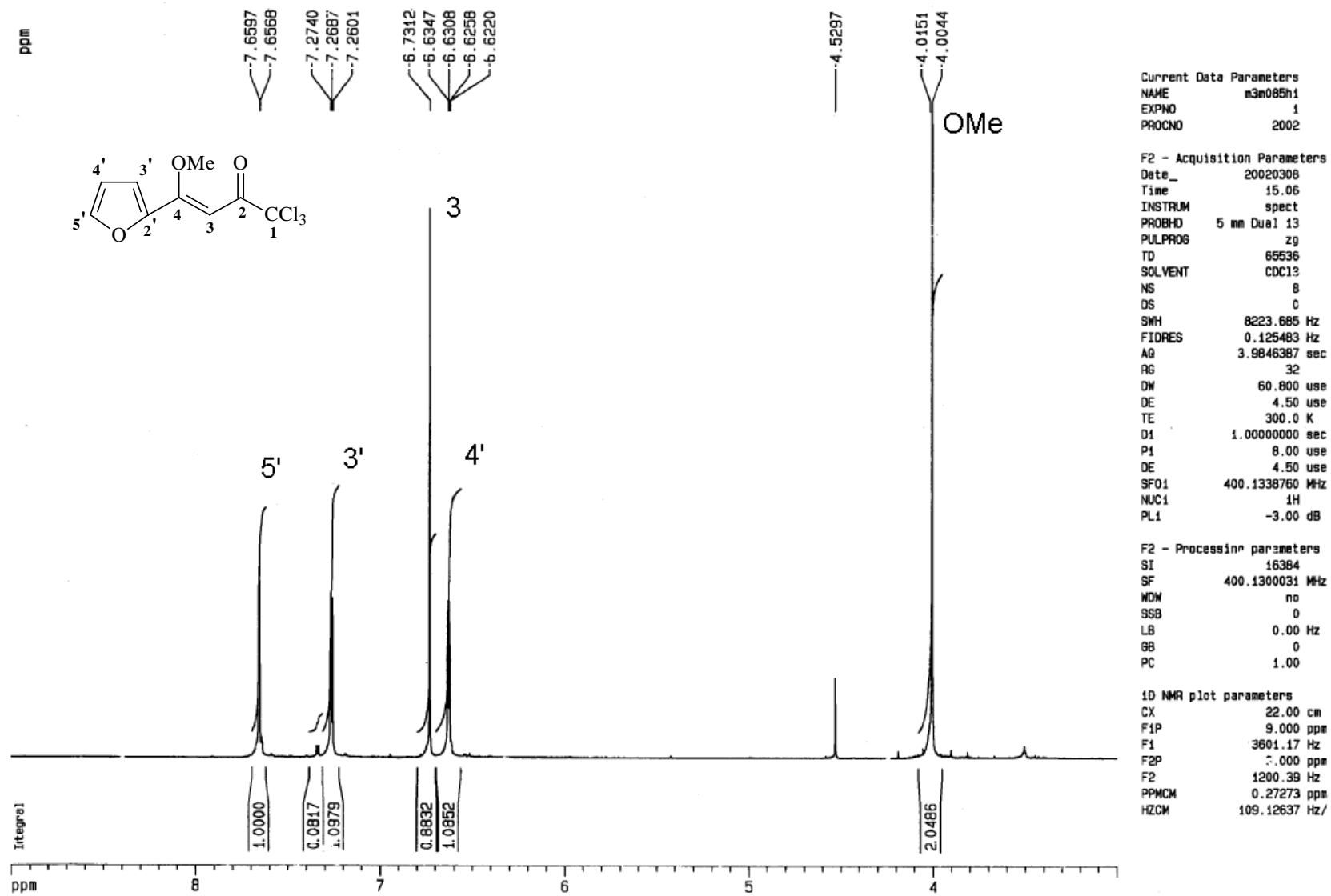


Figura 5. Espectro de RMN (a) ^1H da 1,1,1-Tricloro-4-[2-furil]-4-metoxi-3-buten-2-ona (**2a**) em CDCl_3 .

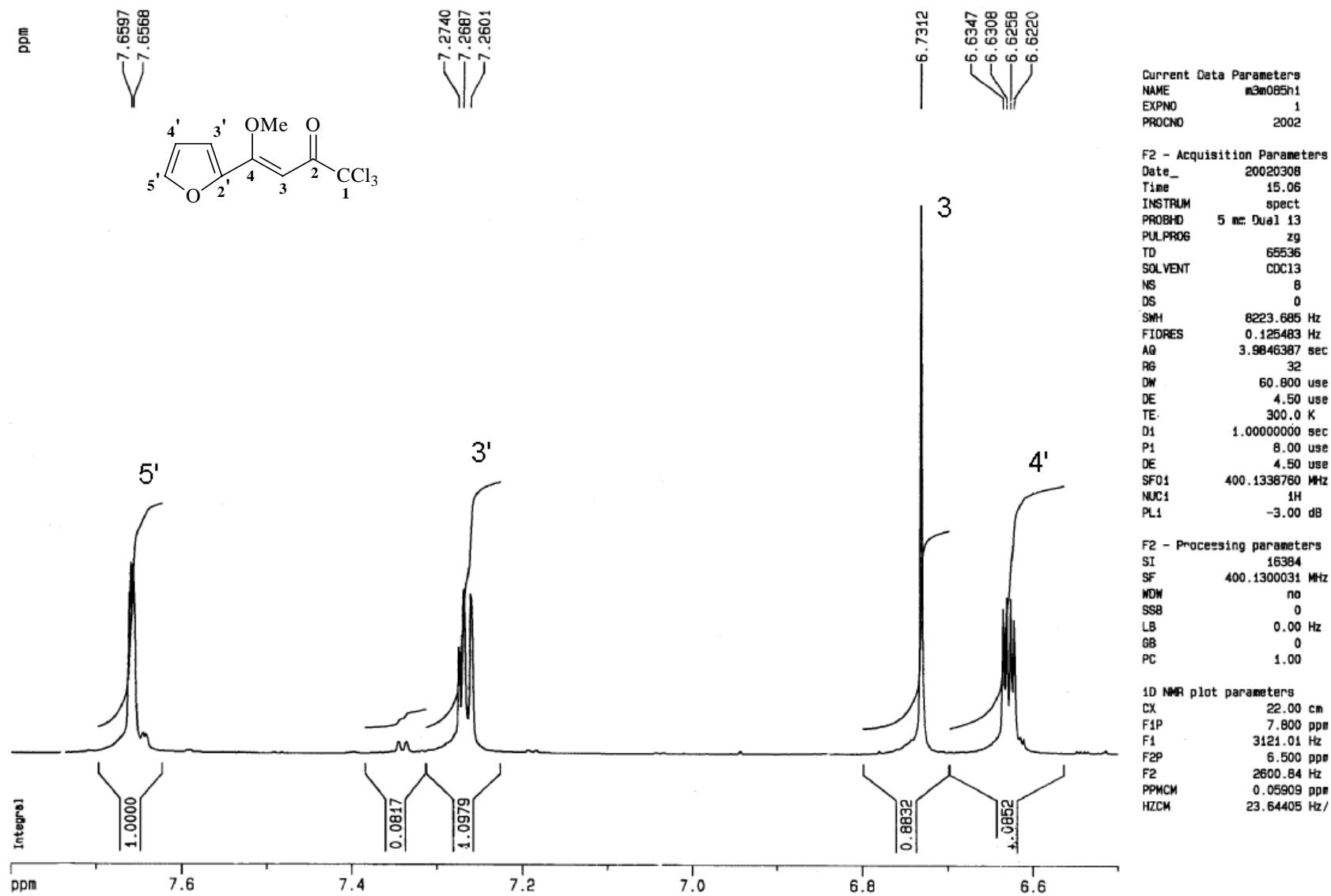


Figura 6. Espectro de ^1H , da 1,1,1-Tricloro-4-[2-furil]-4-metoxi-3-buten-2-ona (**2a**) em CDCl_3 .

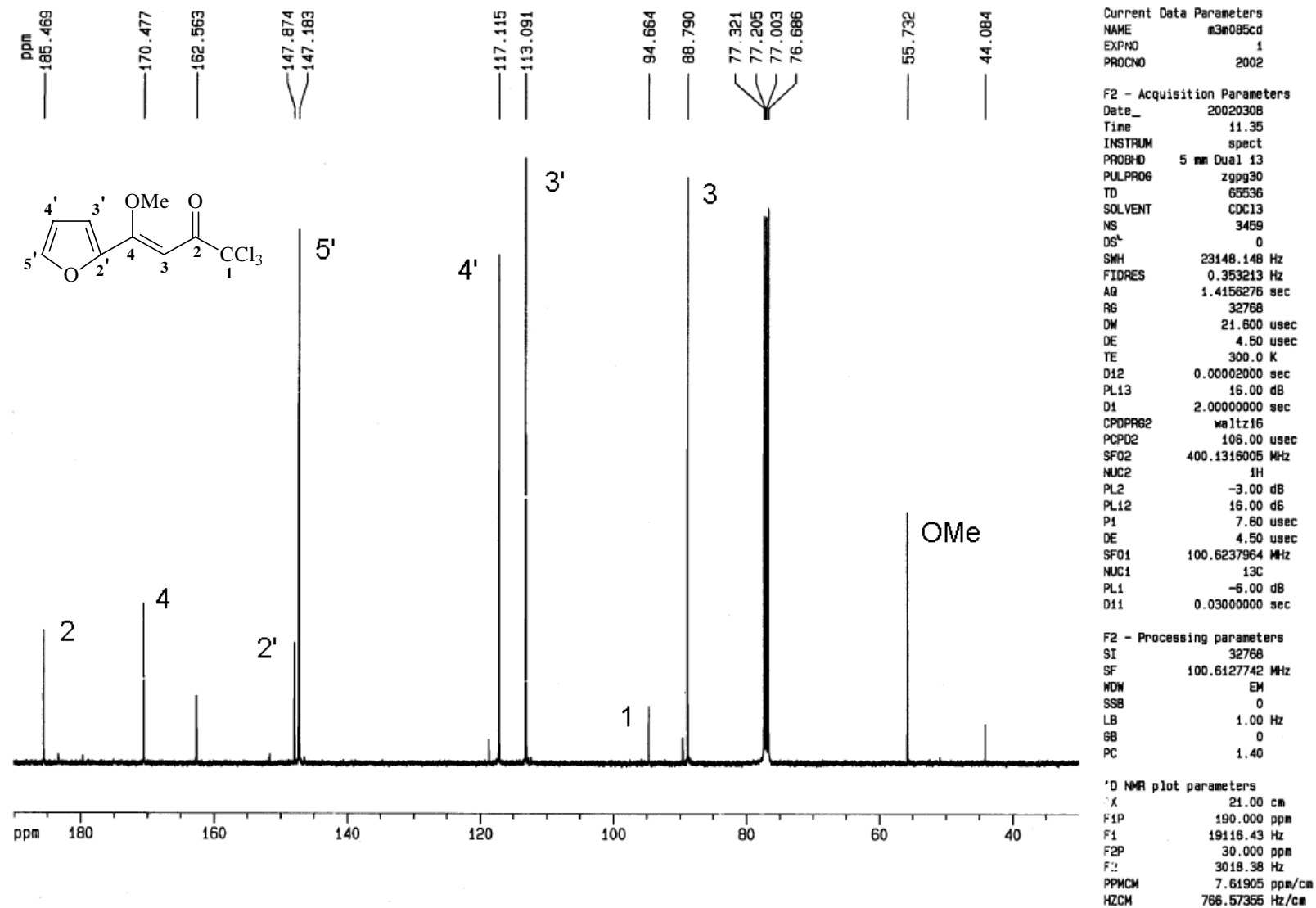


Figura 7. Espectros de RMN ¹³C do 1,1,1-tricloro-4-[2-furil]-4-metoxi-3-buten-2-ona (**2a**) em CDCl₃.

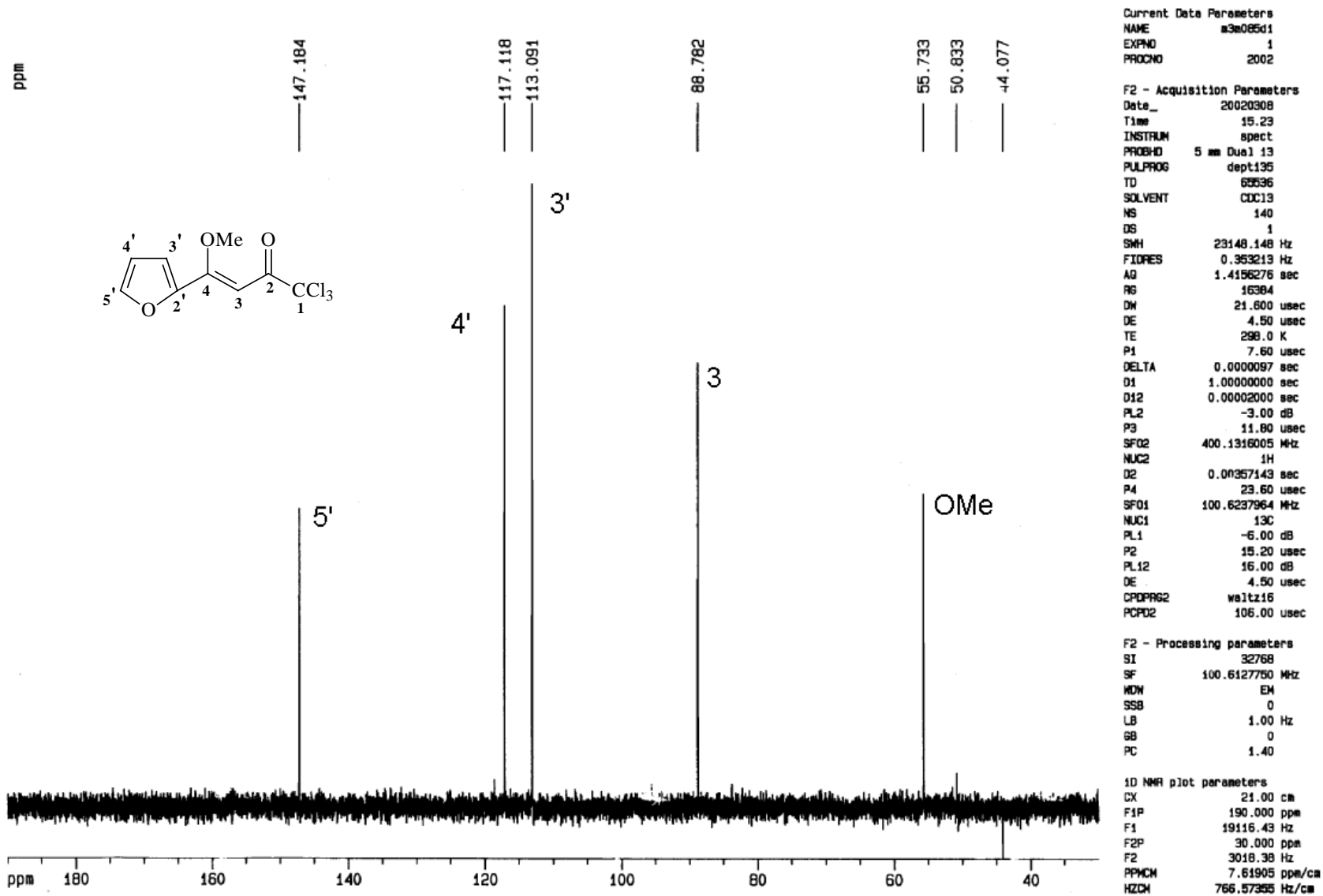


Figura 8. Espectros de RMN DEPT 135 do 1,1,1-tricloro-4-[2-furil]-4-metoxi-3-buten-2-ona (2a) em CDCl₃.

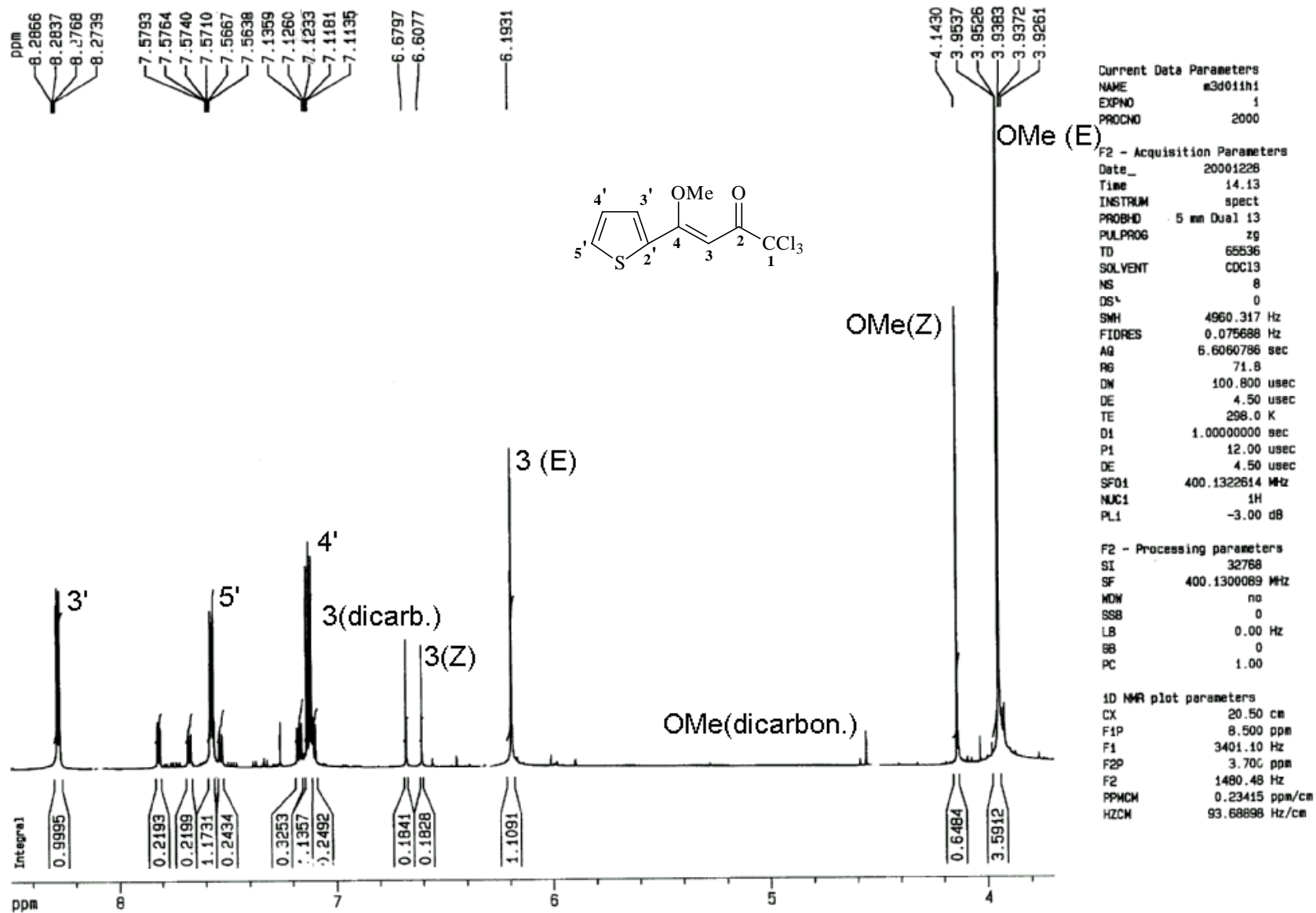


Figura 9. Espectros de RMN ^1H do 1,1,1-tricloro-4-metoxi-4-[2-tienil]-3-buten-2-ona (**2b**) em CDCl_3 .

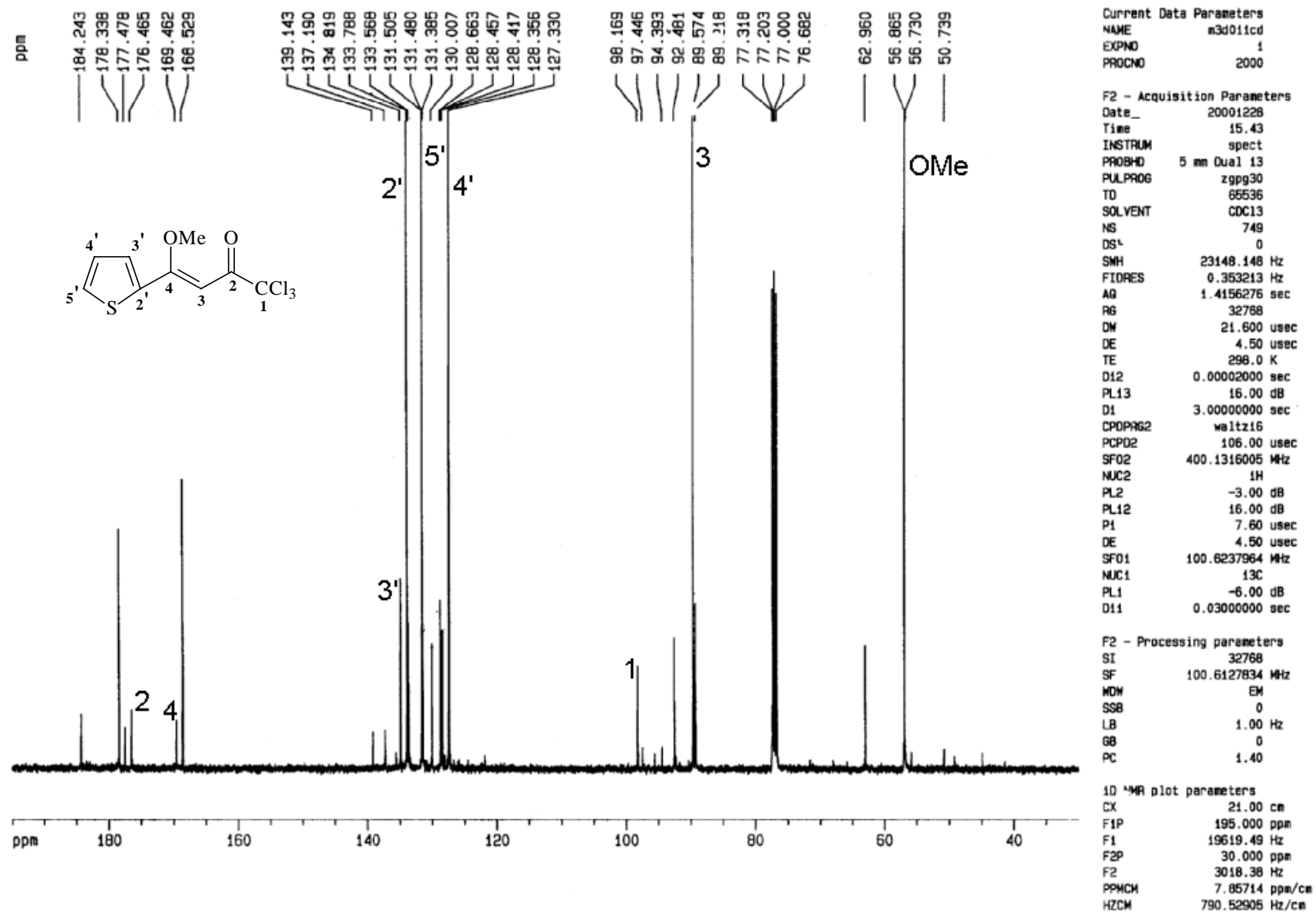


Figura 10. Espectros de RMN $^{13}\text{C}\{^1\text{H}\}$ do 1,1,1-tricloro-4-metoxi-4-[2-tienil]-3-buten-2-ona (**2b**) em CDCl_3 .

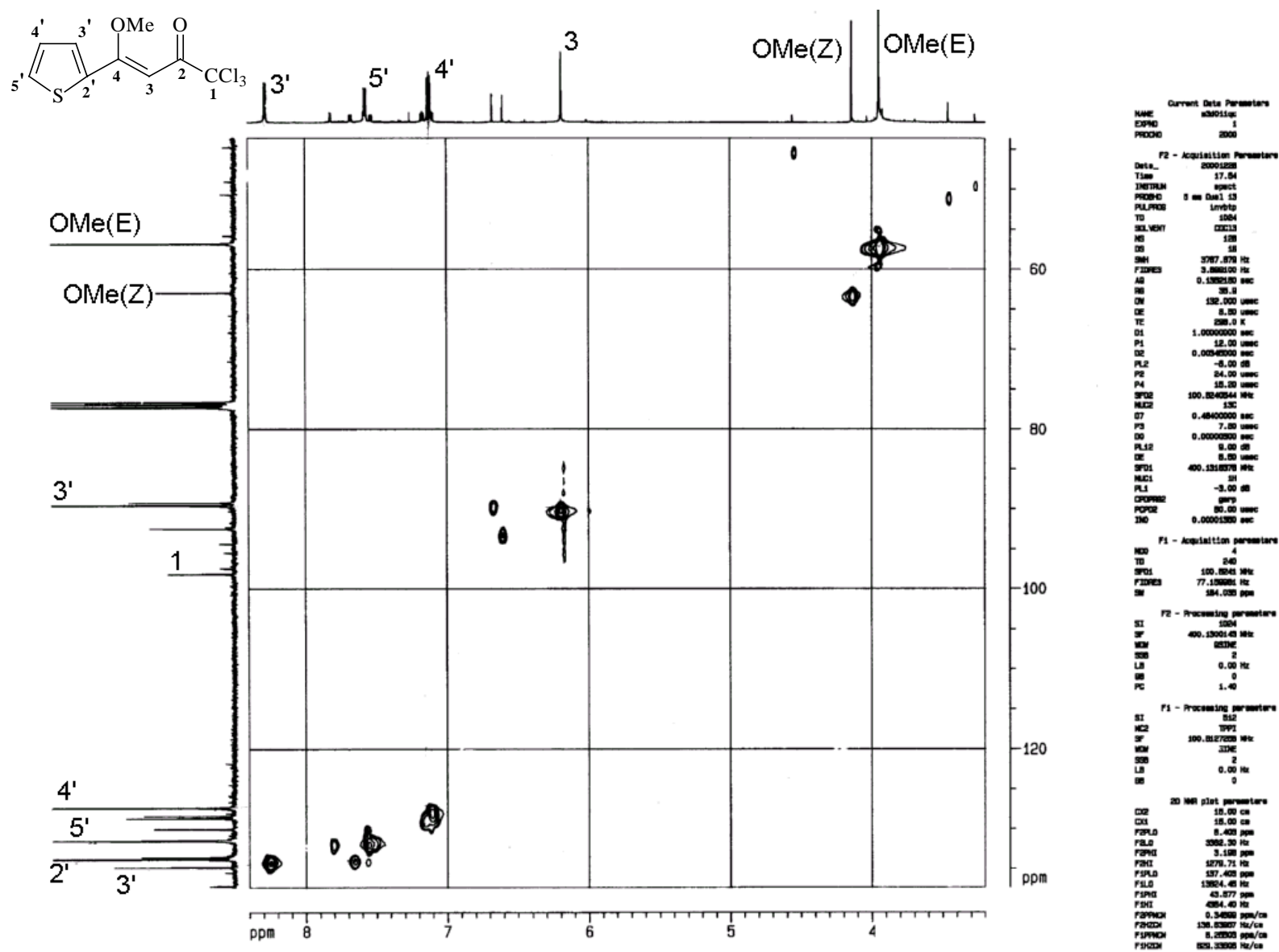
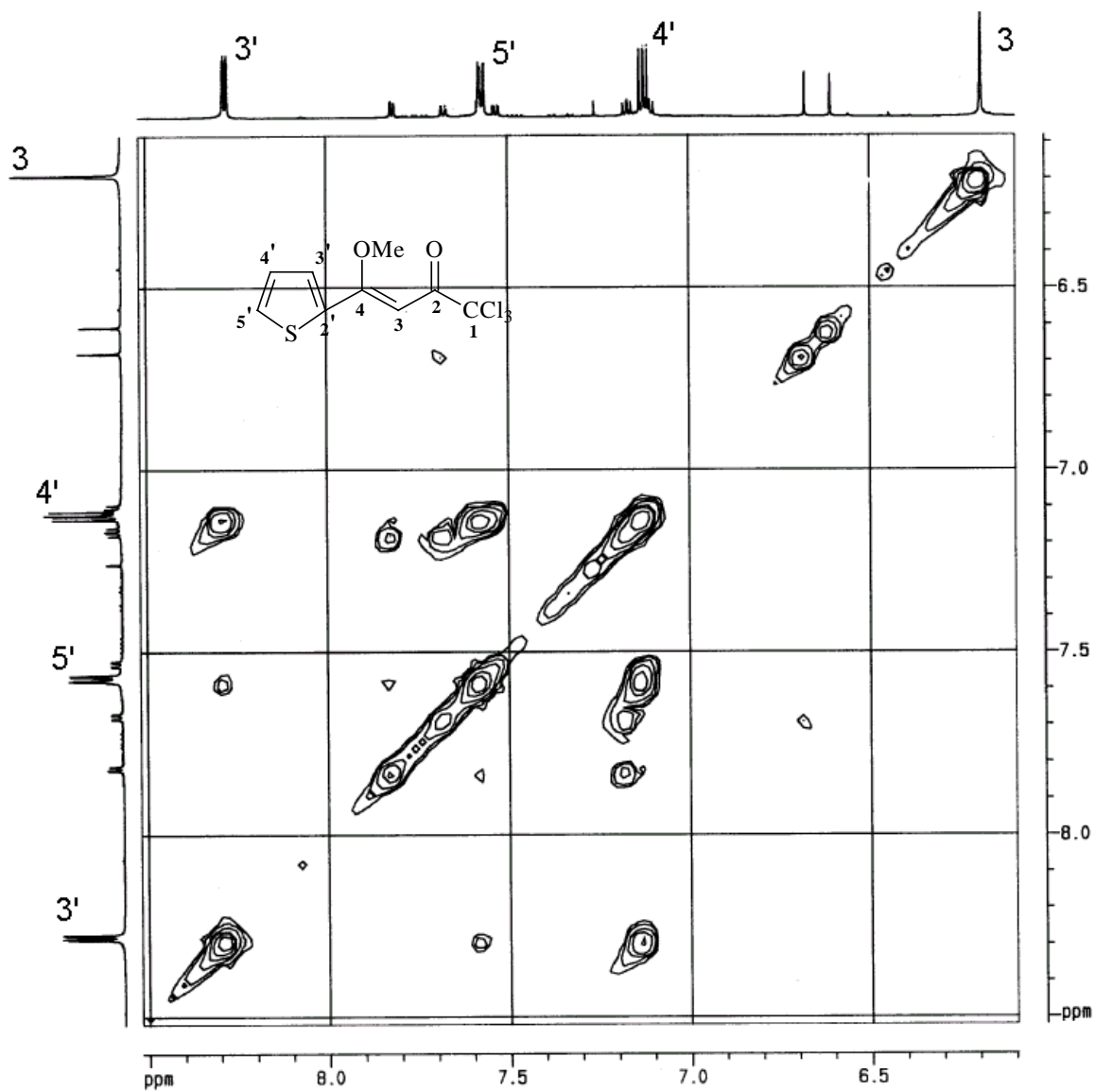


Figura 11. Espectros de RMN correlação C-H (HMQC) do 1,1,1-tricloro-4-metoxi-4-[2-tienil]-3-buten-2-ona (2b) em CDCl₃.



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Current Data Parameters
NAME      a3001sh
EXPNO     1
PROCNO    2000

F2 - Acquisition Parameters
Date_     20001228
Time      14.51
INSTRUM   spect
PROBHD    5 mm Dsl 13
PULPROG   coesy45
TD        1024
SOLVENT   CDCl3
NS         4
DS         16
SWH        3787.879 Hz
FIDRES     3.689100 Hz
AQ         0.1352180 sec
RG         64
CW         132.000 usec
DE         4.50 usec
TE         300.0 K
D1         1.00000000 sec
P1         12.00 usec
D0         0.00000300 sec
DE         4.50 usec
SFO1       400.1318378 MHz
NUC1       13C
PL1        -3.00 dB
IN0        0.00025400 sec

F1 - Acquisition parameters
ND0        1
TD         256
SFO1       400.1318 MHz
FIDRES     14.796483 Hz
SW         9.457 ppm

F2 - Processing parameters
SI         512
SF         400.1300051 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0
PC         1.00

F1 - Processing parameters
SI         512
MC2        OF
SF         400.1300035 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0

2D NMR plot parameters
CK2        15.00 ca
CK1        15.00 ca
F2PL0      8.519 ppm
F2L0       3408.35 Hz
F2PH1      6.796 ppm
F2H1       2436.30 Hz
F1PL0      8.522 ppm
F1L0       3410.00 Hz
F1PH1      6.052 ppm
F1H1       2439.51 Hz
F2PPMCH    0.16147 ppm/ca
F2HZCH     64.61093 Hz/ca
F1PPMCH    0.16271 ppm/ca
F1HZCH     65.10439 Hz/ca

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Figura 12. Espectro de RMN correlação H-H (COSY 45) do 1,1,1-tricloro-4-metoxi-4-[2-tienil]-3-buten-2-ona (**2b**) em CDCl₃.

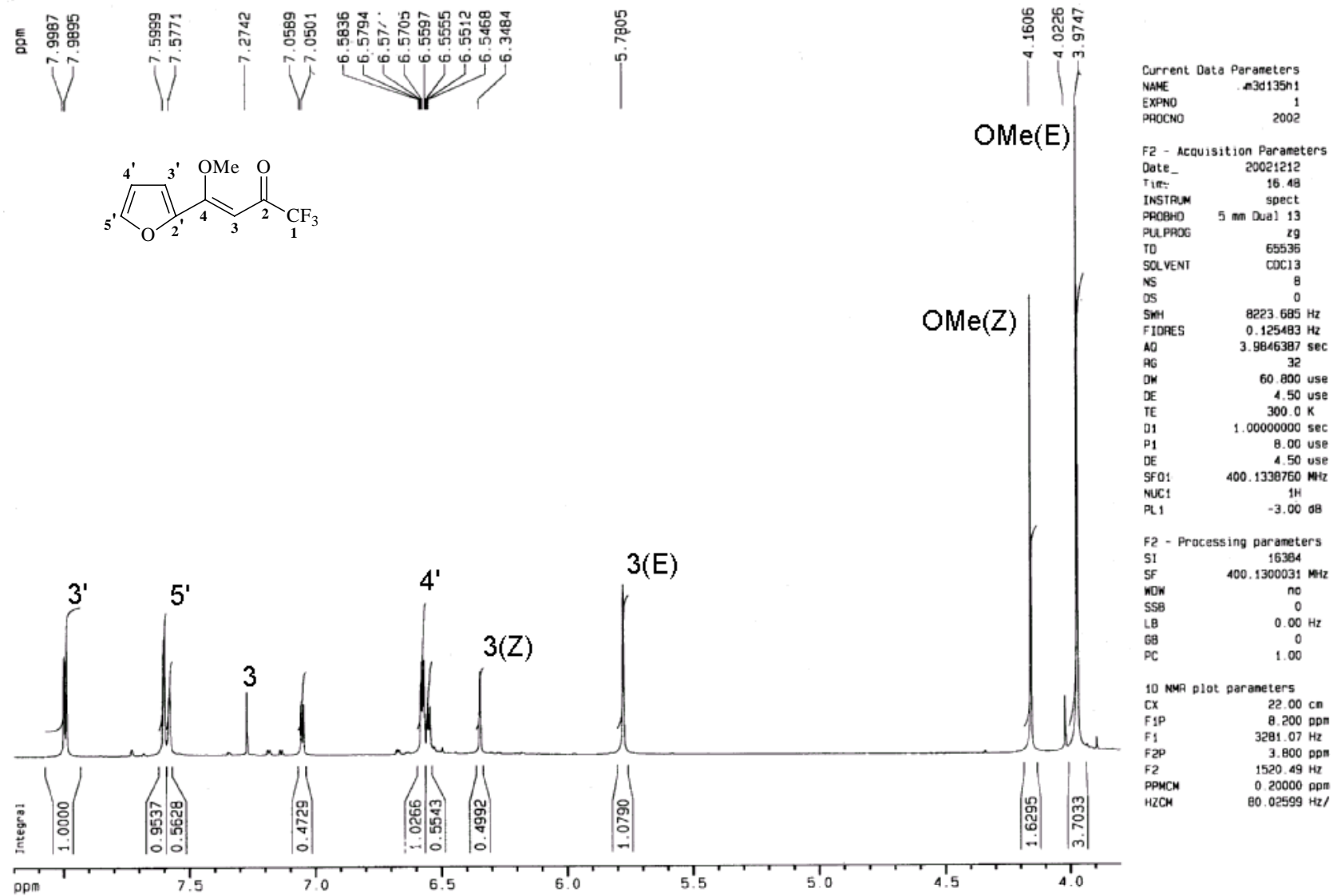


Figura 13. Espectro de RMN ^1H do 1,1,1-trifluor-4-[2-furil]-4-metoxi-3-buten-2-ona (**3a**) em CDCl_3 .

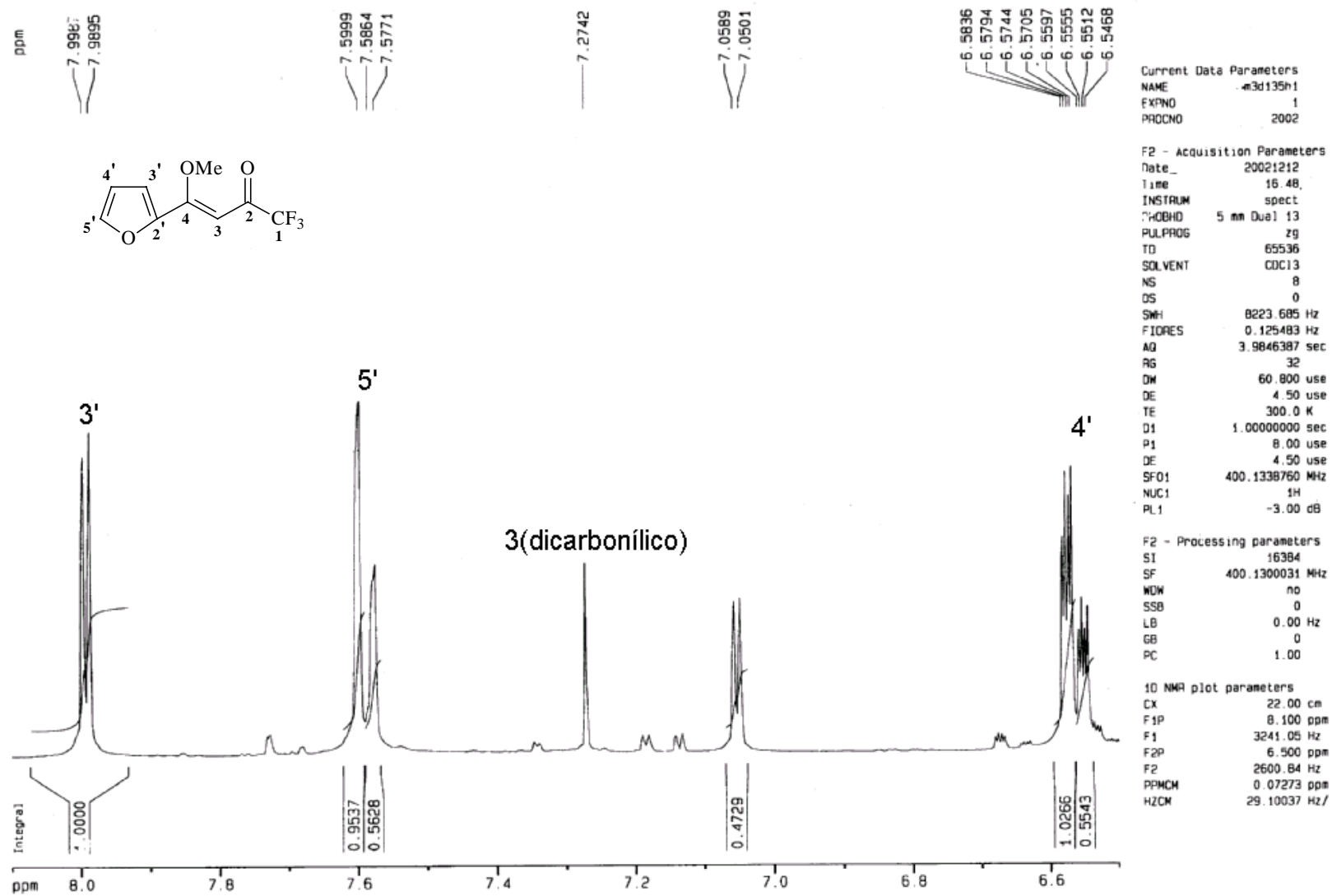
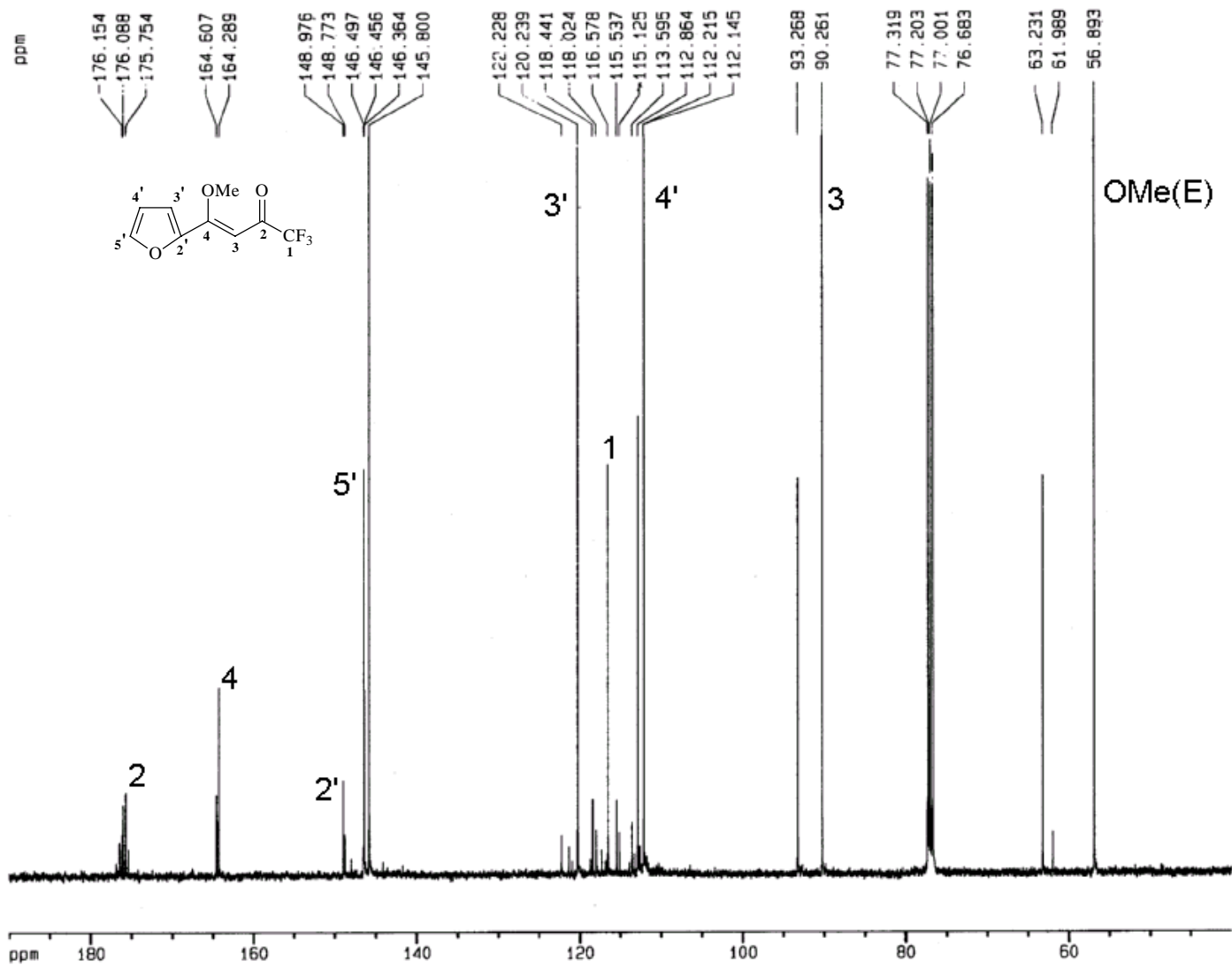


Figura 14. Espectro de RMN ¹H, expansão entre 6,6-8,0 ppm da 1,1,1-trifluor-4-[2-fúril]-4-metoxi-3-buten-2-ona (**3a**) em CDCl₃.



Current Data Parameters
 NAME m3d135cd
 EXPNO 1
 PROCNO 2002

F2 - Acquisition Parameters
 Date_ 20021212
 Time 17:53
 INSTRUM spect
 PROBHD 5 mm Jua1 13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1373
 DS 0
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DM 21.600 usec
 DE 4.50 usec
 TE 300.0 K
 D12 0.00002000 sec
 PL13 16.00 dB
 D1 3.00000000 sec
 CPDPRG2 waltz16
 PCPD2 106.00 usec
 SF02 400.1316005 MHz
 NUC2 13C
 PL2 -3.00 dB
 PL12 16.00 dB
 P1 7.60 usec
 DE 4.50 usec
 SF01 100.6237954 MHz
 NUC1 13C
 PL1 -6.00 dB
 D11 0.03000000 sec

F2 - Processing parameters
 SI 32768
 SF 100.6127728 MHz
 WDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 21.00 cm
 F1P 190.000 ppm
 F1 19116.43 Hz
 F2P 40.000 ppm
 F2 4024.51 Hz
 PPNMC 7.14286 ppm/cm
 HZCM 718.66266 Hz/cm

Figura 15. Espectro de RMN ¹³C {¹H}do 1,1,1-trifluor-4-[2-furil]-4-metoxi-3-buten-2-ona (3a) em CDCl₃.

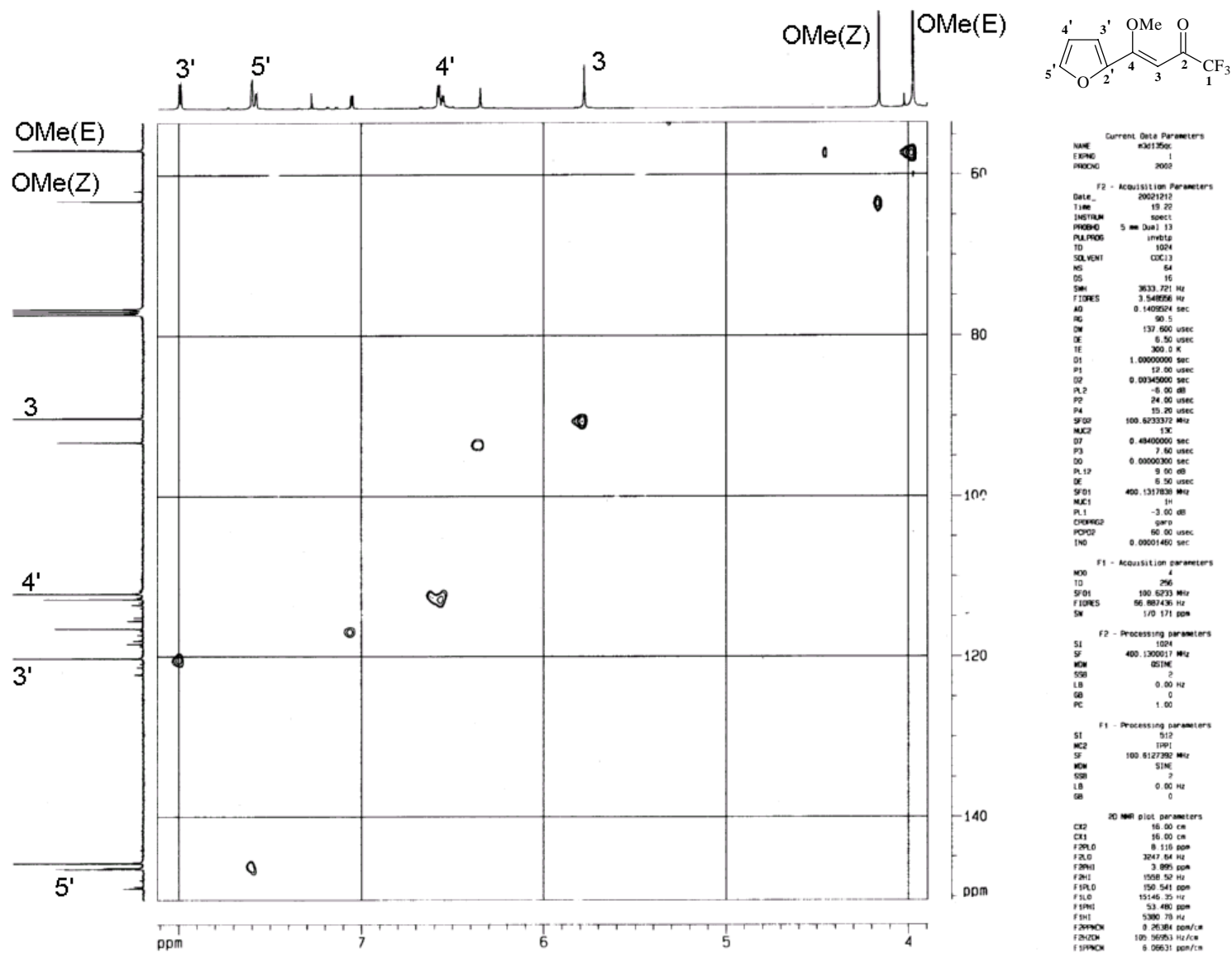
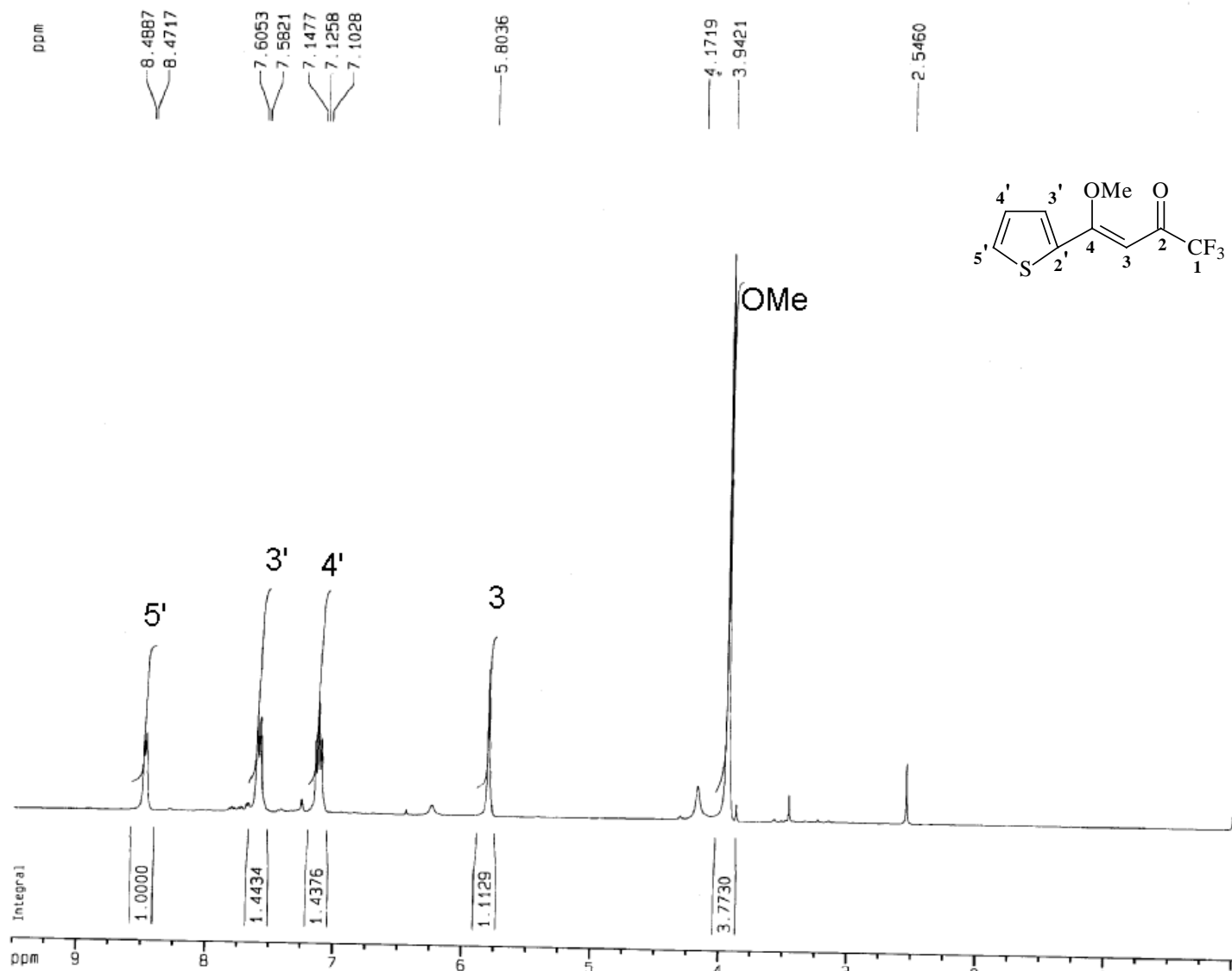


Figura 16. Espectro de RMN ^{13}C correlação C-H (HMBC) do 1,1,1-trifluor-4-metoxi-4-[2-furil]-3-buten-2-ona (**3a**) em CDCl_3 .



Current Data Parameters
 NAME m3d169h1
 EXPNO 1
 PROCNO 2003

F2 - Acquisition Parameters
 Date_ 20031220
 Time 13.53
 INSTRUM spect
 PROBHD 5 mm Multinu
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 2408.478 Hz
 FIDRES 0.073501 Hz
 AQ 6.8026867 sec
 RG 35.9
 DW 207.600 use
 DE 7.07 use
 TE 300.0 K
 D1 0.00100000 sec
 P1 7.00 use
 DE 7.07 use
 SFO1 200.1310007 MHz
 NUC1 1H
 PL1 -3.00 dB

F2 - Processing parameters
 SI 32768
 SF 200.1300095 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 22.00 cm
 F1P 9.500 ppm
 F1 901.24 Hz
 F2P -0.100 ppm
 F2 -20.01 Hz
 PPMCM 0.43636 ppm
 HZCM 87.32946 Hz/

Figura 17. Espectro de RMN ¹H do 1,1,1-trifluor-4-metoxi-4-[2-tienil]-3-buten-2-ona (**3b**) em CDCl₃.

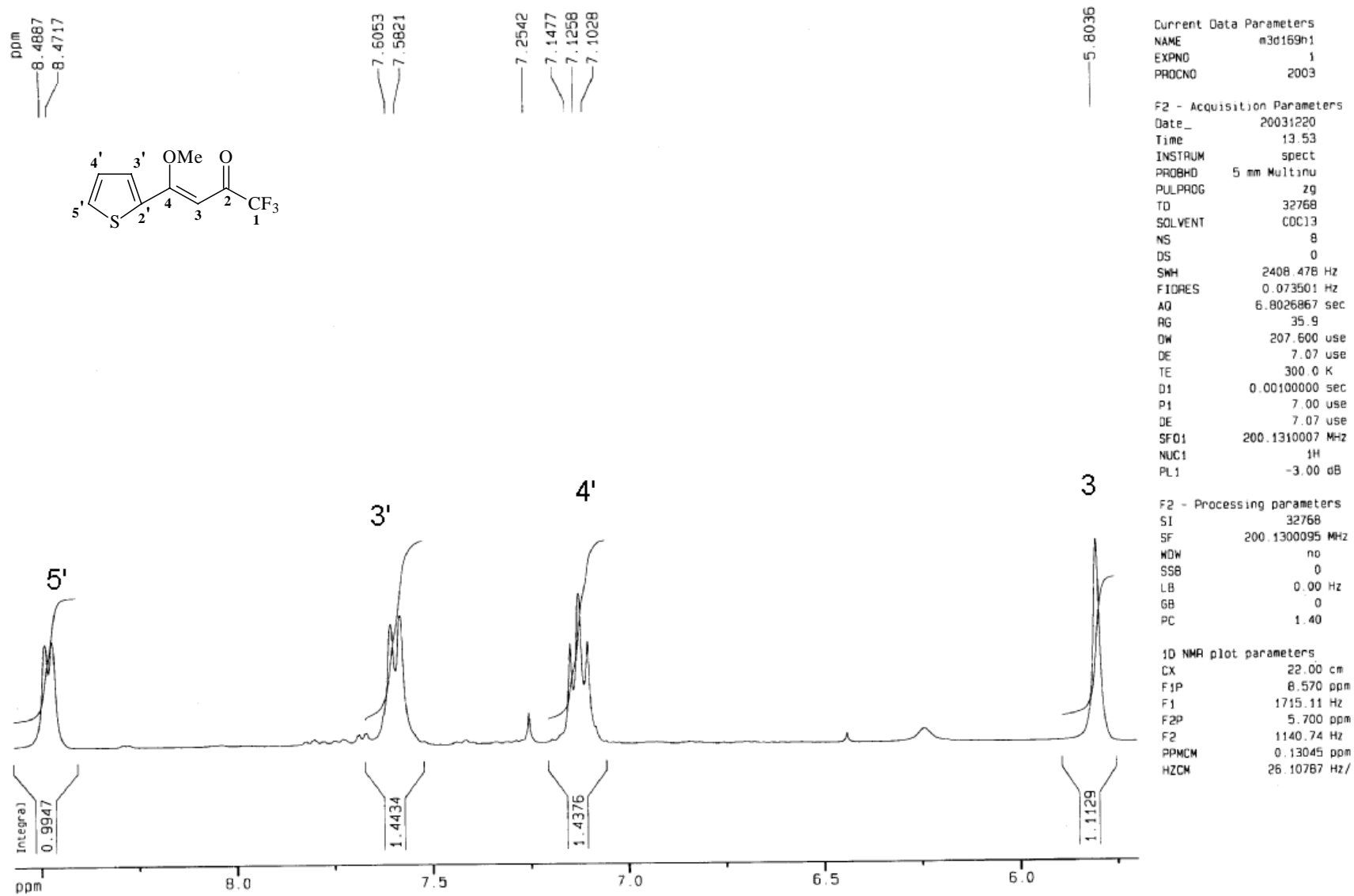


Figura 18. Espectro de RMN ^1H , expansão entre 6,0-8,5 ppm do 1,1,1-trifluor-4-metoxi-4-[2-tienil]-3-buten-2-ona (**3b**) em CDCl_3 .

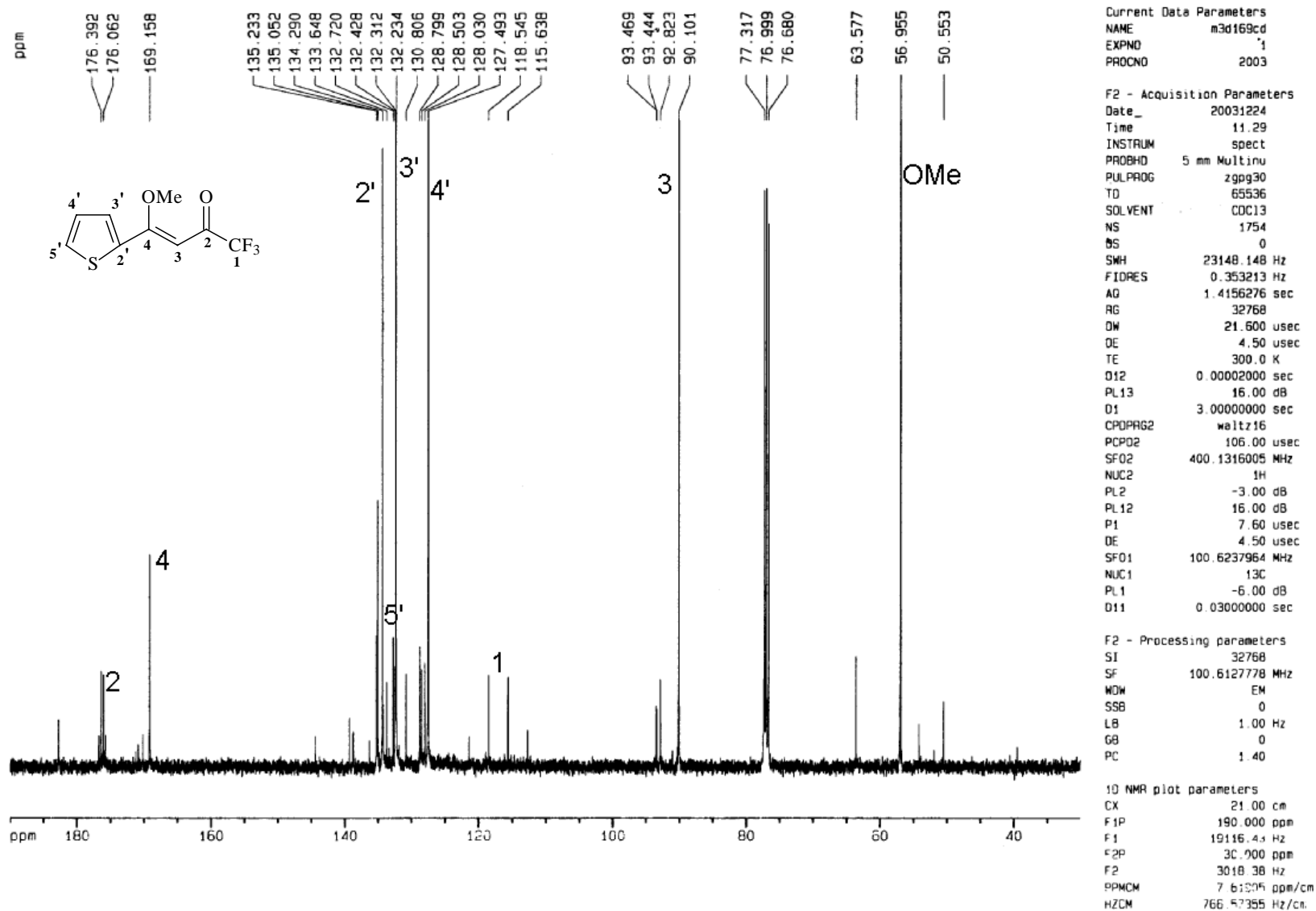


Figura 19. Espectro de RMN ^{13}C do 1,1,1-trifluor-4-metoxi-4-[2-tienil]-3-buten-2-ona (**3b**) em CDCl_3 .

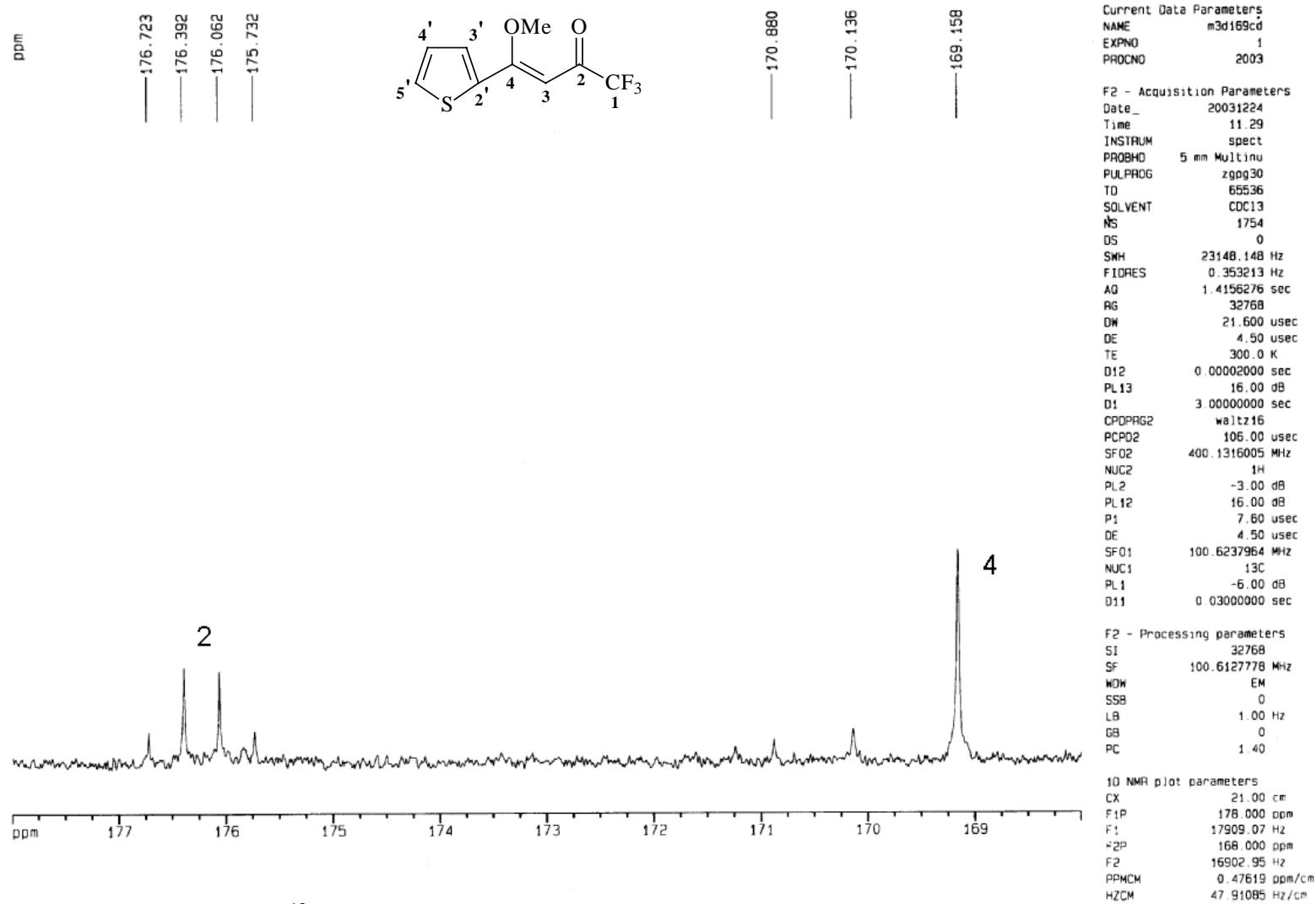


Figura 20. Espectro de RMN ^{13}C expansão entre 169-177 ppm do 1,1,1-trifluor-4-metoxi-4-[2-tienil]-3-buten-2-ona (**3b**) em CDCl_3 .

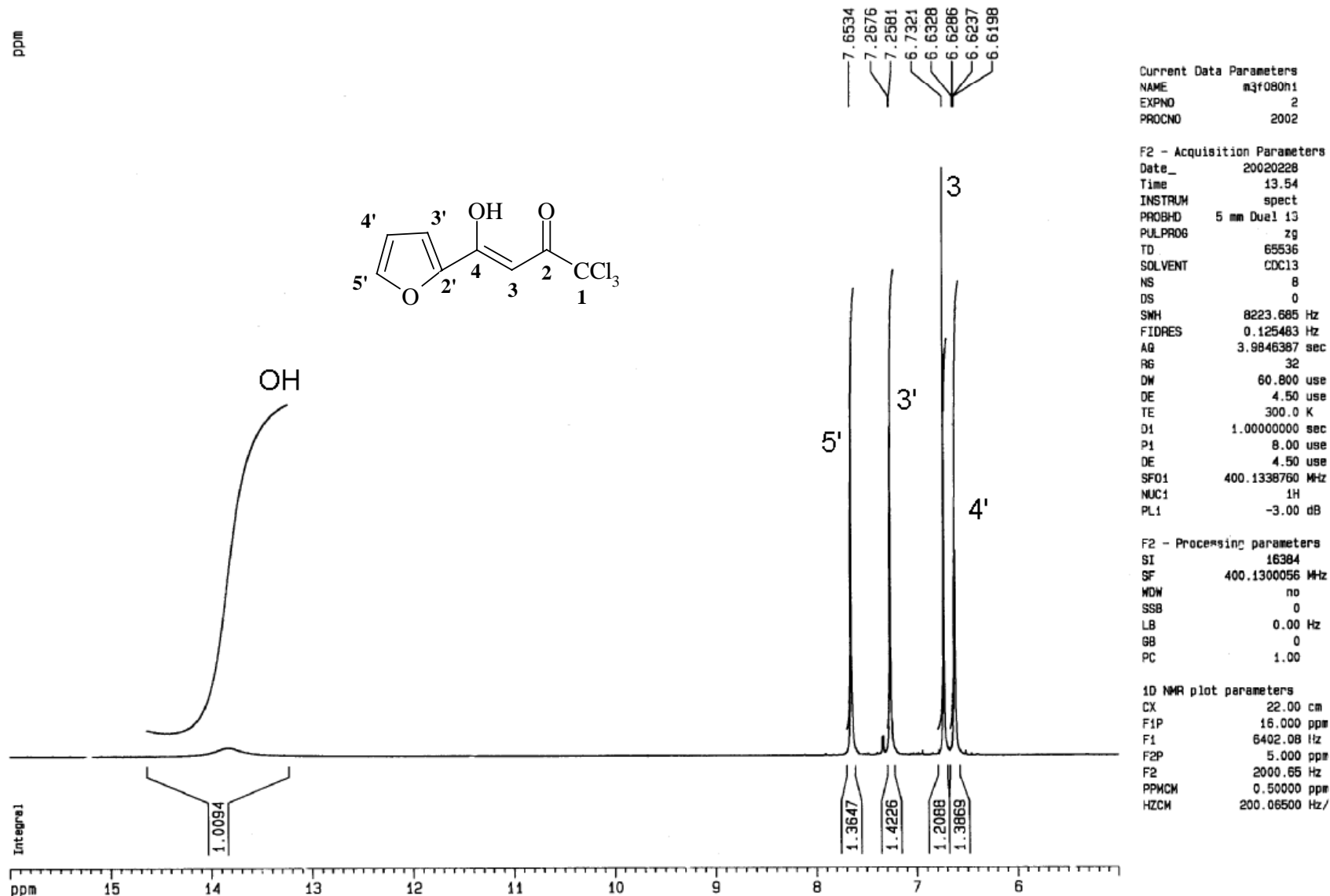


Figura 21. Espectro de RMN de ^1H do 1,1,1-tricloro-4-[2-furil]-buten-1,3-diona (**4a**) em CDCl_3 .

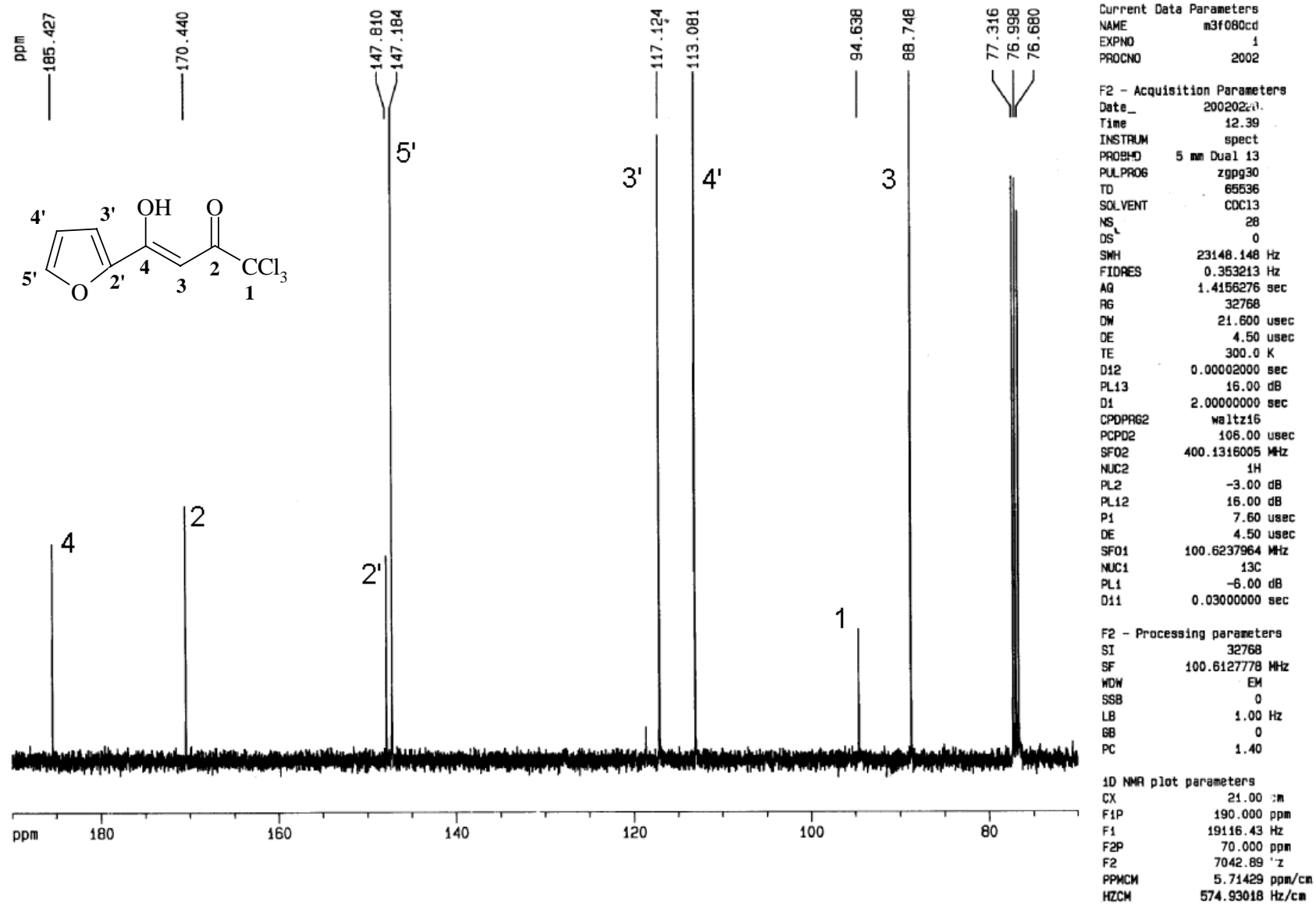


Figura 22. Espectro de RMN de ¹³C do 1,1,1-tricloro-4-[2-furil]-buten-1,3-diona (4a) em CDCl₃.

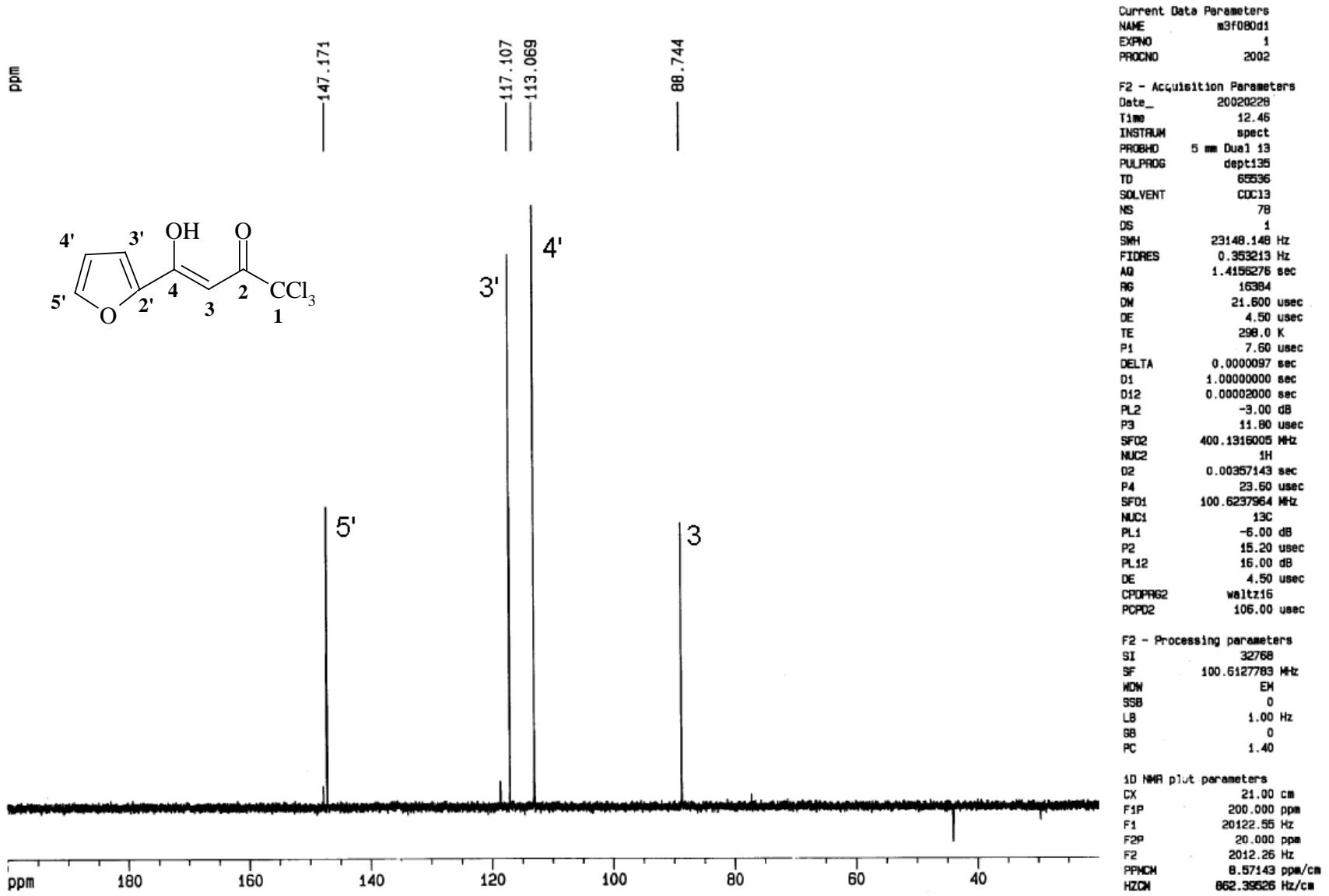
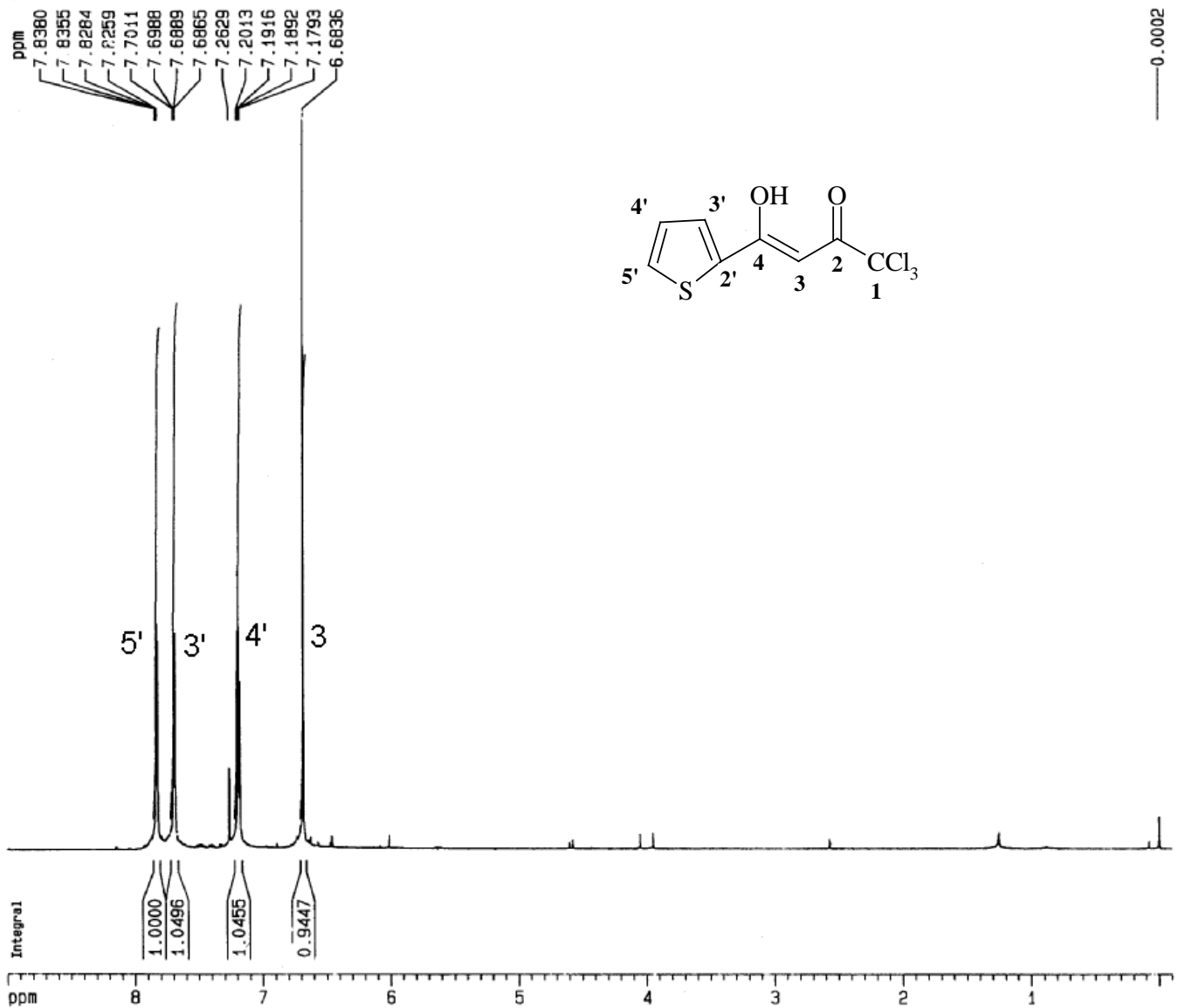


Figura 23. Espectro de RMN de ¹³C, DEPT 135 do 1,1,1 -triclouro-4-[2-furil]-buten-1,3-diona (**4a**) em CDCl₃.



Current Data Parameters
 NAME n3m081h1
 EXPNO 1
 PROCNO 2002

F2 - Acquisition Parameters
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 Time 12.59
 INSTRUM spect
 PROBHD 5 mm Dual 13
 PULPROG zg
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4960.317 Hz
 FIDRES 0.075688 Hz
 AQ 6.6060786 sec
 RG 35.9
 DW 100.800 usec
 DE 4.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 P1 12.00 usec
 DE 4.50 usec
 SFO1 400.1322614 MHz
 NUC1 1H
 PL1 -3.00 dB

F2 - Processing parameters
 SI 32768
 SF 400.1300075 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.50 cm
 F1P 9.000 ppm
 F1 3601.17 Hz
 F2P -0.170 ppm
 F2 -40.01 Hz
 PPMCM 0.44390 ppm/cm
 HZCM 177.61870 Hz/cm

Figura 24. Espectro de RMN de ¹H do 1,1,1-tricloro-4-[2-tienil]-buten-1,3-diona (4a) em CDCl₃.

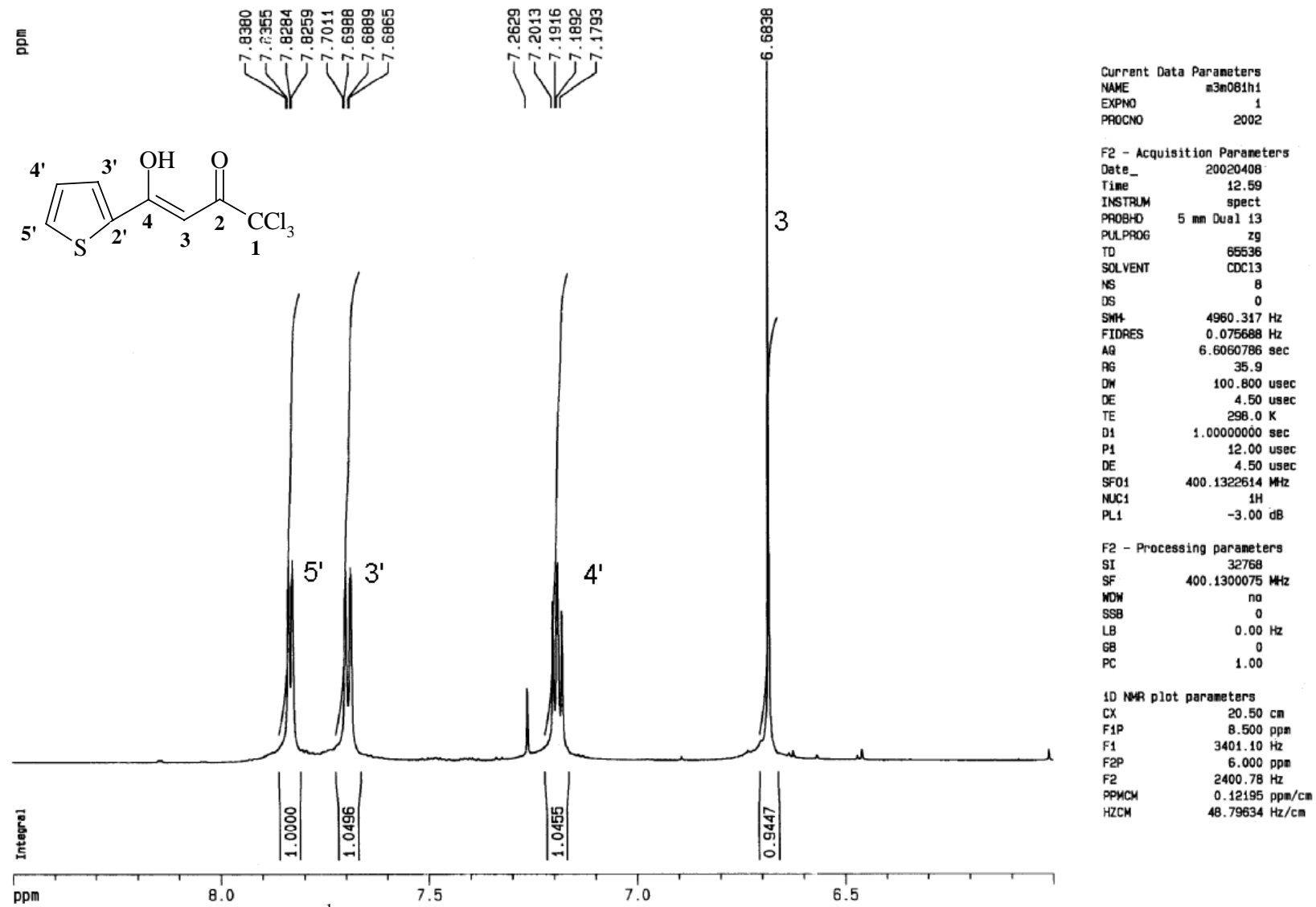
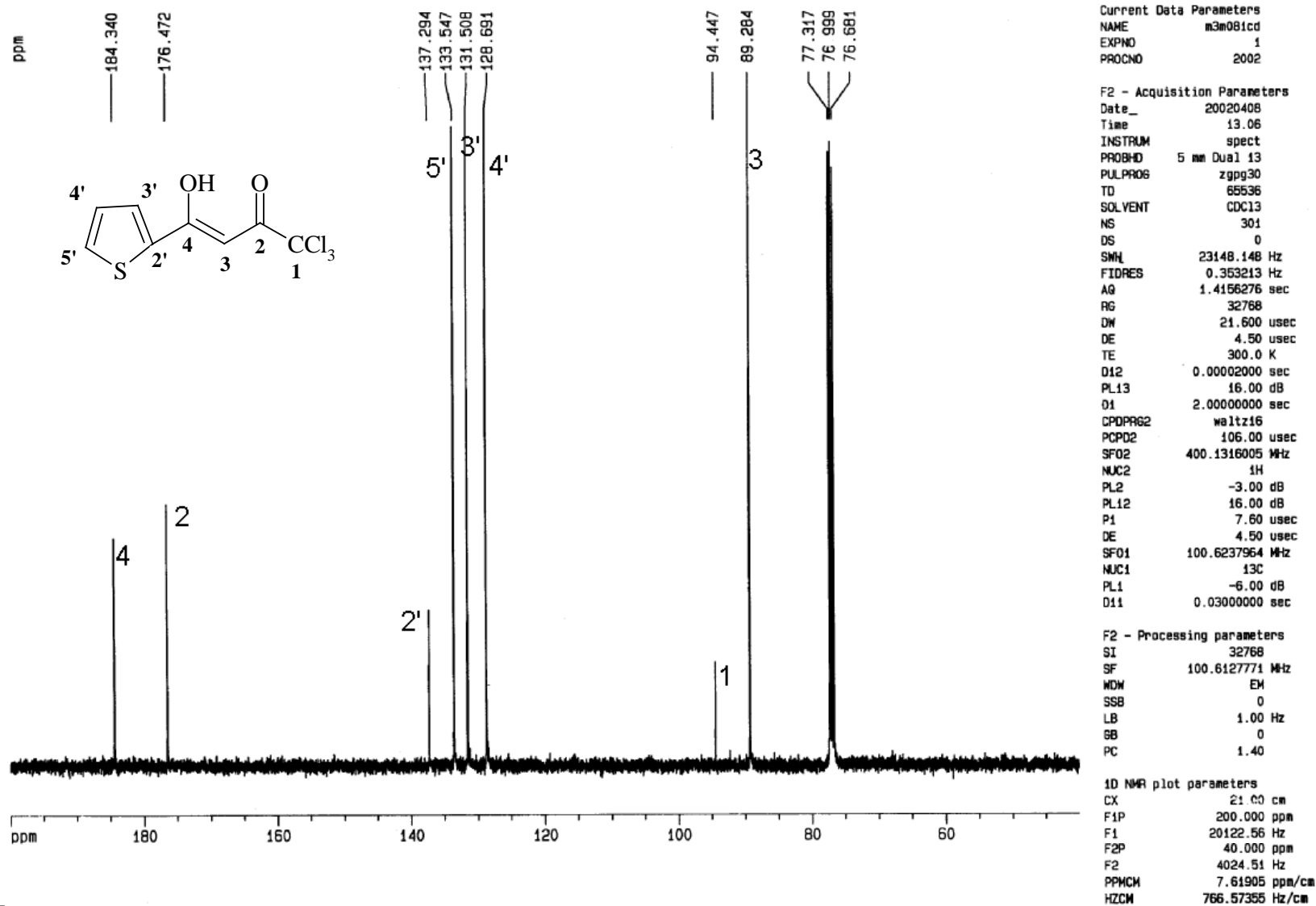


Figura 25. Espectro de RMN de ^1H , expansão entre 6,5-8,0 ppm do 1,1,1-tricloro-4-[2-tienil]-buten-1,3-diona (**4b**) em CDCl_3 .



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 Figura 26. Espectro de RMN de ¹³C do 1,1,1-tricloro-4-[2-tienil]-buten-1,3-diona (**4b**) em CDCl₃.

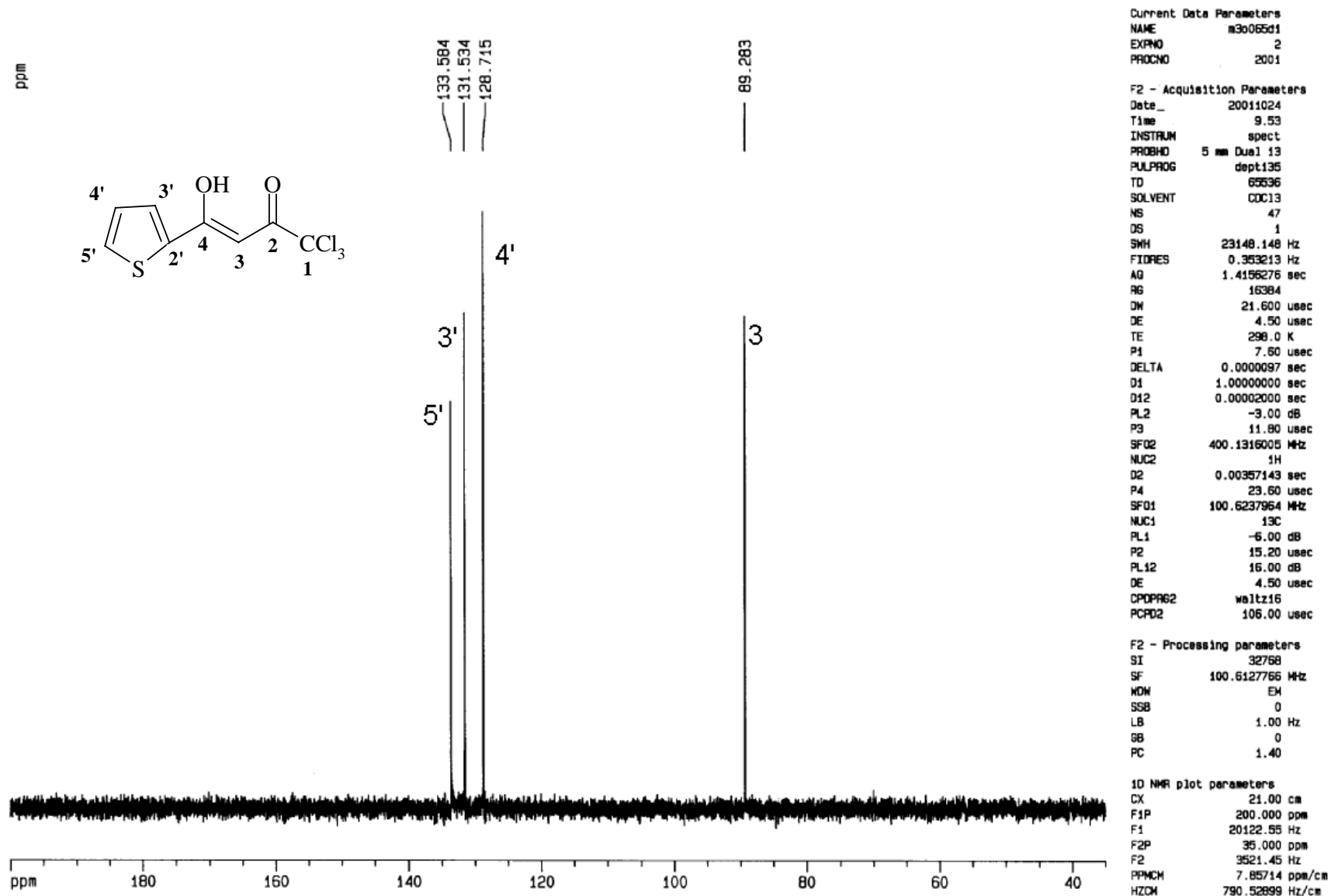


Figura 27. Espectro de RMN de ^{13}C (DEPT 135) do 1,1,1-tricloro-4-[2-tienil]-buten-1,3-diona (**4b**) em CDCl_3 .

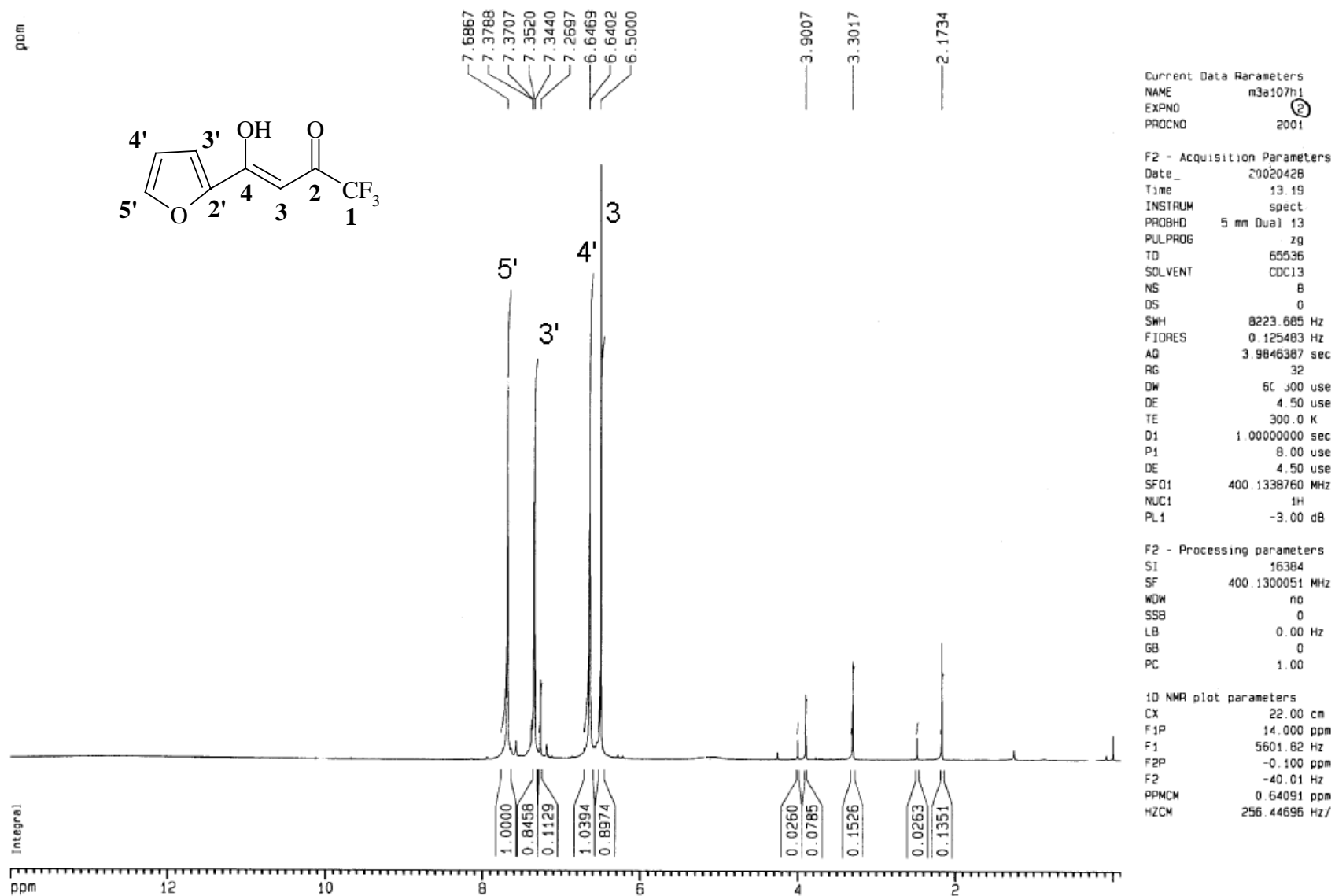


Figura 28. Espectro de RMN ¹H do 1,1,1-trifluor-4-[2-furil]-buten-1,3-diona (**5a**) em CDCl₃.

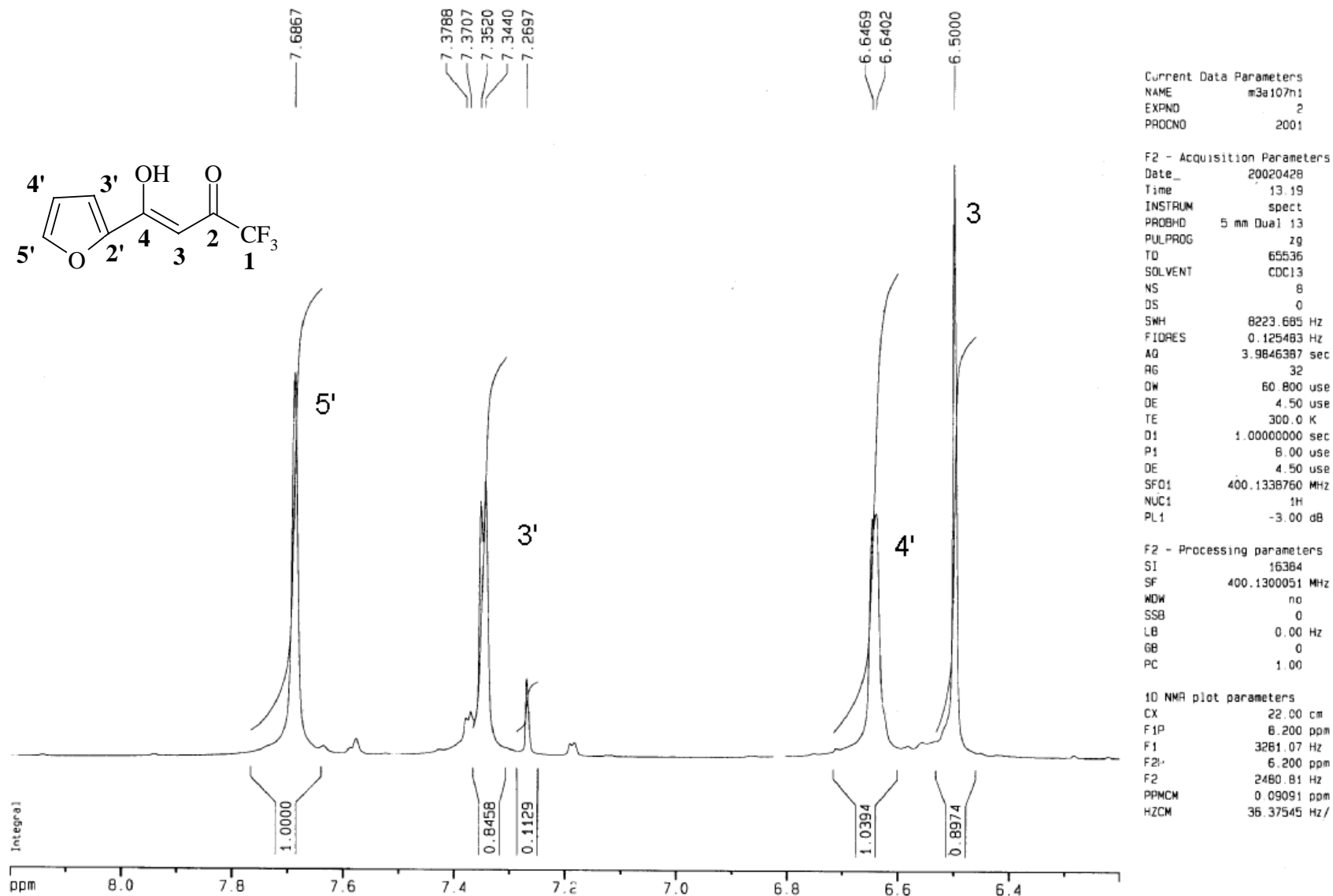


Figura 29. Espectro de RMN ¹H, expansão entre 6,4-8,0 ppm do 1,1,1-trifluor-4-[2-furil]-buten-1,3-diona (**5a**) em CDCl₃.

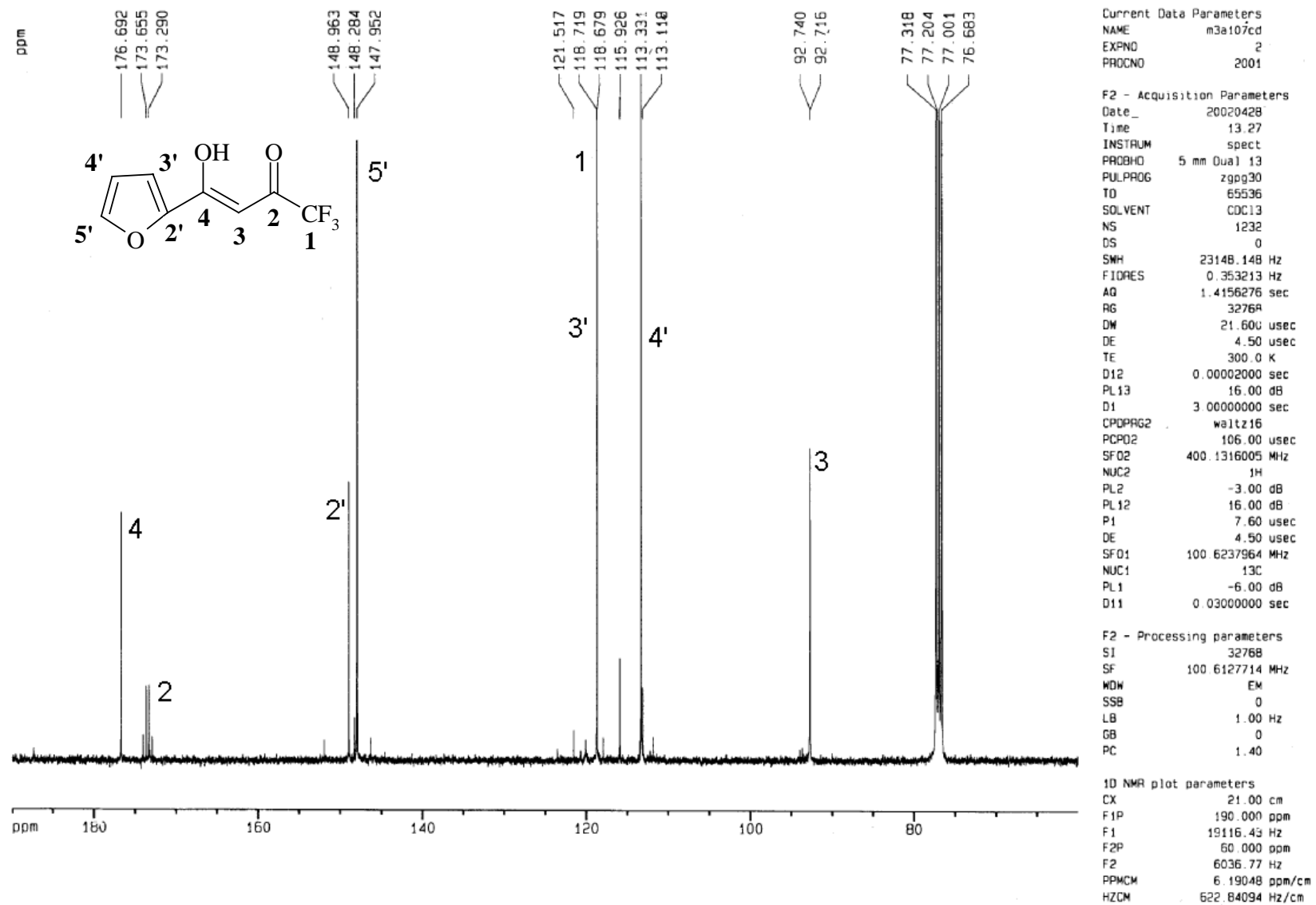


Figura 30. Espectro de ^{13}C do 1,1,1-trifluor-4-[2-furil]-buten-1,3-diona (**5a**) em CDCl_3 .

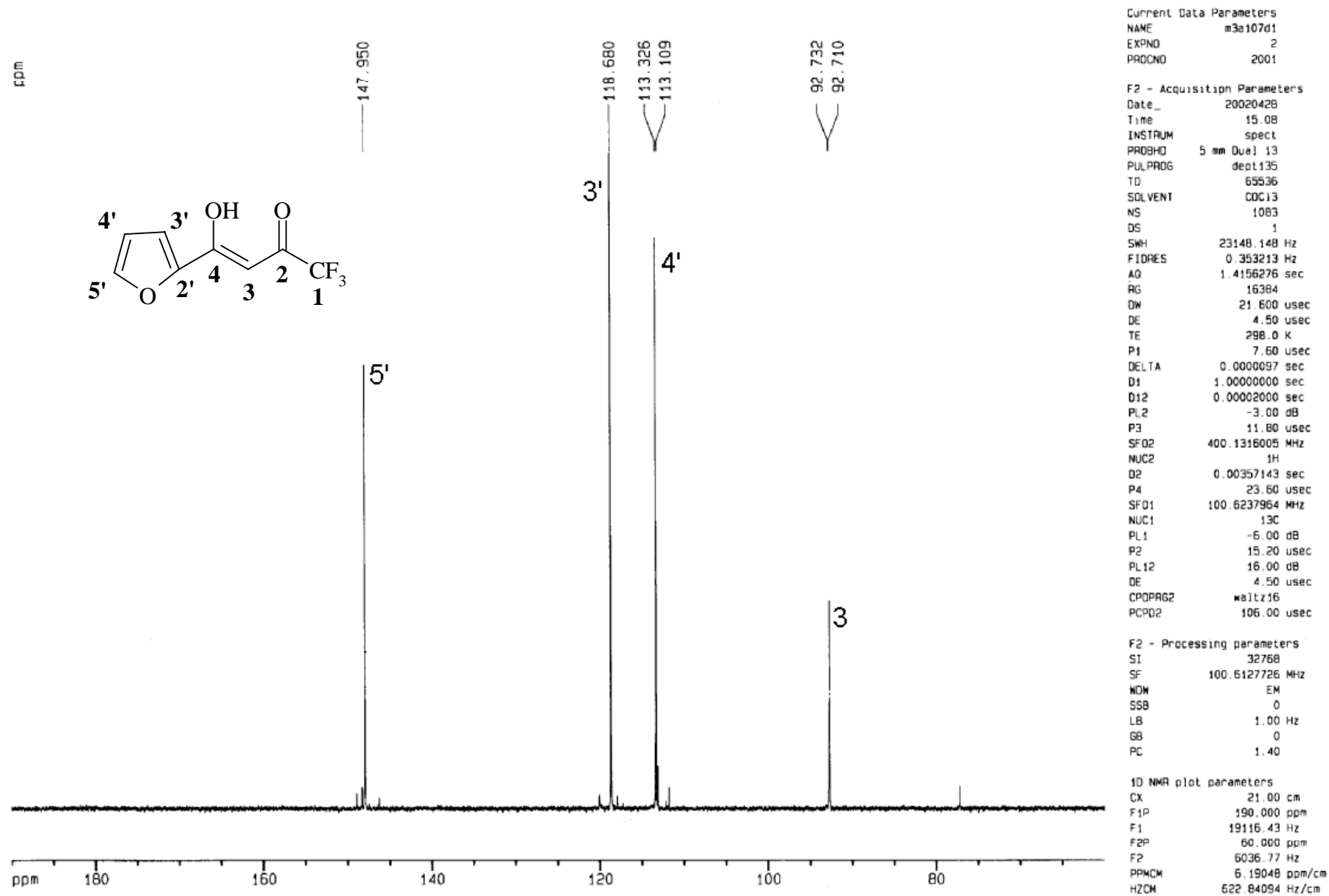


Figura 31. Espectro de ^{13}C , experimento DEPT 135 do 1,1,1-trifluor-4-[2-furil]-buten-1,3-diona (**5a**) em CDCl_3 .

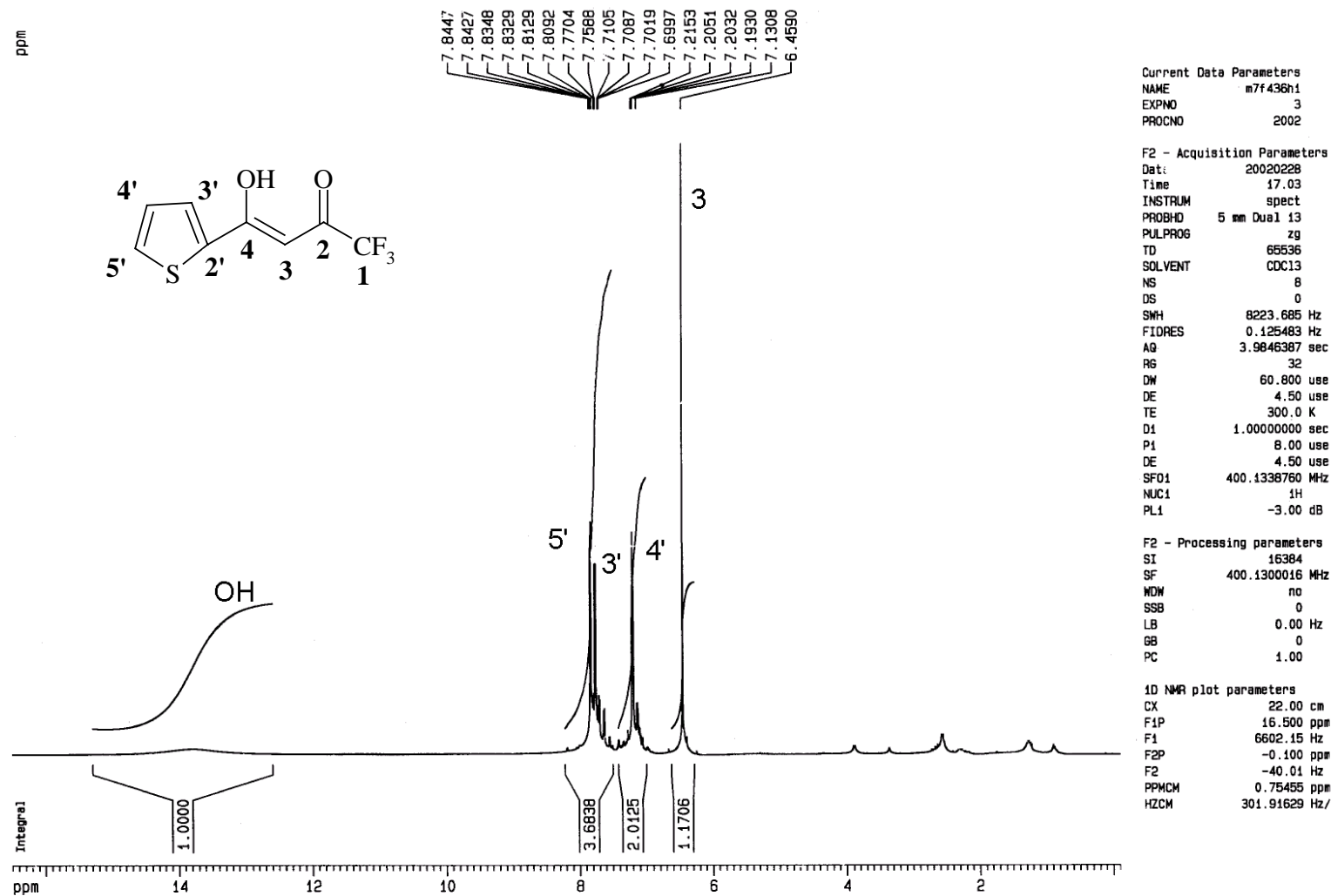


Figura 32. Espectro de ^1H do 1,1,1-trifluor-4-[2-tienil]-buten-1,3-diona (**5b**) em CDCl_3 .

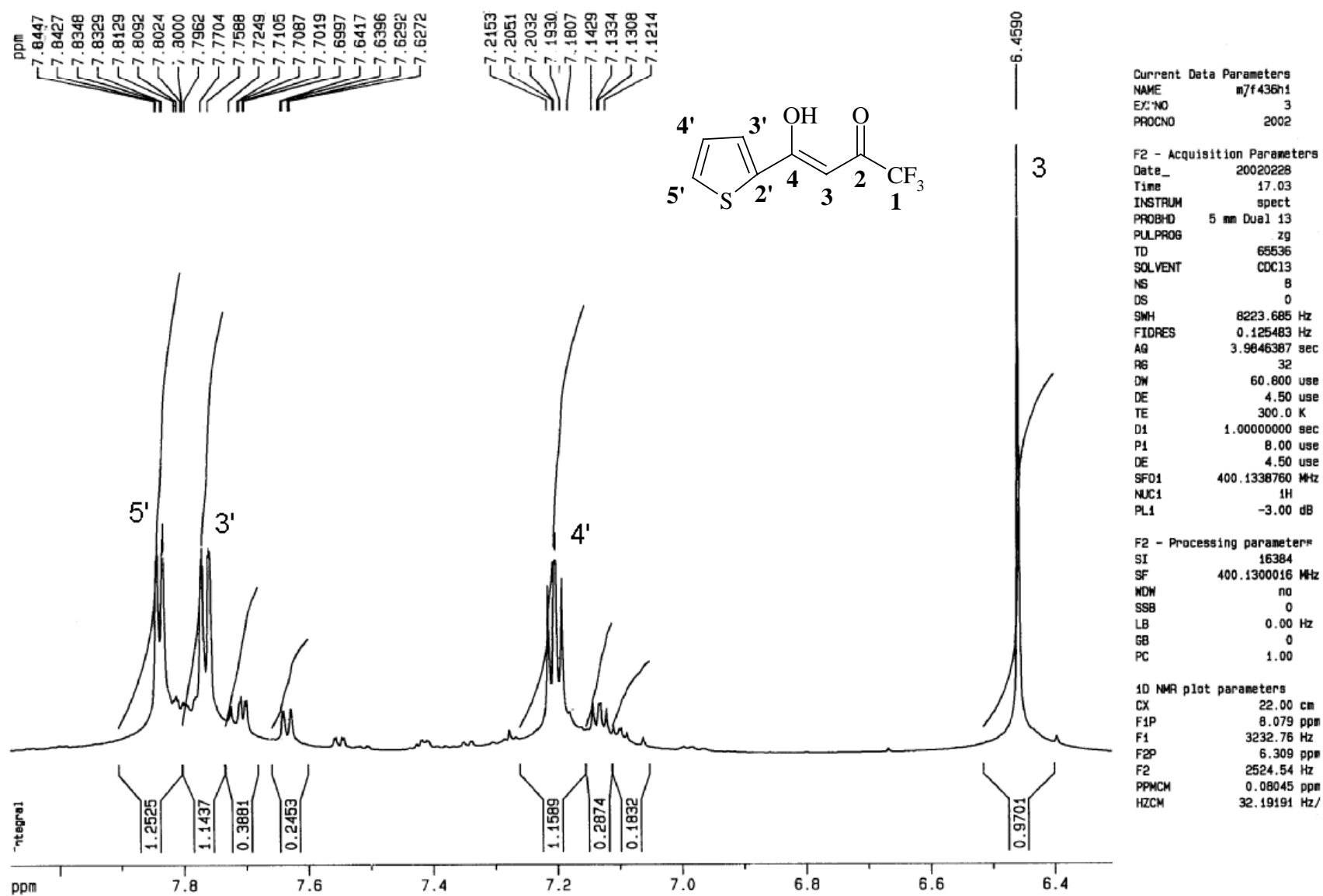


Figura 33. Espectro de ^1H , expansão entre 6,4-7,8 ppm do 1,1,1-trifluor-4-[2-tienil]-buten-1,3-diona (**5b**) em CDCl_3 .

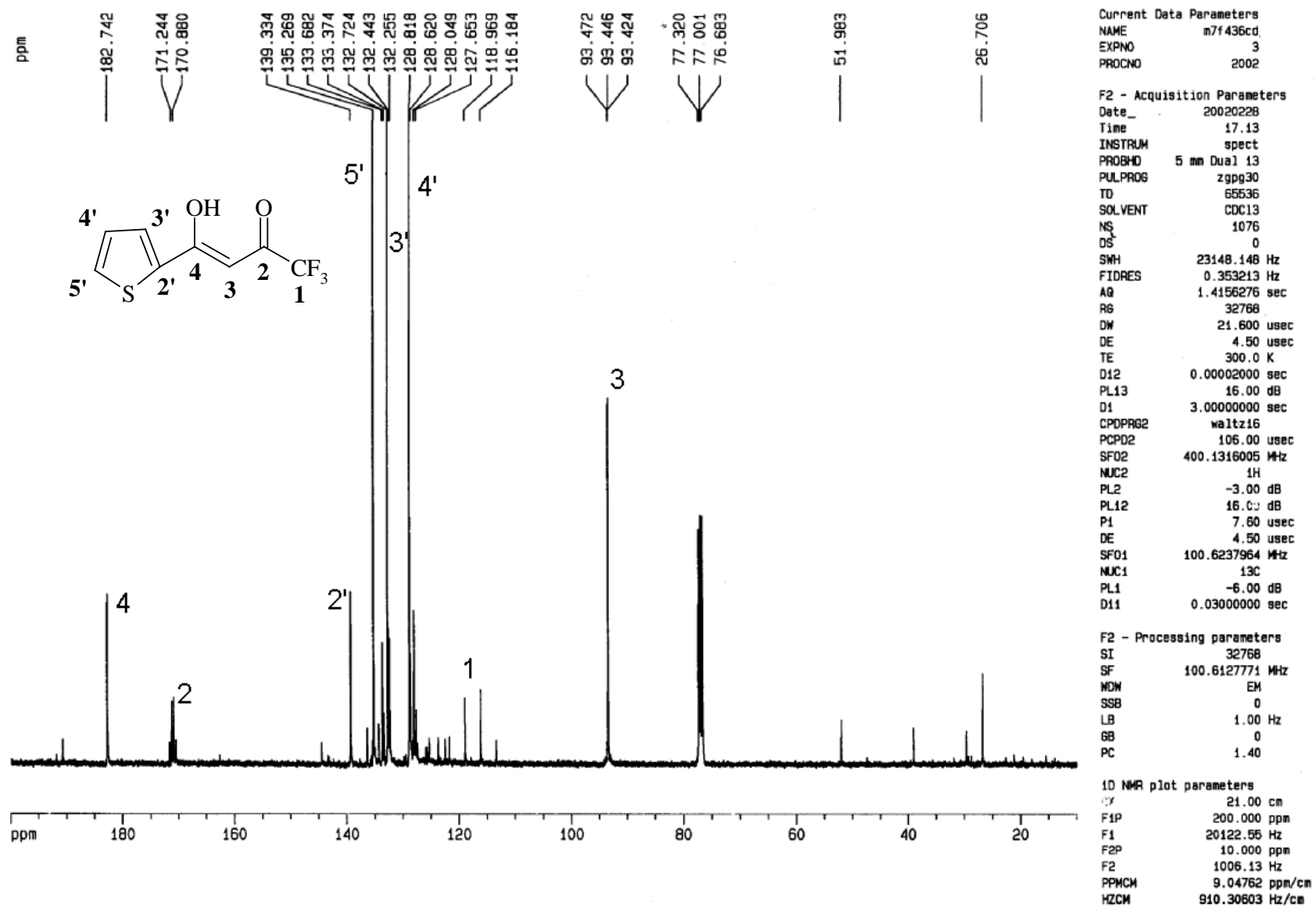


Figura 34. Espectros de RMN ^{13}C do 1,1,1-trifluor-4-[2-tienil]-buten-1,3-diona (**5b**) em CDCl_3 .

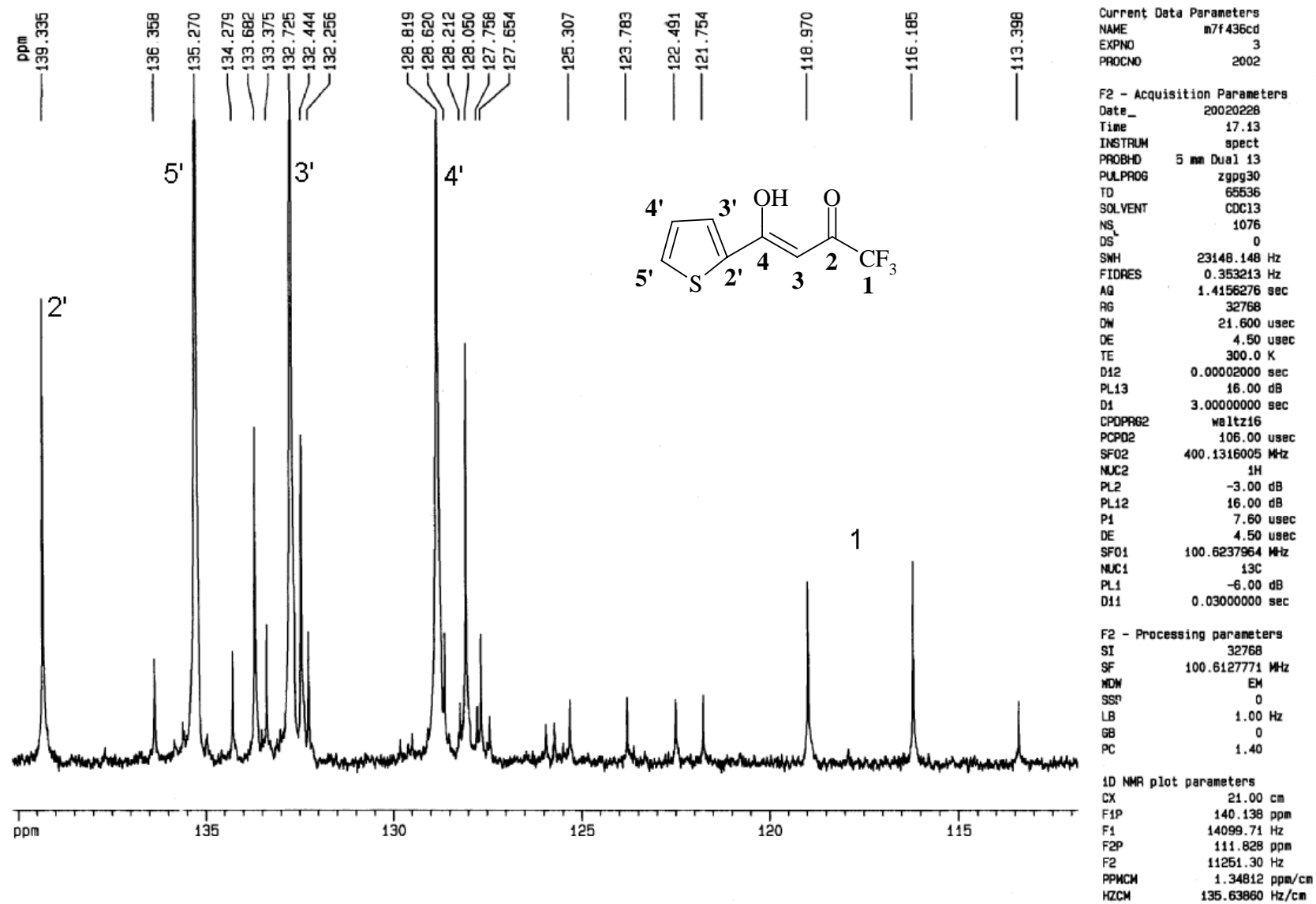


Figura 35. Espectros de RMN ^{13}C , expansão entre 115-145 ppm do 1,1,1-trifluor-4-[2-tienil]-buten-1,3-diona (**5b**) em CDCl_3 .

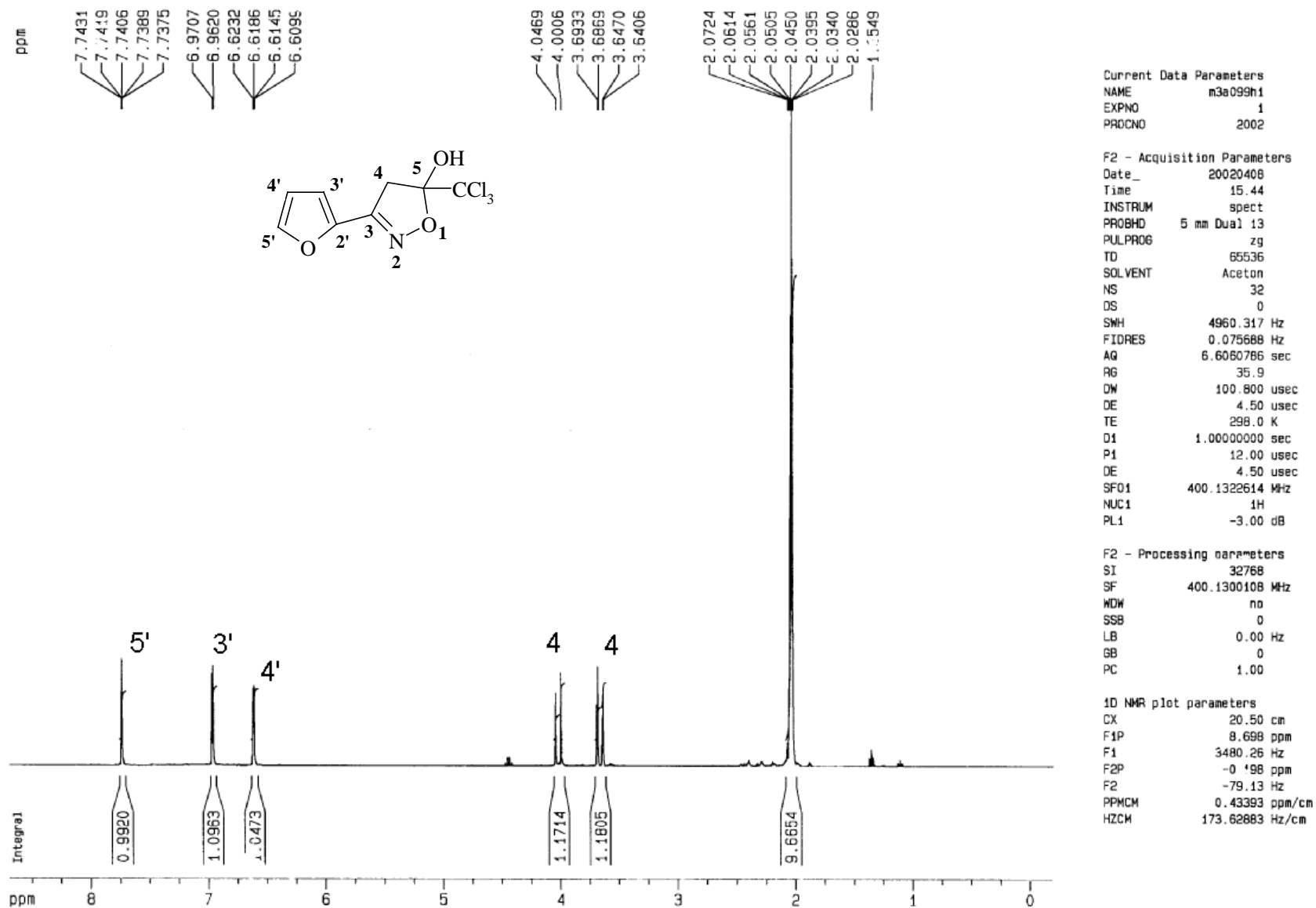


Figura 36. Espectros de RMN ^1H do 5-triclorometil-3-[2-furil]-5-hidroxi-4,5-diidro-isoxazol (**6a**) em acetona.

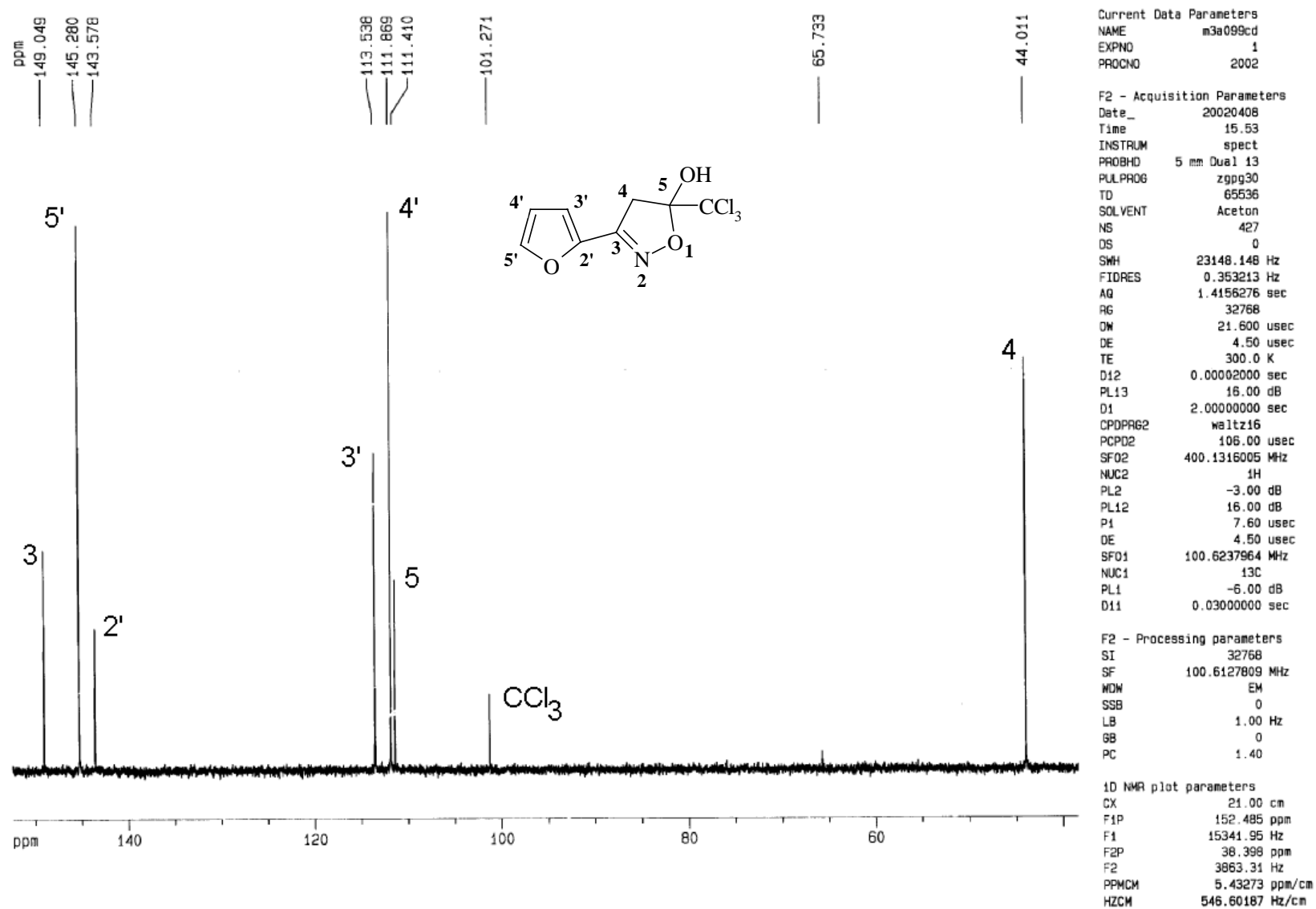


Figura 37. Espectros de RMN ^{13}C do 5-triclorometil-3-[2-furil]-5-hidroxi-4,5-diidro-isoxazol (**6a**) em acetona.

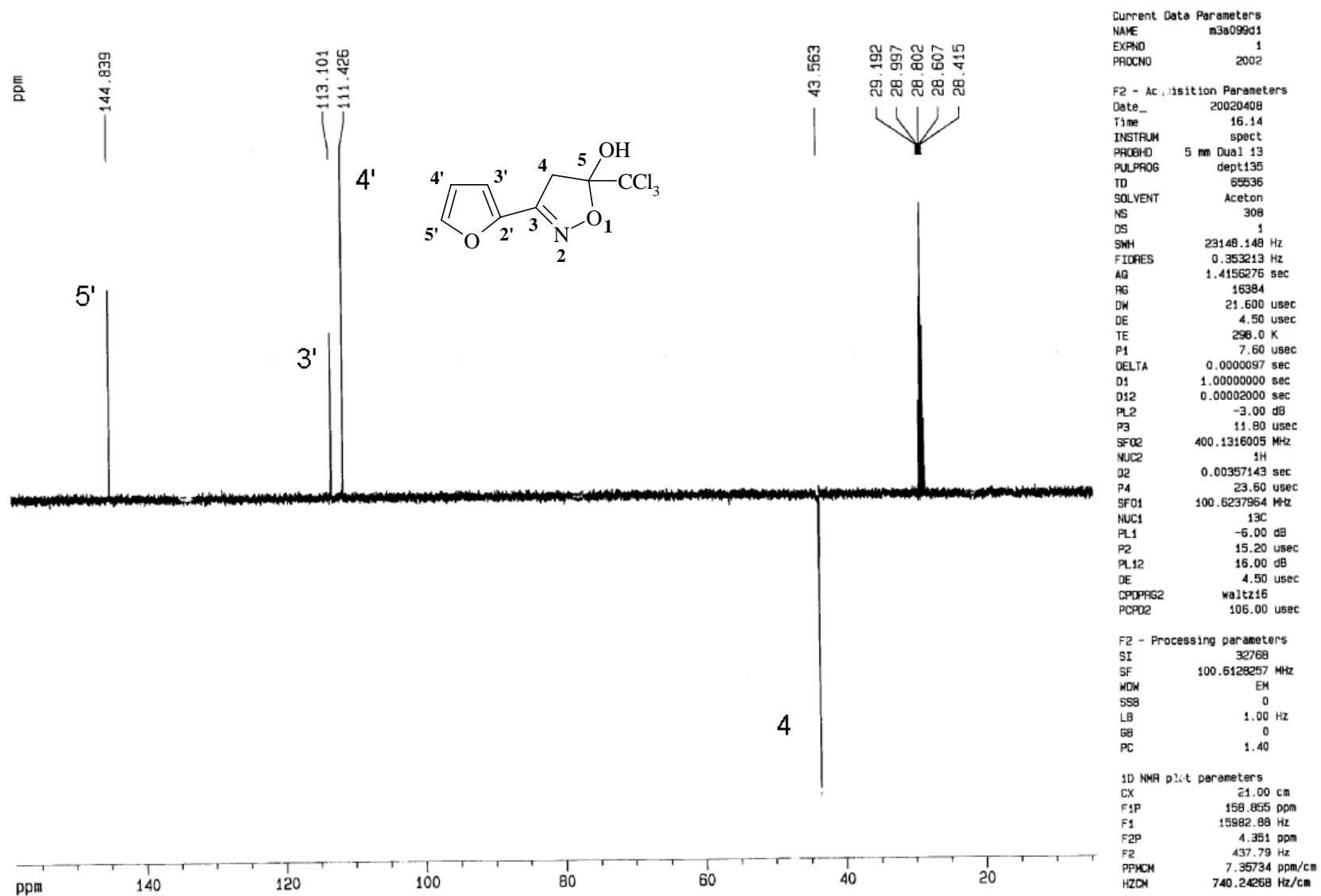


Figura 38. Espectros de RMN ^{13}C (DEPT 135) do 5-triclorometil-3-[2-furil]-5-hidroxi-4,5-diidro-isoxazol (**6a**) em acetona.

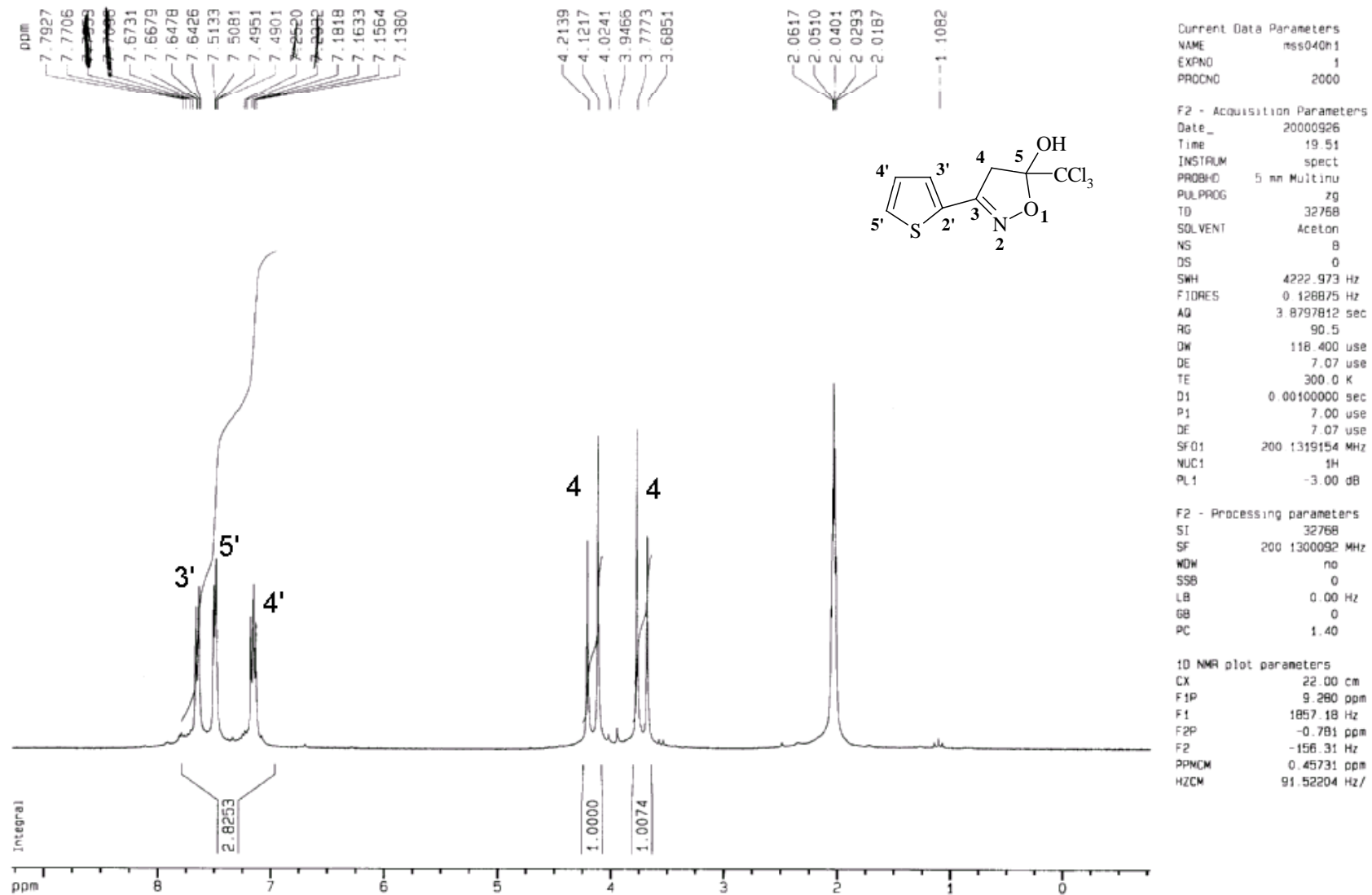


Figura 39. Espectros de RMN ^1H do 5-triclorometil-3-[2-tienil]-5-hidroxi-4,5-diidro-isoxazol (**6b**) em acetona.

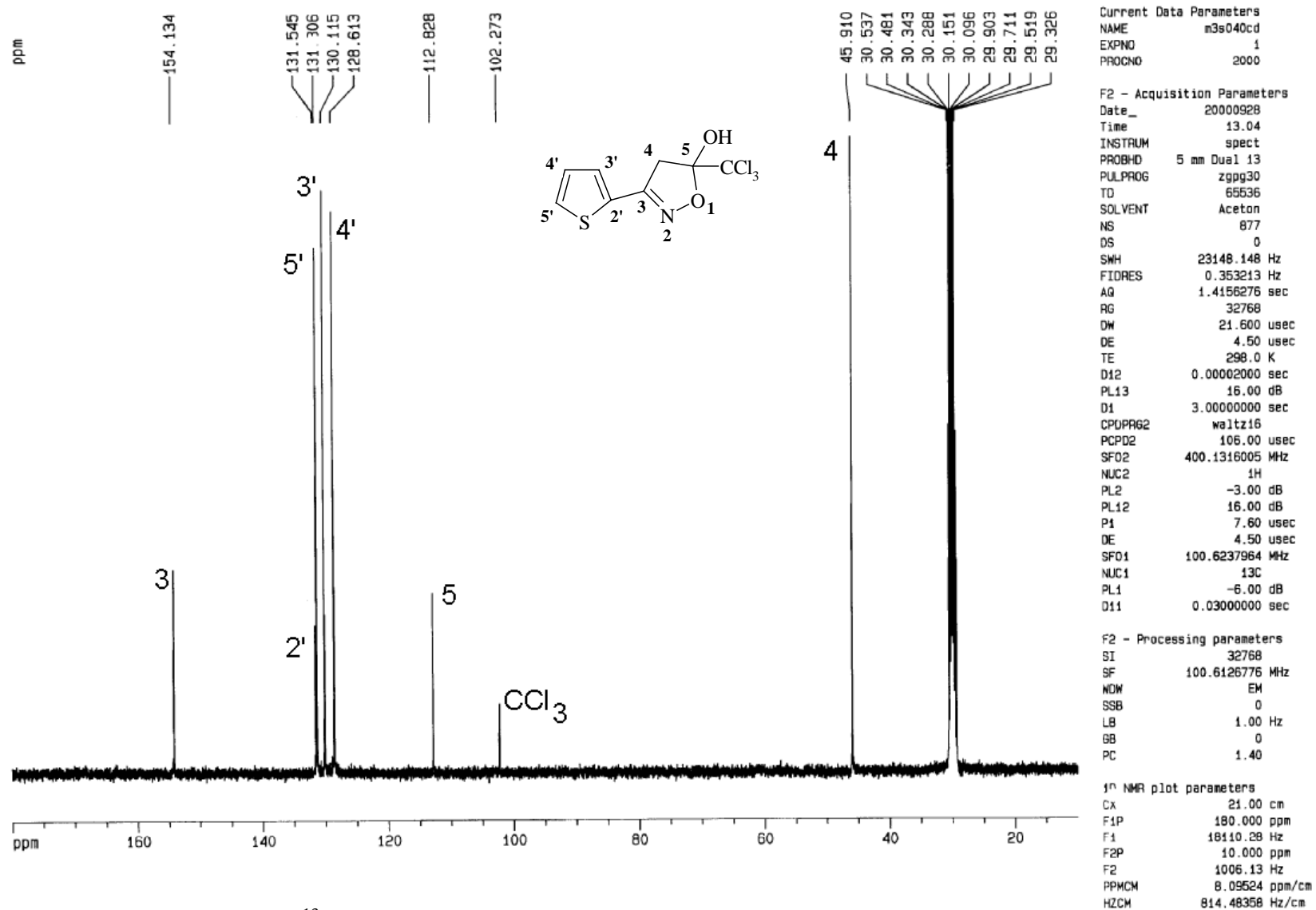


Figura 40. Espectros de RMN ^{13}C do 5-triclorometil-3-[2-tienil]-5-hidroxi-4,5-diidro-isoxazol (**6b**) em acetona.

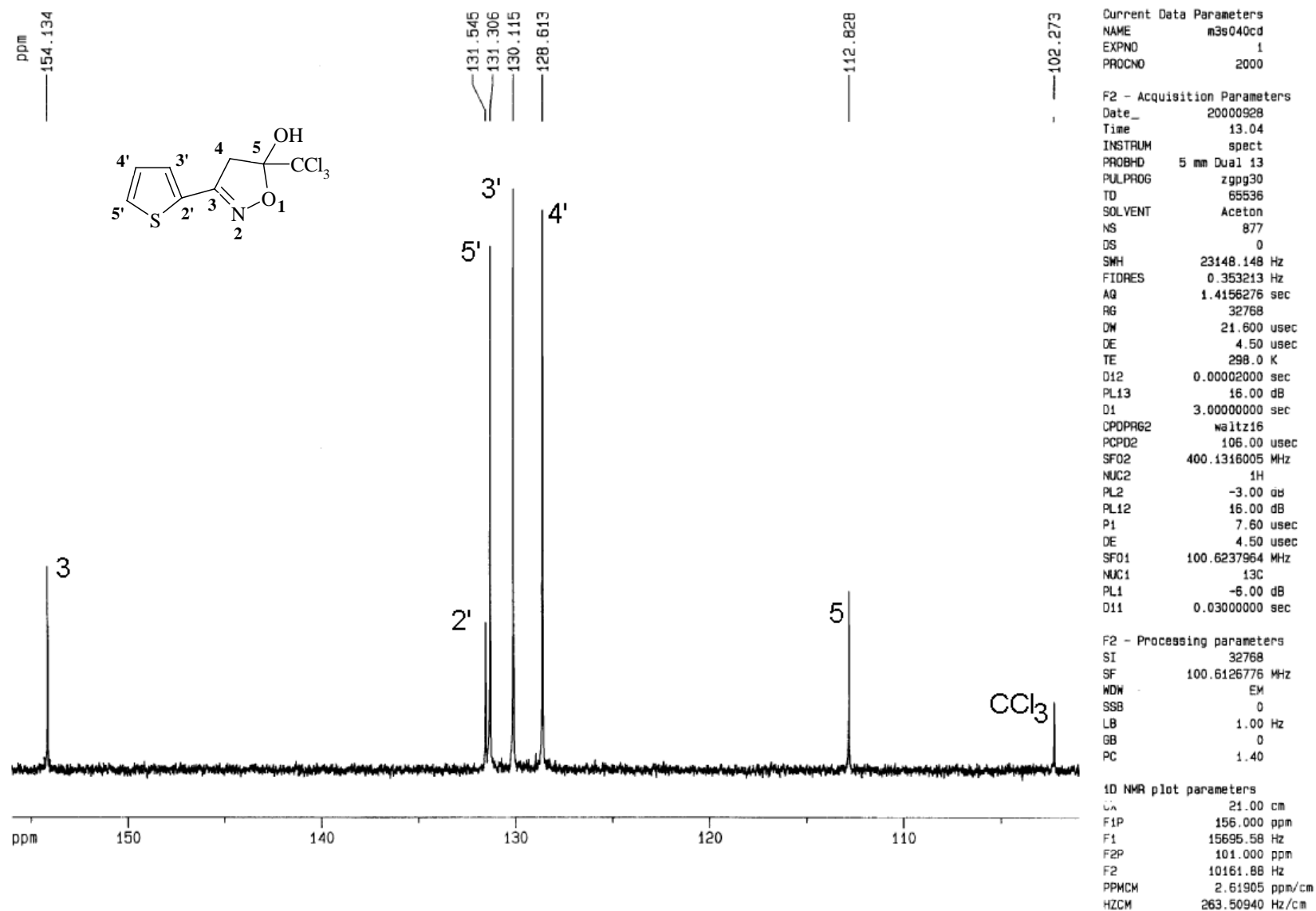


Figura 41. Espectros de RMN ¹³C do 5-triclorometil-3-[2-tienil]-5-hidroxi-4,5-diidro-isoxazol (**6b**) em acetona.

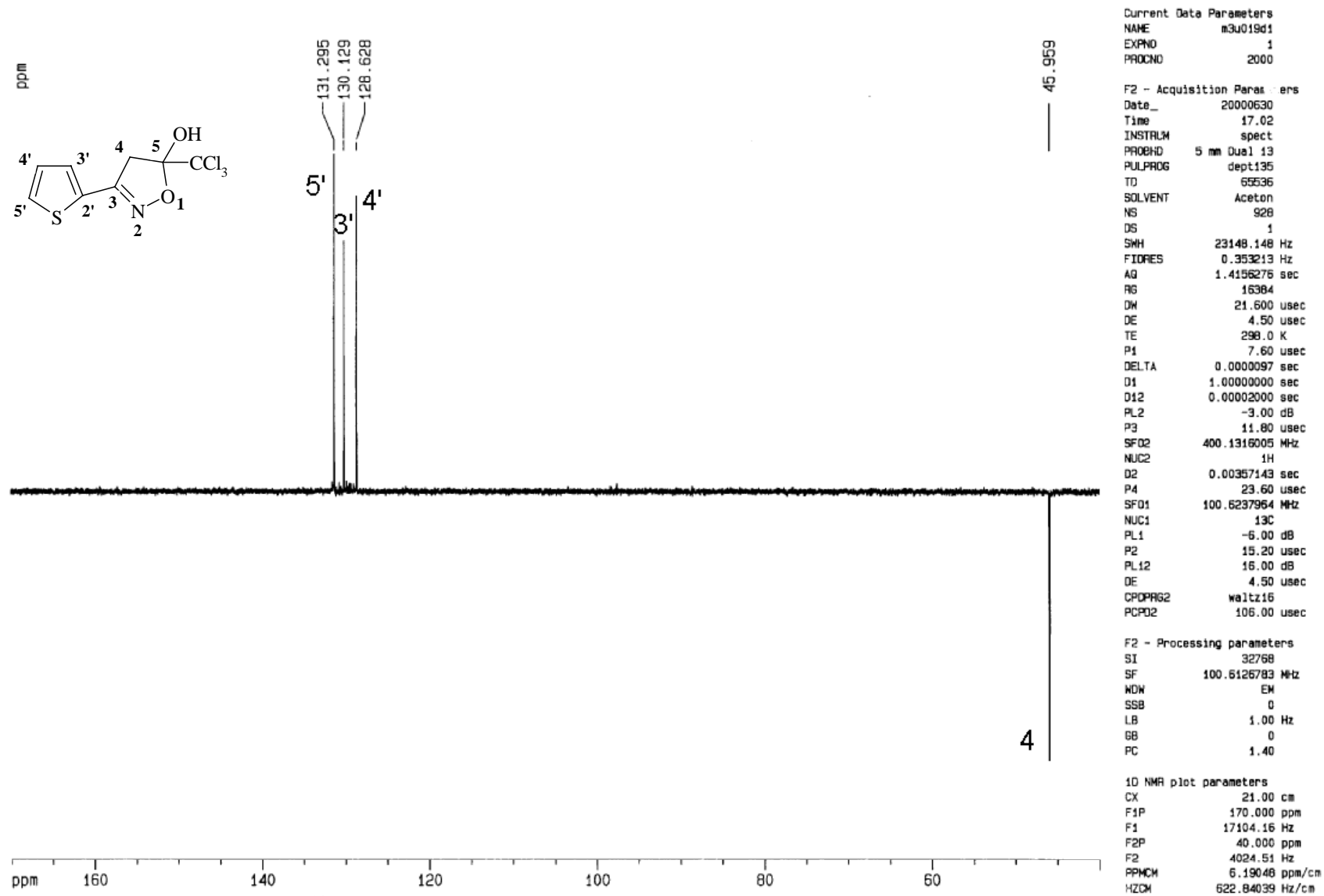


Figura 42. Espectros de RMN ^{13}C (DEPT 135) do 5-triclorometil-3-[2-tienil]-5-hidroxi-4,5-diidro-isoxazol (**6b**) em acetona.

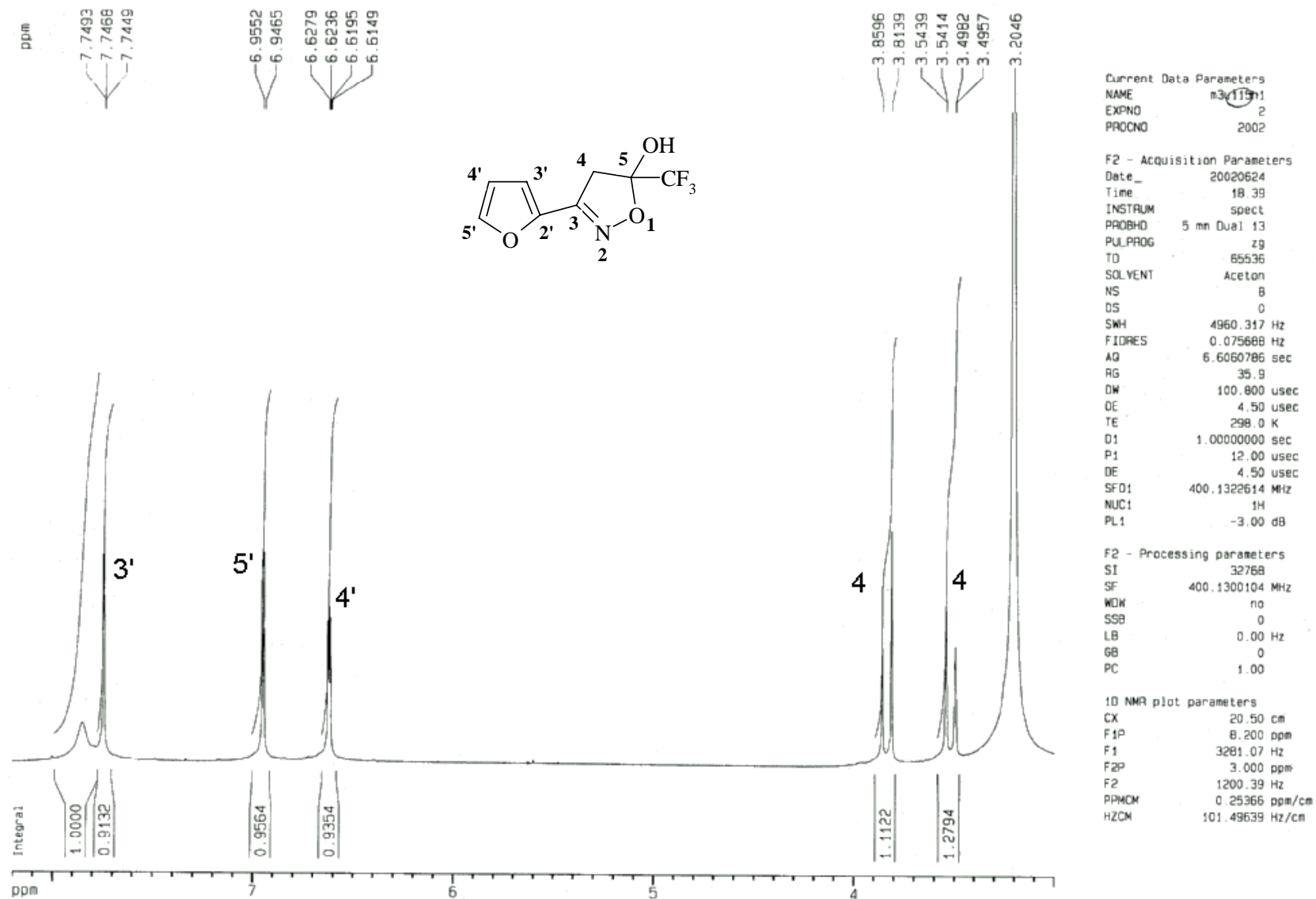


Figura 43. Espectros de RMN ^1H do 5-trifluormetil-3-[2-furil]-5-hidroxi-4,5-diidro-isoxazol (**7a**) em acetona.

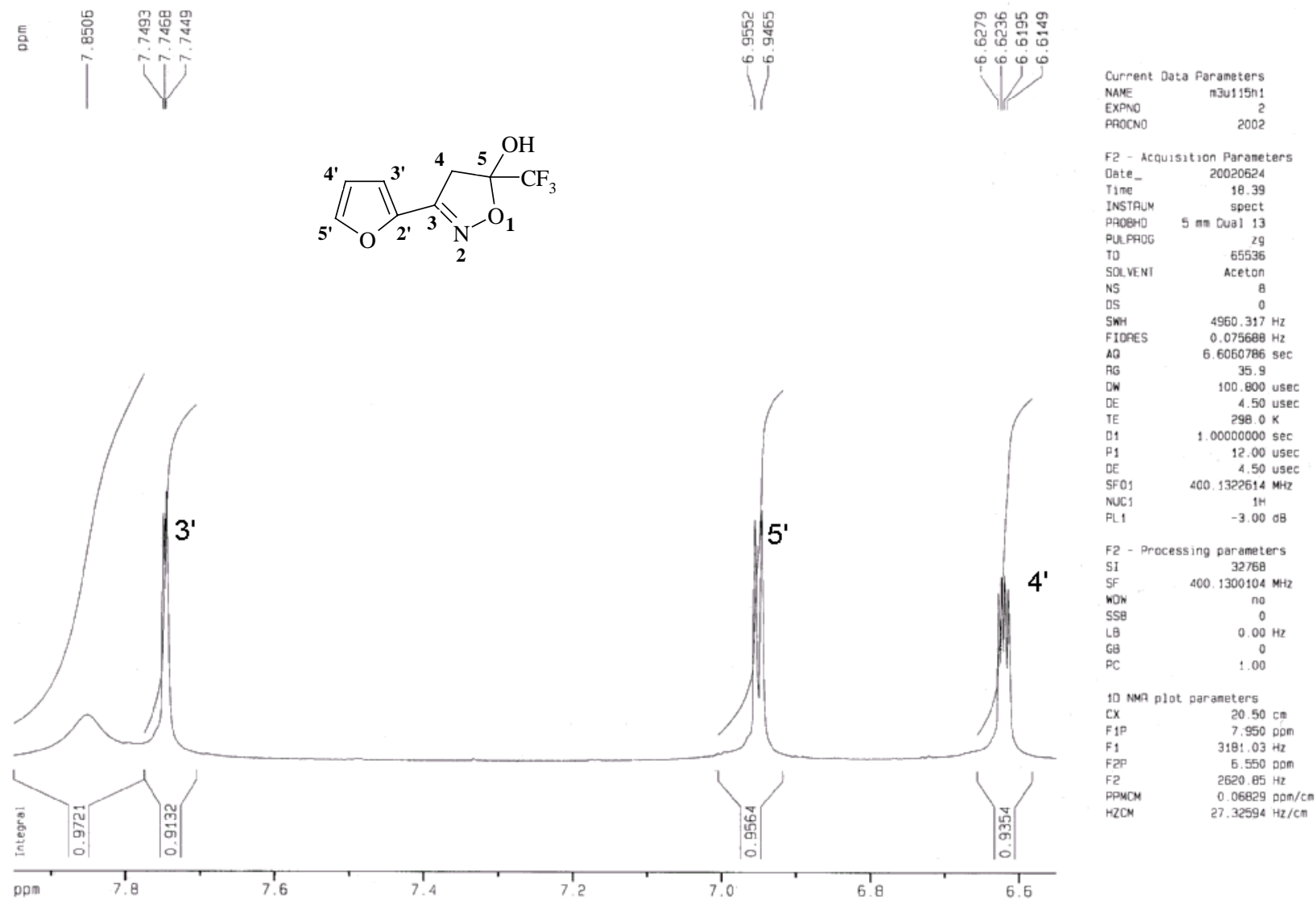


Figura 44. Espectros de RMN ^1H , expansão entre 6,6-7,8 ppm do 5-trifluorometil-3-[2-furil]-5-hidroxi-4,5-diidro-isoxazol (**7a**) em acetona.

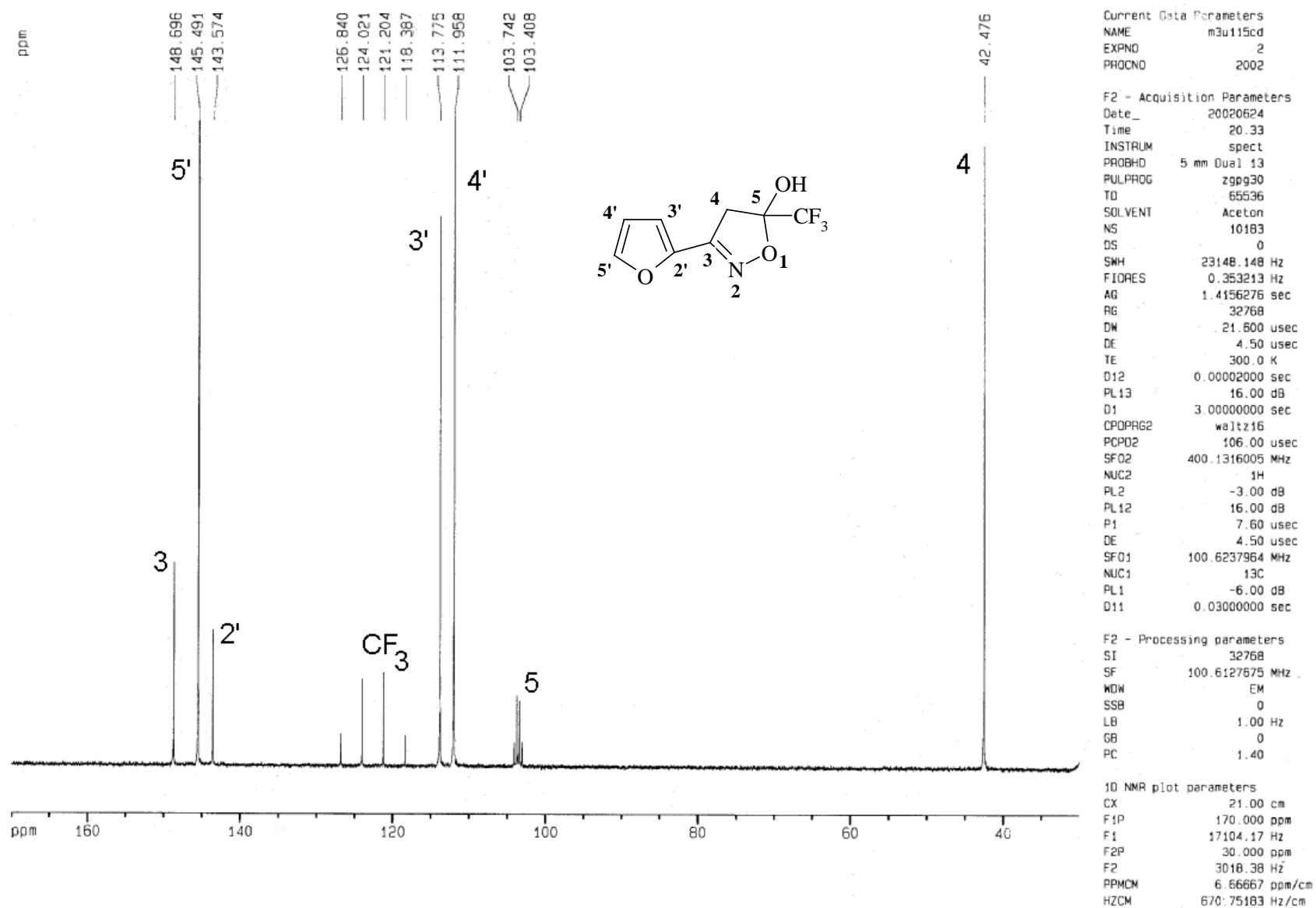


Figura 45. Espectros de RMN ¹³C do 5-trifluormetil-3-[2-furil]-5-hidroxi-4,5-diidro-isoxazol (**7a**) em acetona.