

**Investigação Fitoquímica, Atividade Antioxidante, Antifúngica e Antibacteriana da Parte Aérea da Macrófita *Paspalum Repens* P. J. Bergius
Wust, K. M.; Cornelius, M. T. F.; Schirmann, J.; Braun, G.; Sarragiotto, M. H.; Olguin, C. F. A.***

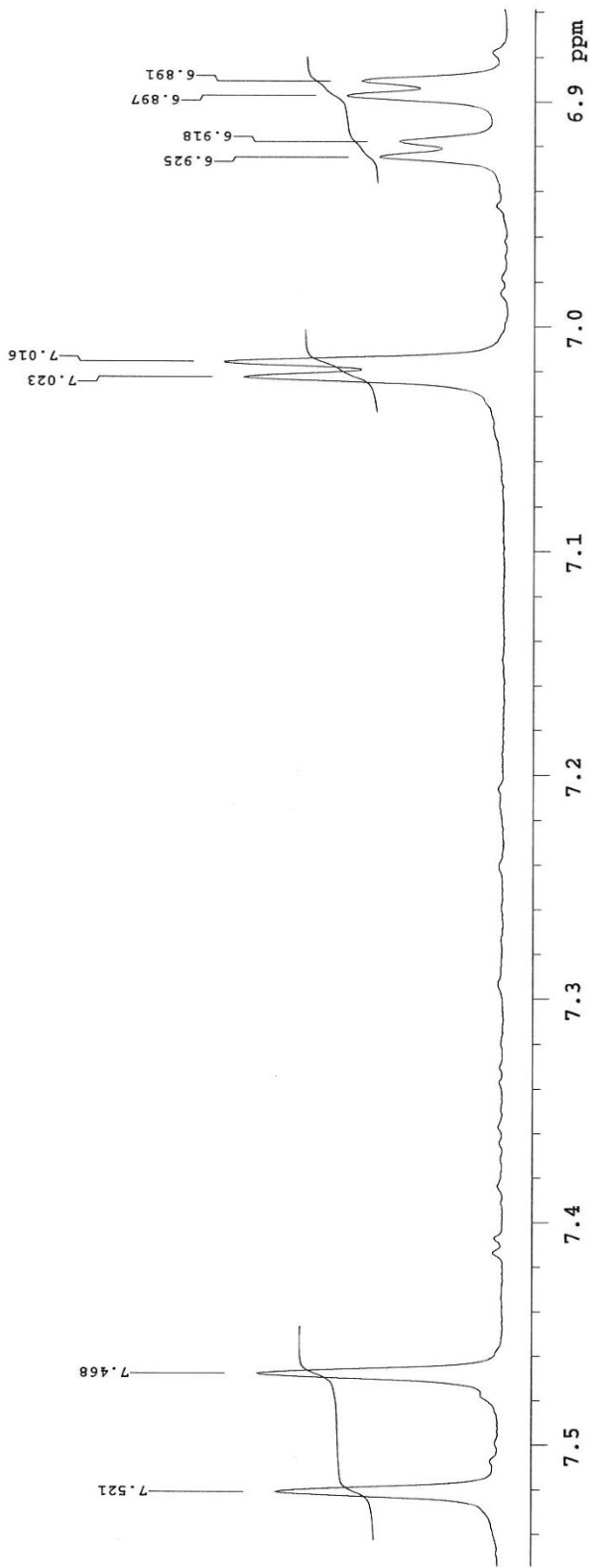
Rev. Virtual Quim., 2016, X (X), S1-S20. Data de publicação na Web: 19 de setembro de 2016

<http://rvq.sbq.org.br>

MATERIAL SUPLEMENTAR

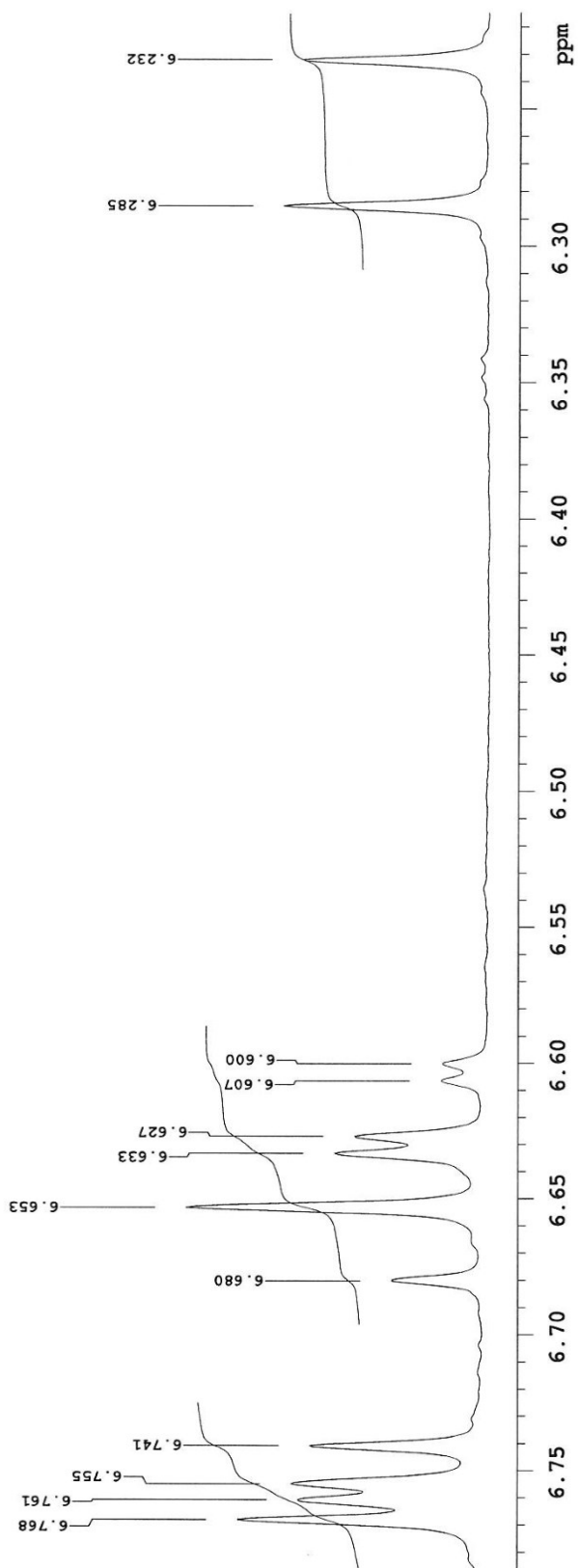
Espectros de RMN ^1H e ^{13}C (1D e 2D)

MHIK42-46-H1
Keli Maiara-DQI
File: MHIK42-46-H1
Pulse Sequence: s2pul



b) Expansão do espectro de RMN de próton (região de 7,7 a 6,7 ppm) do composto 1.

MHIK42-46-H1
Keli Maiana-DQI
File: MHIK42-46-H1
Pulse Sequence: s2pul



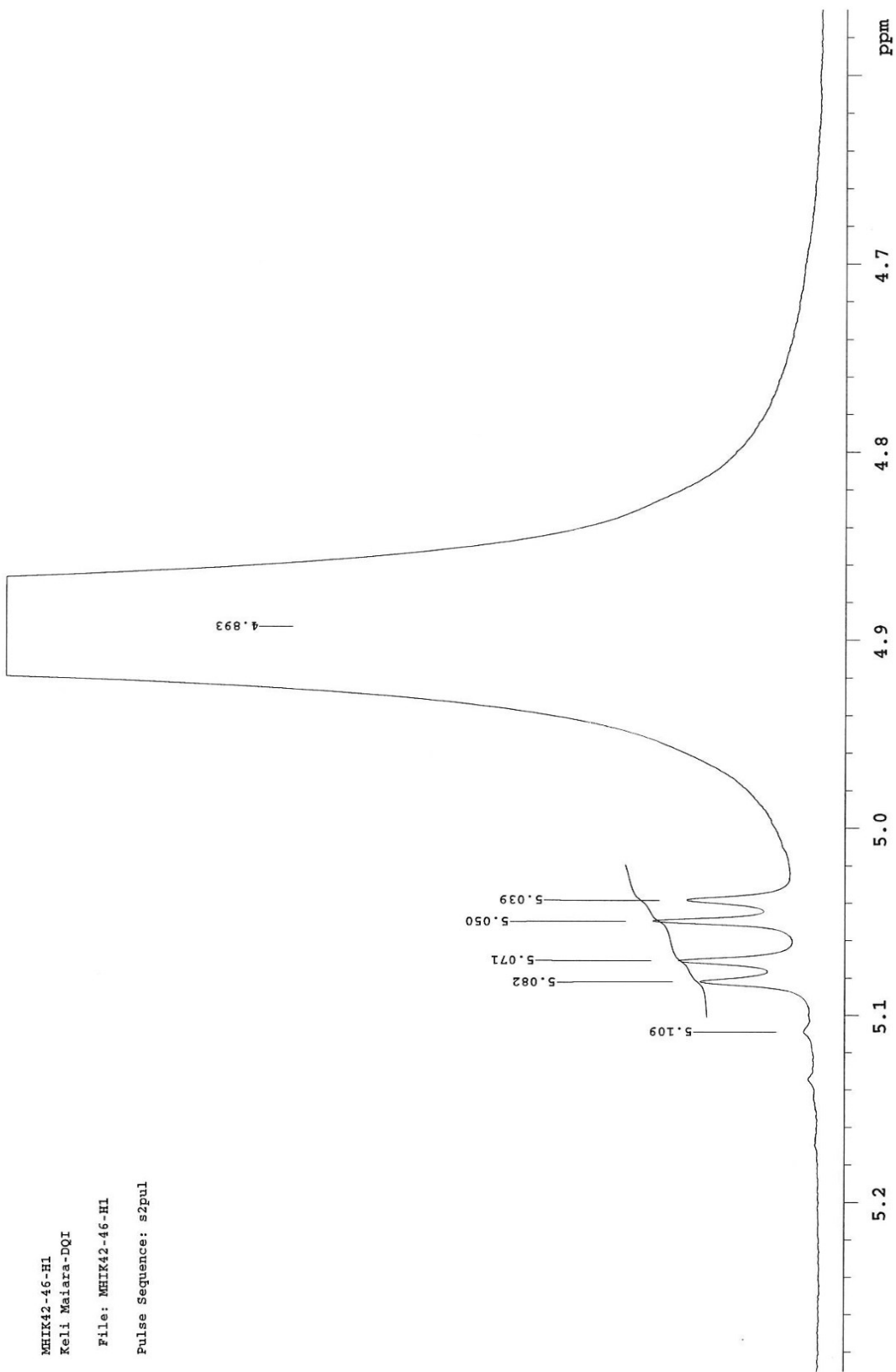
c) Expansão do espectro de RMN de próton (região de 6,9 a 6,2 ppm) do composto 1.

impresso na UNIVERSIDADE FEDERAL DO RIO DE JANEIRO

MHIK42-46-H1
Keli Máia-DQI

File: MHIK42-46-H1

Pulse Sequence: s2pul



d) Expansão do espectro de RMN de próton (região de 5,5 a 4,6 ppm) do composto 1.

impresso na UNIVES-LE - catala.terraira

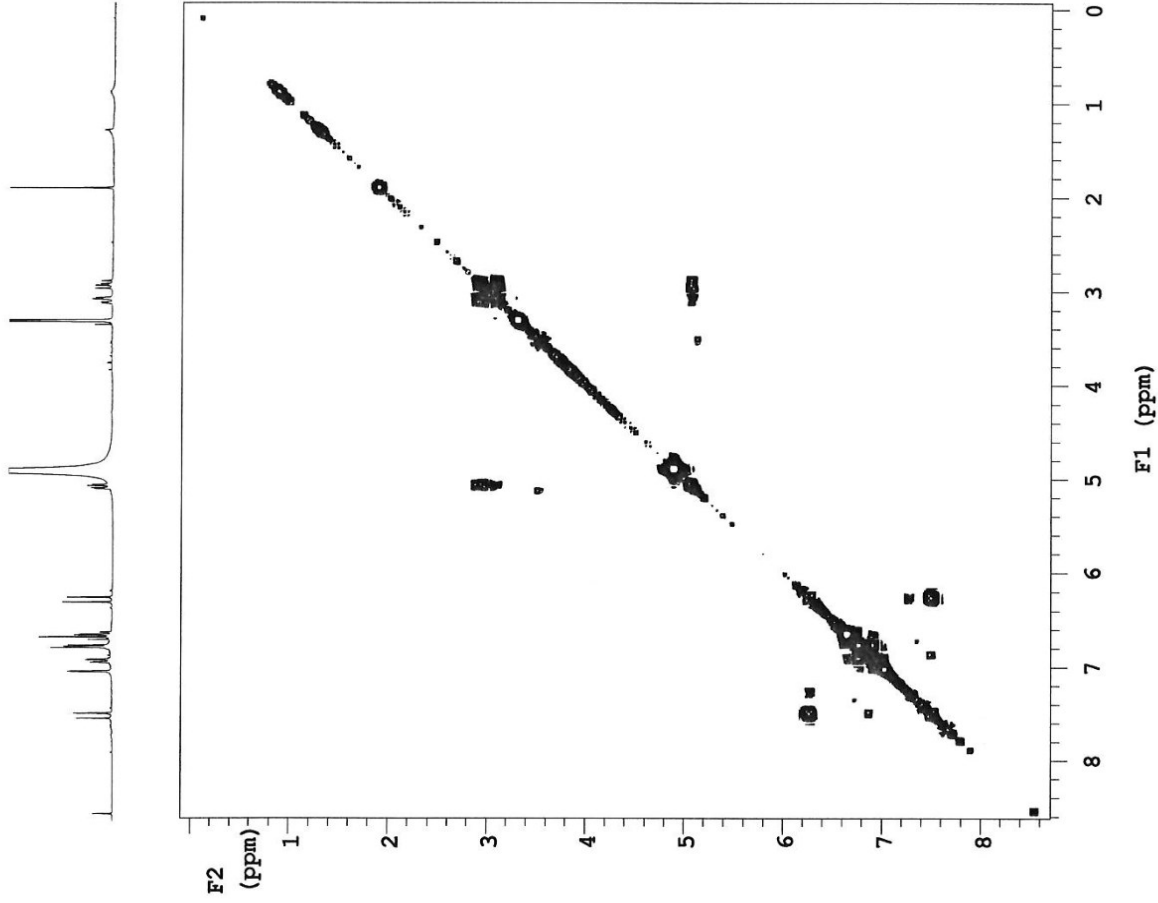
MHIK42-46-gCOSY
Keli-DQI

File: MHIK42-46-gCOSY

Pulse Sequence: gCOSY

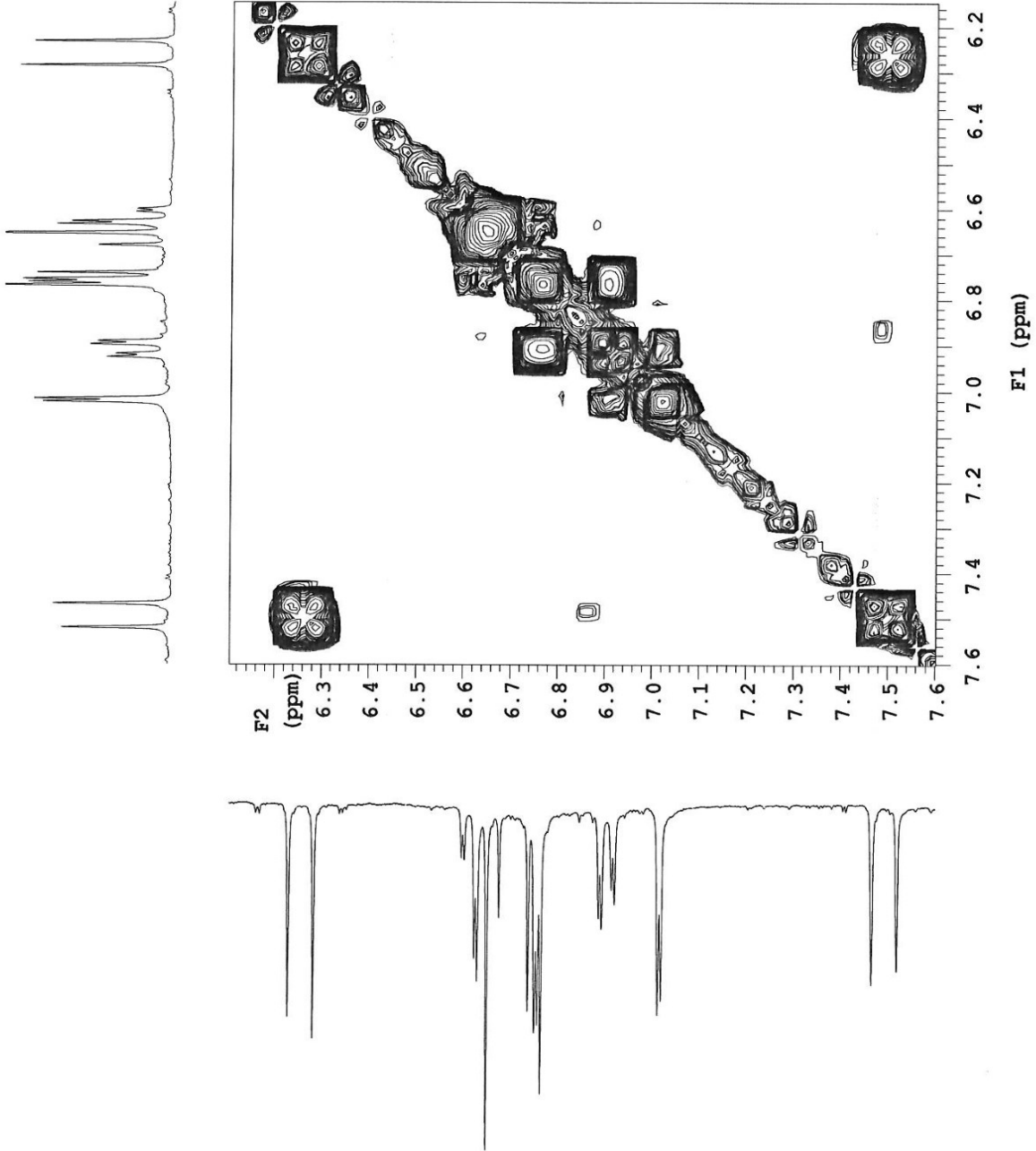
Solvent: cd3od
Ambient temperature
Operator: ivania
File: MHIK42-46-gCOSY
Mercury-300BB "uem-dqi-rmn"

Relax. delay 1.301 sec
Acq. time 0.166 sec
Width 3084.5 Hz
2D Width 3084.5 Hz
4 repetitions
128 increments
OBSERVE H1, 300.0581265 MHz
DATA PROCESSING
Sq. sine bell 0.083 sec
F1 DATA PROCESSING
Sq. sine bell 0.041 sec
FT size 2048 x 2048
Total time 14 min, 7 sec



e) Mapa de contornos COSY ($^1\text{H} \times ^1\text{H}$) do composto 1.

MHIK42-46-gCOSY
 Keli-DQI
 File: MHIK42-46-gCOSY
 Pulse Sequence: gCOSY



f) Expansão do mapa de contornos COSY (região de 7,6 a 6,2 ppm) do composto 1.

MHIK42-46-C13
Keli-DQI

File: MHIK42-46-C13

Pulse Sequence: s2pul

Solvent: cd3od

Ambient temperature

Operator: ivania

File: MHIK42-46-C13

Mercury-300BB "uem-dqi-rmr"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.301 sec

Width 18115.9 Hz

13008 repetitions

OBSERVE C13, 75.4496759 MHz

DECOUPLE H1, 300.0596027 MHz

Low power 10 dB atten.

continuously on

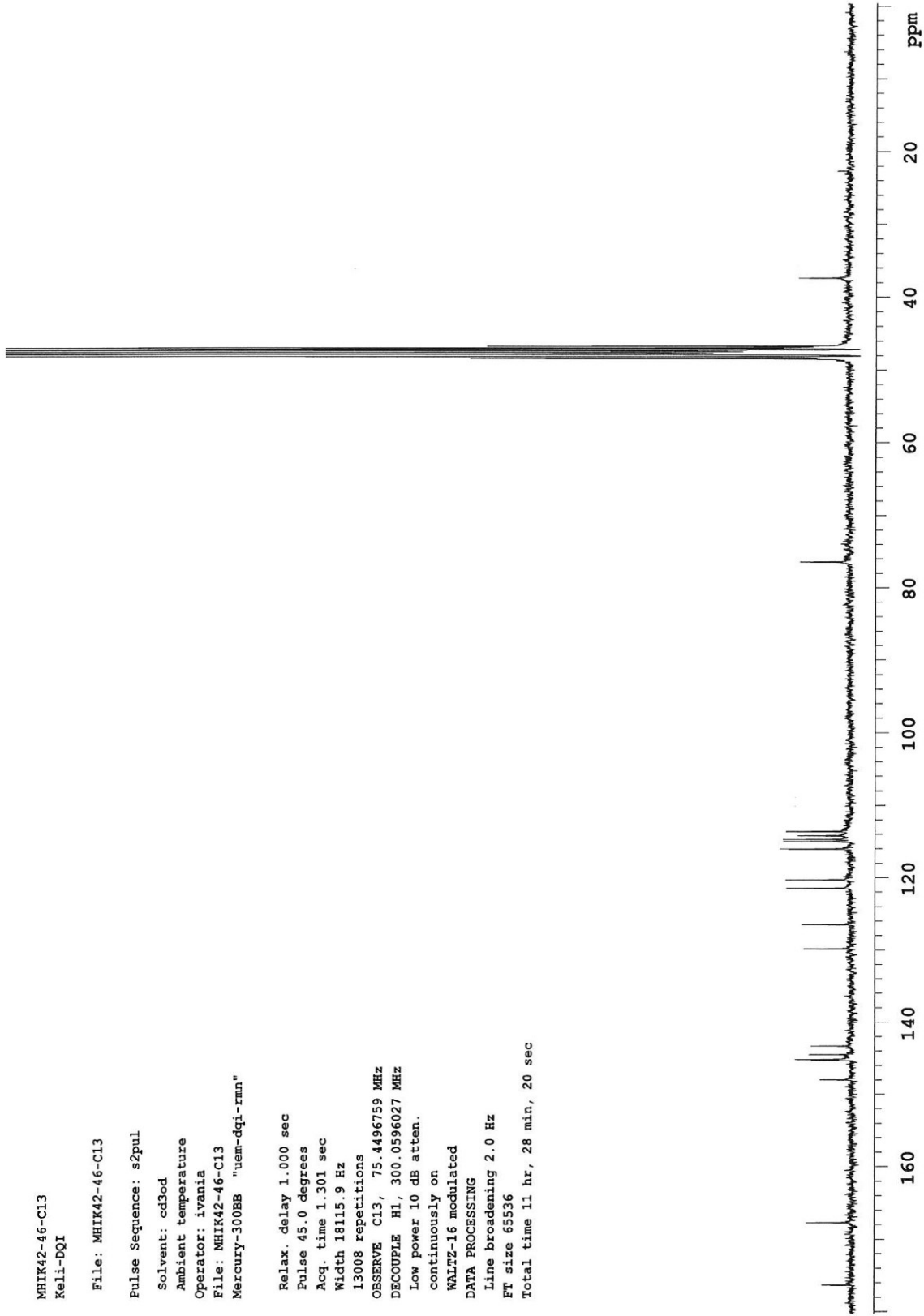
WALTZ-16 modulated

DATA PROCESSING

Line broadening 2.0 Hz

FT size 65536

Total time 11 hr, 28 min, 20 sec



g) Espectro de RMN de carbono-13 (75,5 MHz, CD₃OD) do composto 1.

MHIK42-46-gHSQC
Keli-DQI

File: MHIK42-46-gHSQC

Pulse Sequence: gHSQC

Solvent: cd3od

Ambient temperature

Operator: ivania

File: MHIK42-46-gHSQC

Mercury-300BB "nem-dqi-rmn"

Relax. delay 1.301 sec

Acq. time 0.199 sec

Width 3084.5 Hz

2D Width 12826.7 Hz

16 repetitions

2 x 128 increments

OBSERVE H1, 300.0581265 MHz

DECOUPLE C13, 75.4553346 MHz

Low power 10 dB atten.

on during acquisition

off during delay

GARP-1 modulated

DATA PROCESSING

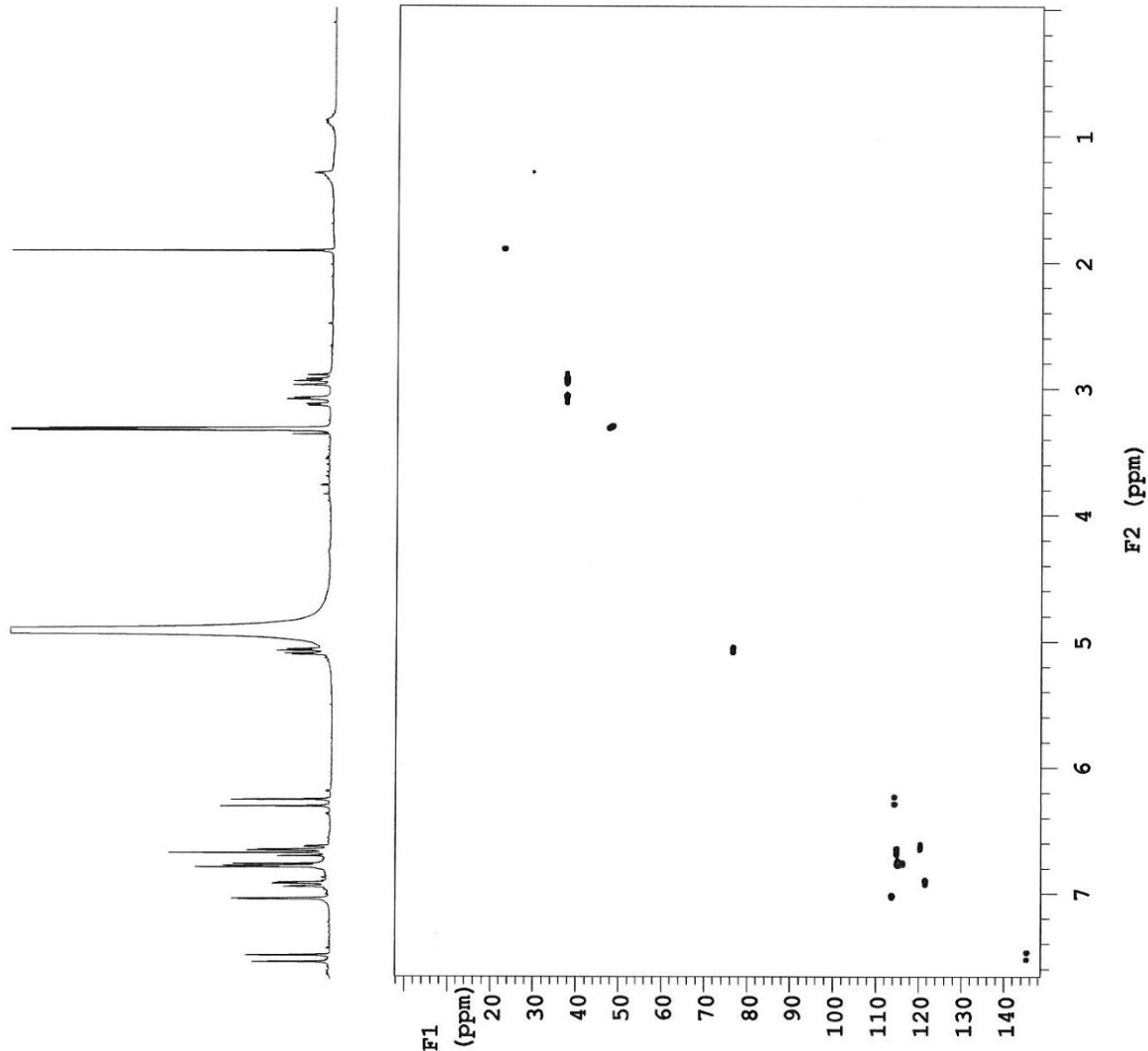
Gauss apodization 0.092 sec

F1 DATA PROCESSING

Gauss apodization 0.009 sec

FT size 2048 x 2048

Total time 1 hr, 54 min, 1 sec



h) Mapa de contornos HSQC ($^1\text{H} \times ^{13}\text{C}$) do composto I.

impresso na UNIVESITE - caixa,terreira

J5Fr53234-H1
Manuela/Maria Helena-DQI

File: Proton

Pulse Sequence: s2pul

Solvent: cd3od

Ambient temperature

Operator: ivania

Mercury-300BB "uem-dqi-rmn"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 3.333 sec

Width 4800.8 Hz

64 repetitions

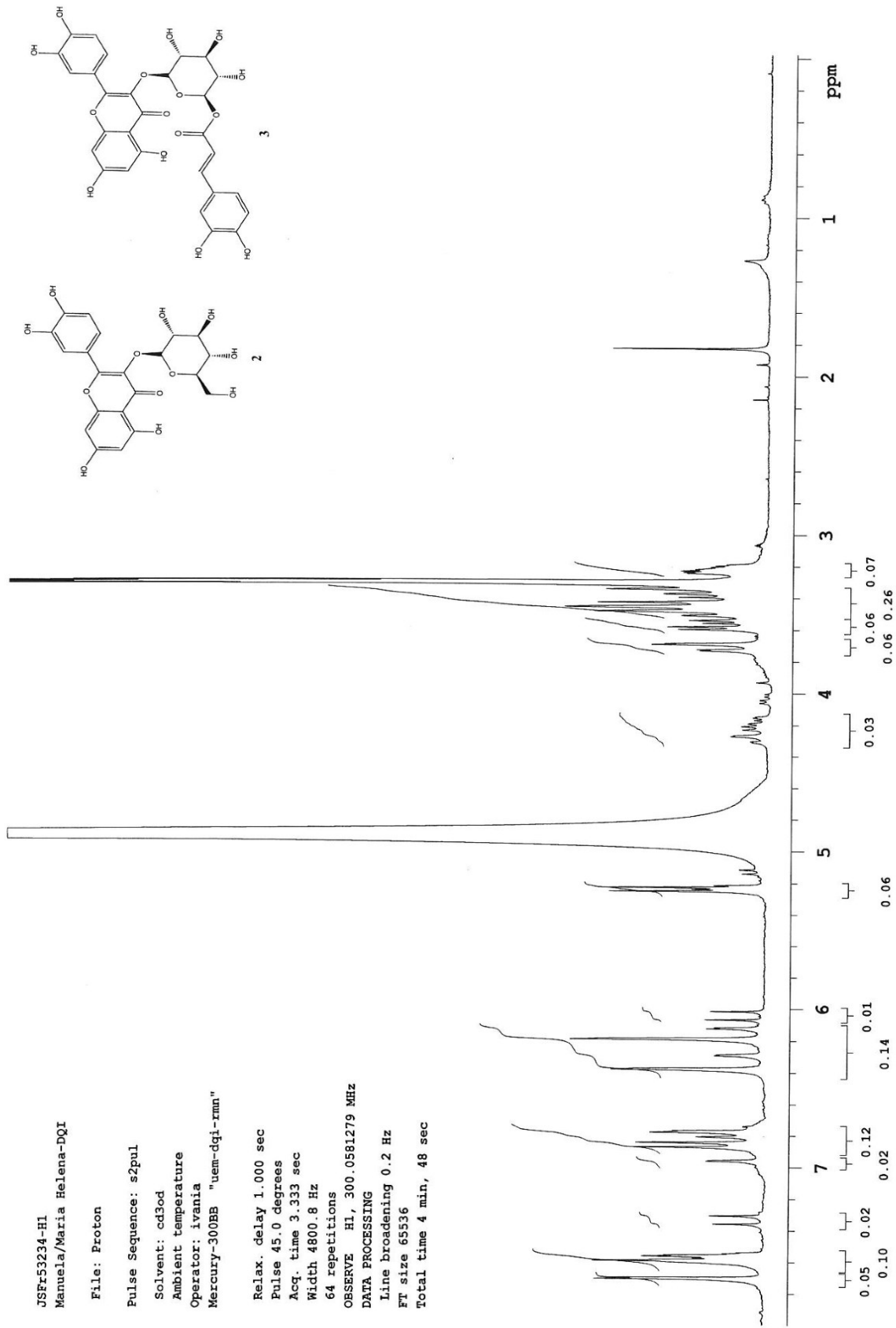
OBSERVE H1, 300.0581279 MHz

DATA PROCESSING

Line broadening 0.2 Hz

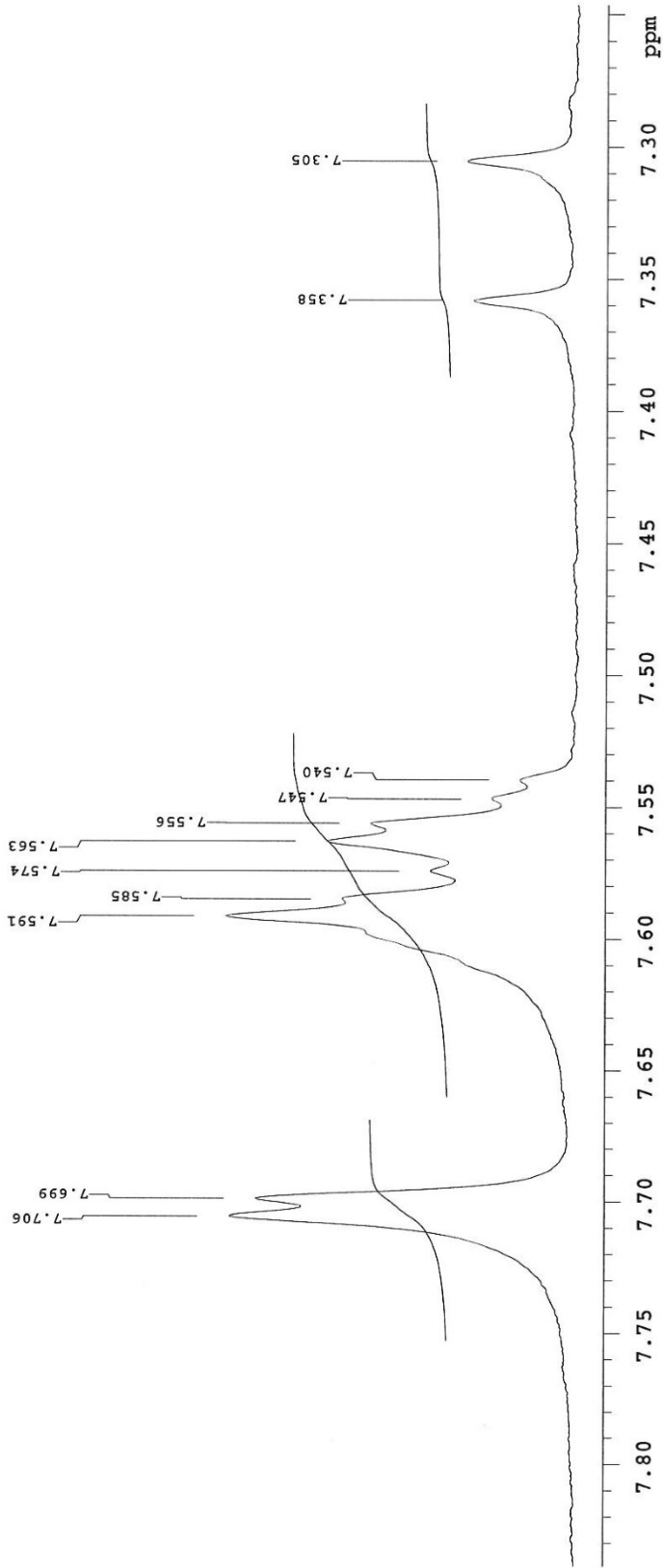
FT size 65536

Total time 4 min, 48 sec



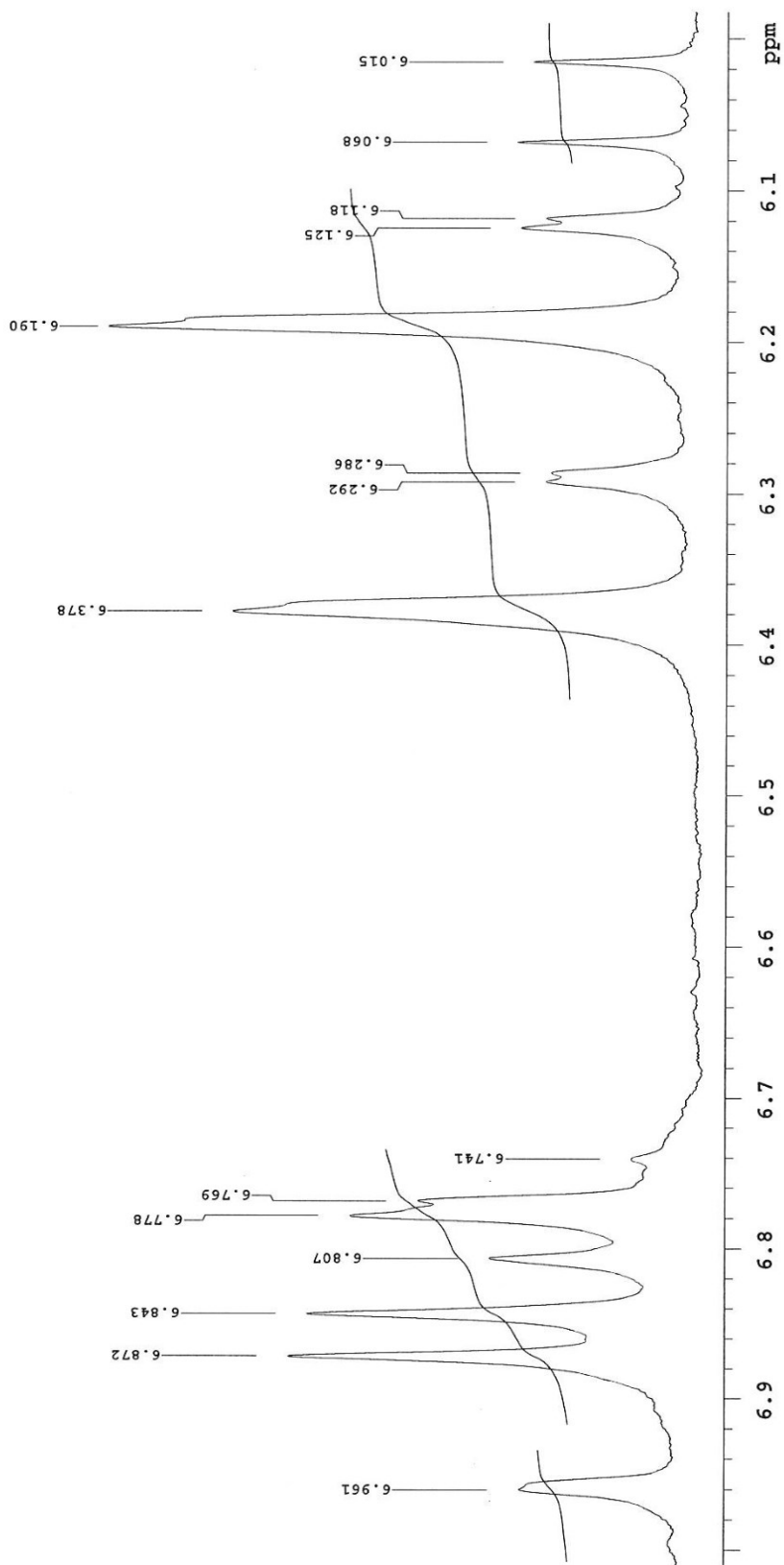
i) Espectro de RMN de próton (300 MHz, CD₃OD) dos compostos 2 + 3.

JSF153234-H1
 Manuela/Maria Helena-DQI
 File: Proton
 Pulse Sequence: s2pul

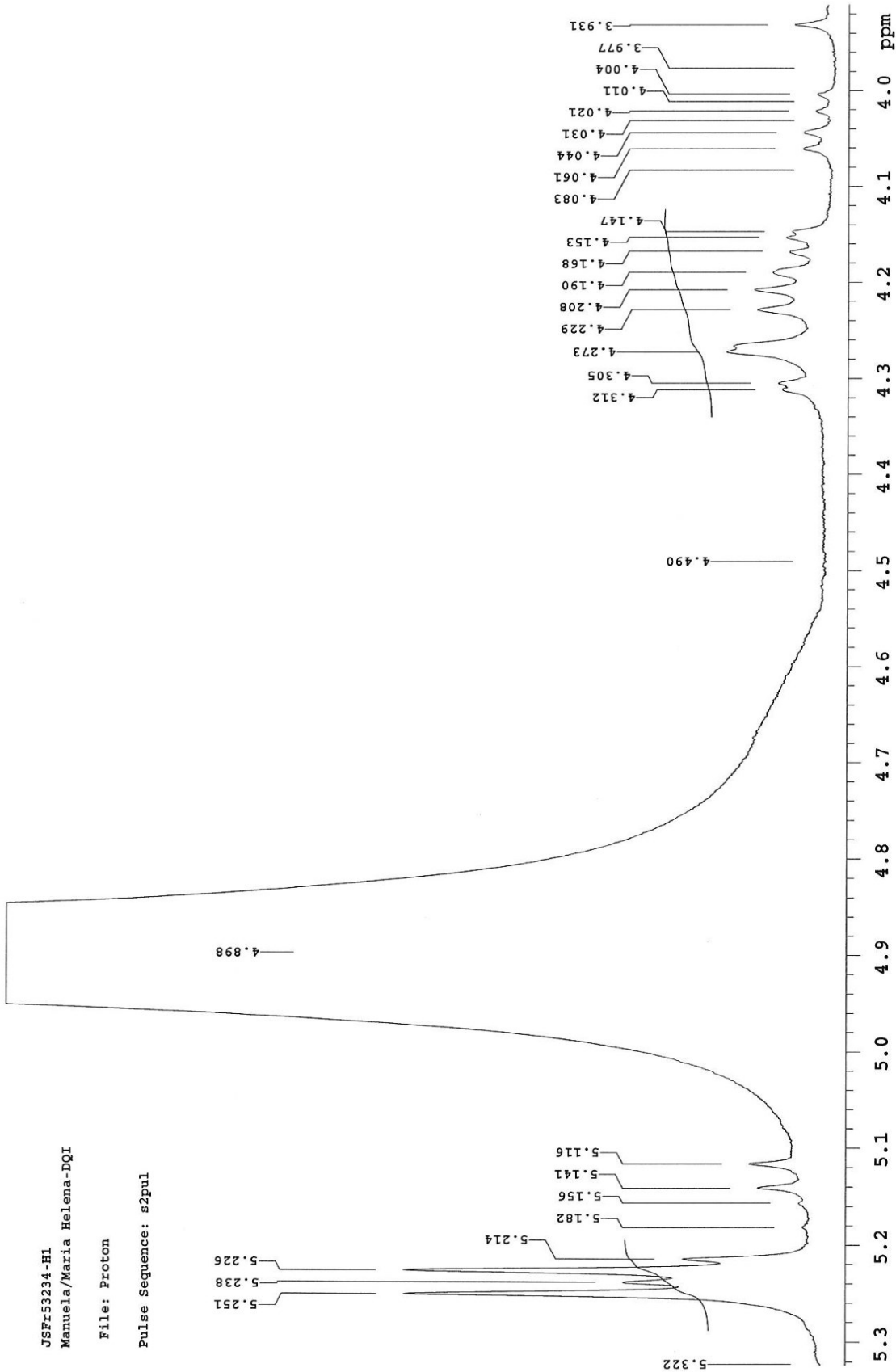


j) Expansão do espectro de RMN de próton (região de 7,8 a 7,2 ppm) dos compostos 2 + 3.

JSPF53234-H1
Manuela/Maria Helena-DQI
File: Proton
Pulse Sequence: s2pul

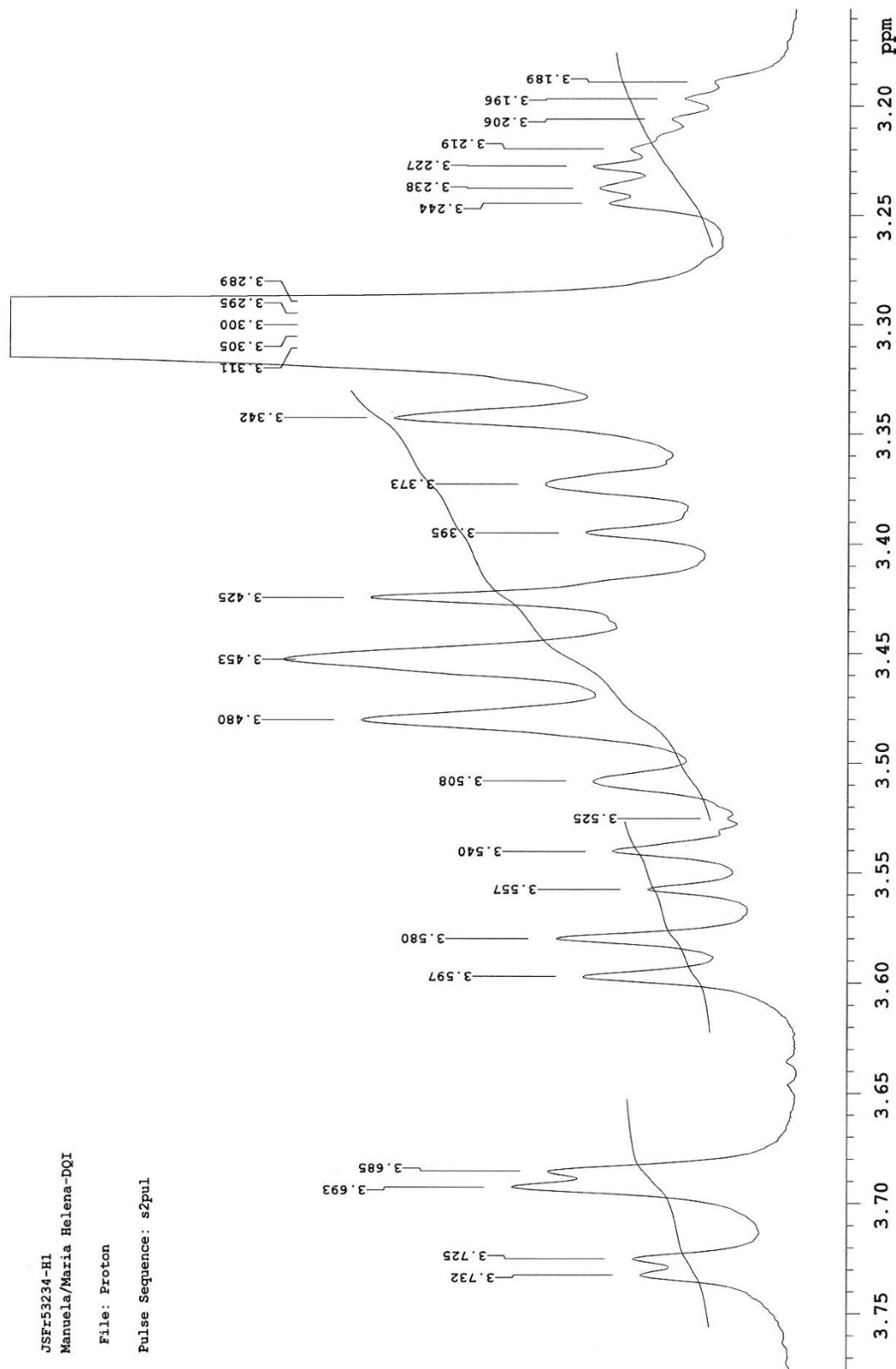


k) Expansão do espectro de RMN de próton (região de 7,0 a 6,0 ppm) dos compostos 2 + 3.



JSF53234-H1
Manuela/Maria Helena-DQI
File: Proton
Pulse Sequence: s2pul

1) Expansão do espectro de RMN de próton (região de 5,3 a 3,8 ppm) dos compostos 2 + 3.



JSF53234-H1
Manuela/Maria Helena-DQ1

File: Proton

Pulse Sequence: s2pul

m) Expansão do espectro de RMN de próton (região de 3,7 a 3,2 ppm) dos compostos 2 + 3.

J5Fr53234-gCOSY
 Maria Helena-DQI

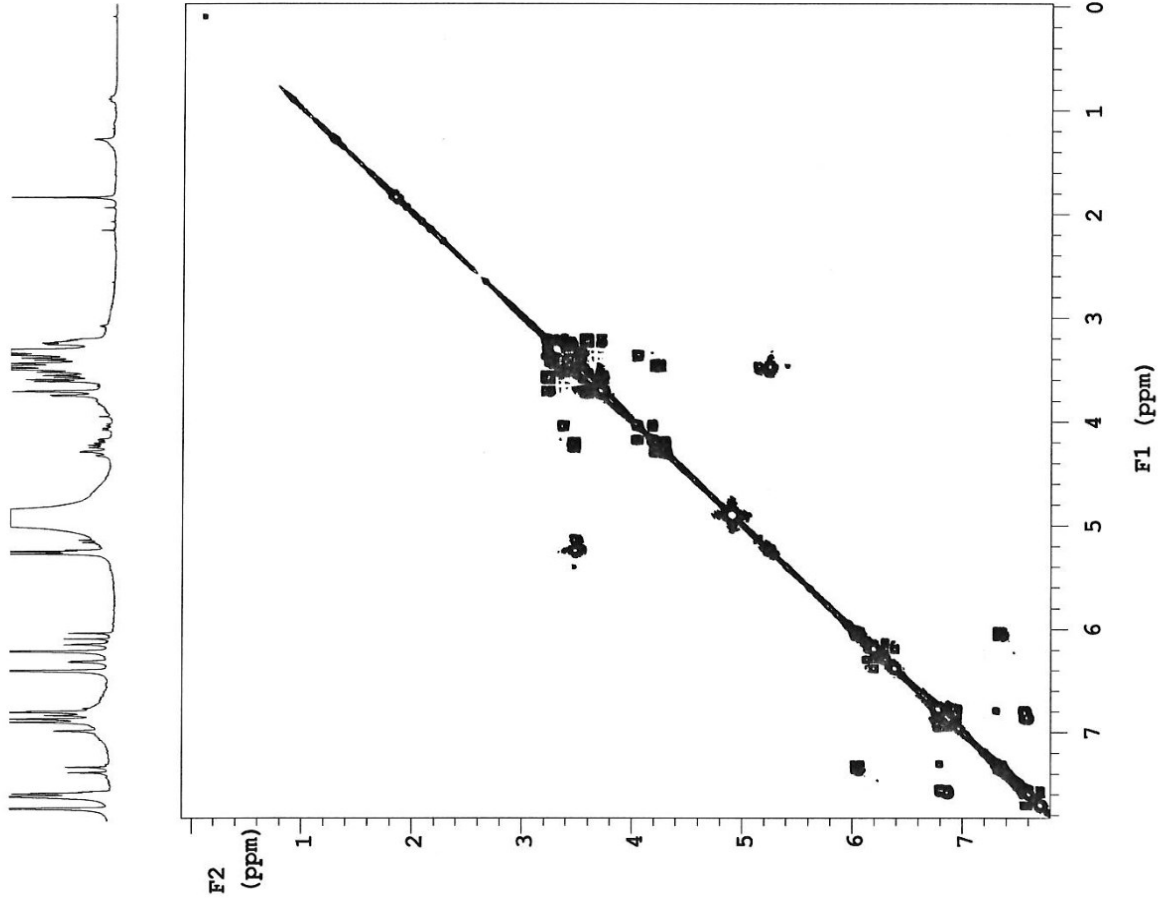
File: J5Fr53234-gCOSY

Pulse Sequence: gCOSY

Solvent: cd3od
 Ambient temperature
 Operator: ivania
 File: J5Fr53234-gCOSY
 Mercury-300BB "uem-dqi-zmn"

Relax. delay 1.301 sec
 Acq. time 0.179 sec
 Width 2861.2 Hz
 2D Width 2861.2 Hz
 8 repetitions
 256 increments
 OBSERVE H1, 300.0581265 MHz
 DATA PROCESSING
 Sg. sine bell 0.089 sec

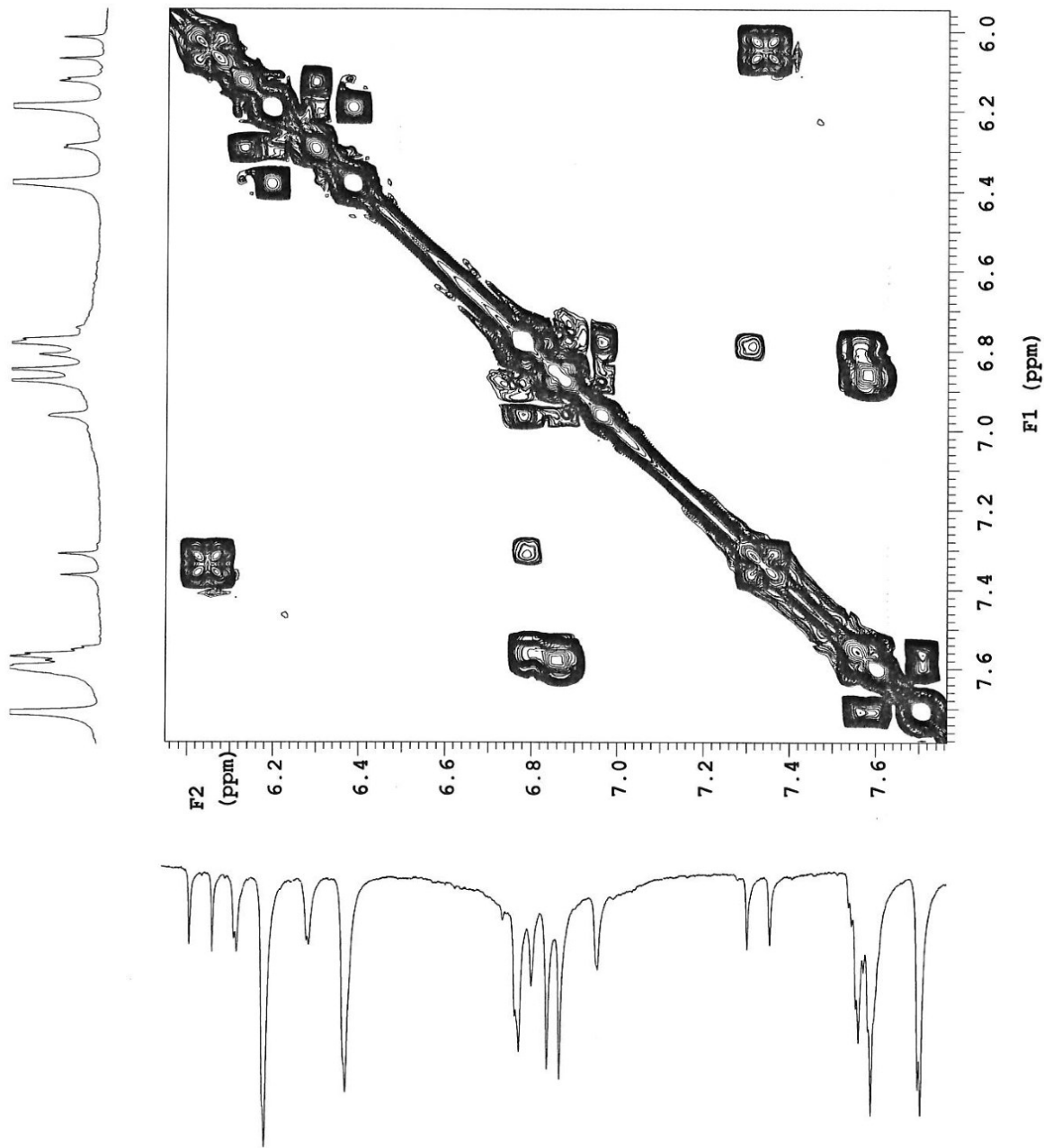
F1 DATA PROCESSING
 Sg. sine bell 0.089 sec
 FT size 4096 x 4096
 Total time 56 min, 16 sec



n) Mapa de contornos COSY ($^1\text{H} \times ^1\text{H}$) dos compostos 2 + 3.

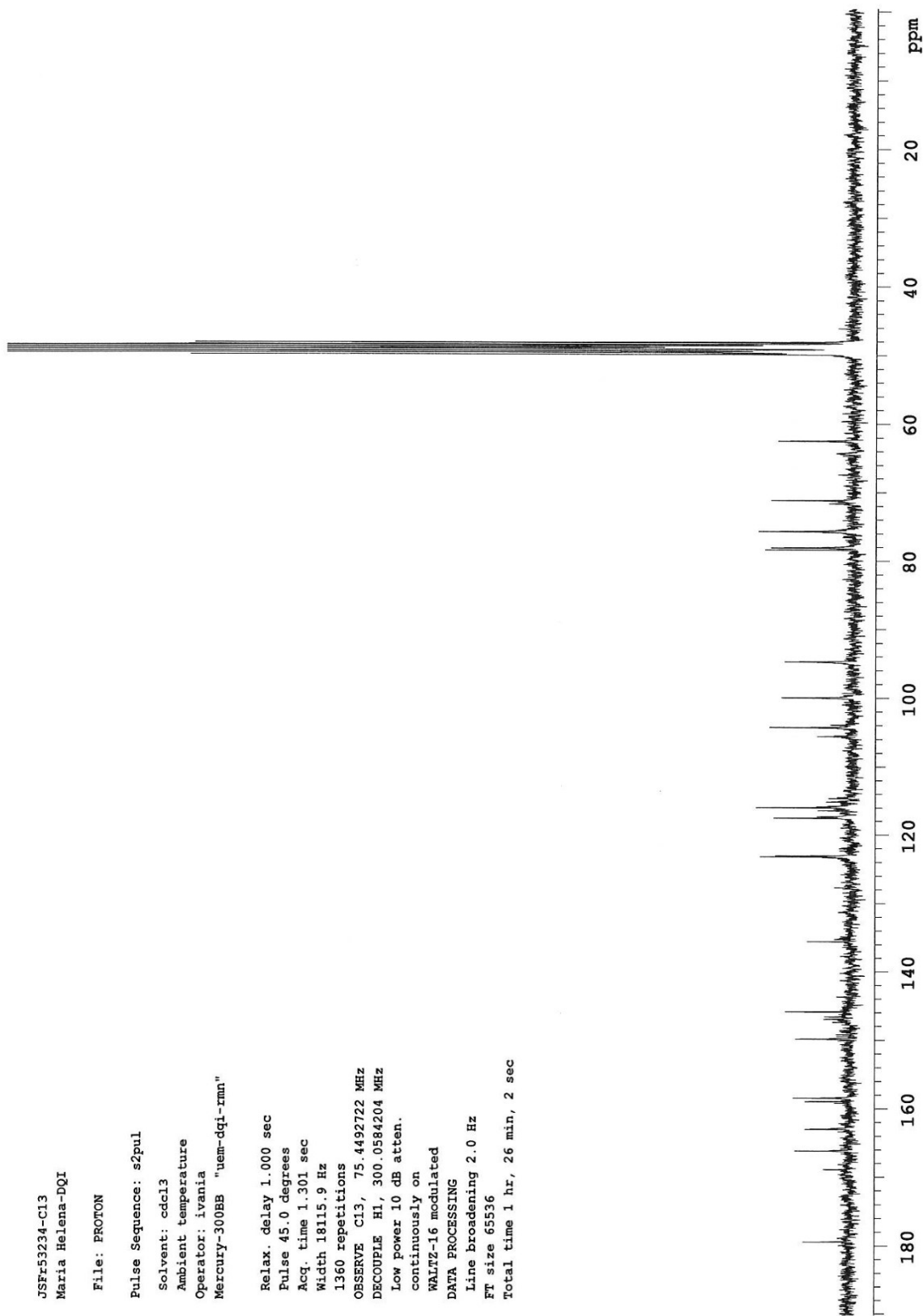
impresso na UNIVES-LE - callia.erroira

JSFr53234-gCOSY
Maria Helena-DQI
File: JSFr53234-gCOSY
Pulse Sequence: gCOSY



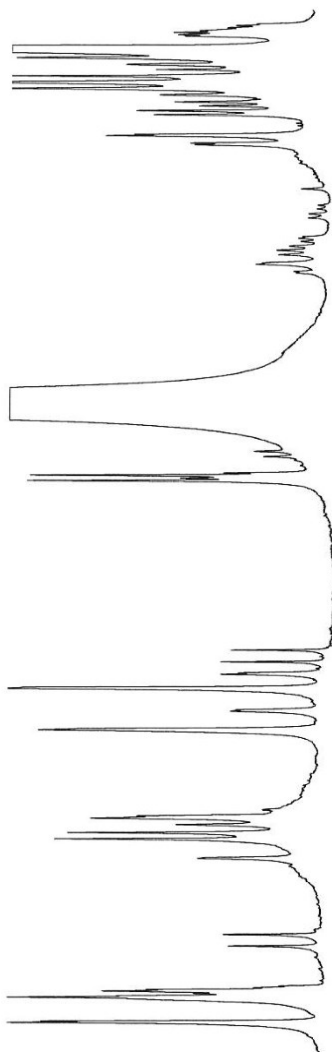
o) Expansão do mapa de contornos COSY (região de 7,6 a 6,2 ppm) dos compostos 2 + 3.

JSFR53234-C13
 Maria Helena-DQI
 File: PROTON
 Pulse Sequence: s2pul
 Solvent: cdcl3
 Ambient temperature
 Operator: ivania
 Mercury-300BB "nem-dqi-rmn"
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.301 sec
 Width 18115.9 Hz
 1360 repetitions
 OBSERVE C13, 75.4492722 MHz
 DECOUPLE H1, 300.0584204 MHz
 Low power 10 dB atten.
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 2.0 Hz
 FT size 65536
 Total time 1 hr, 26 min, 2 sec



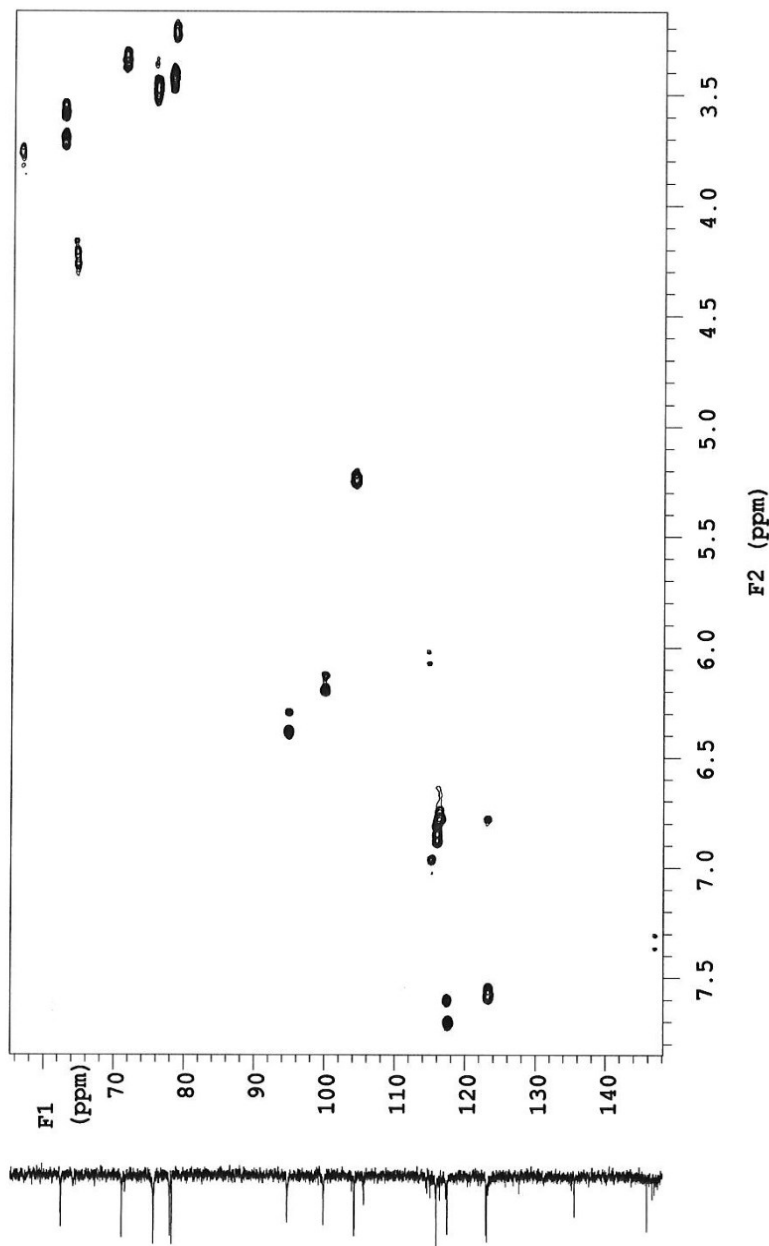
p) Espectro de RMN de carbono-13 (75,5 MHz, CD₃OD) dos compostos 2 + 3.

impresso na UNIVESITE - caua.rerreira



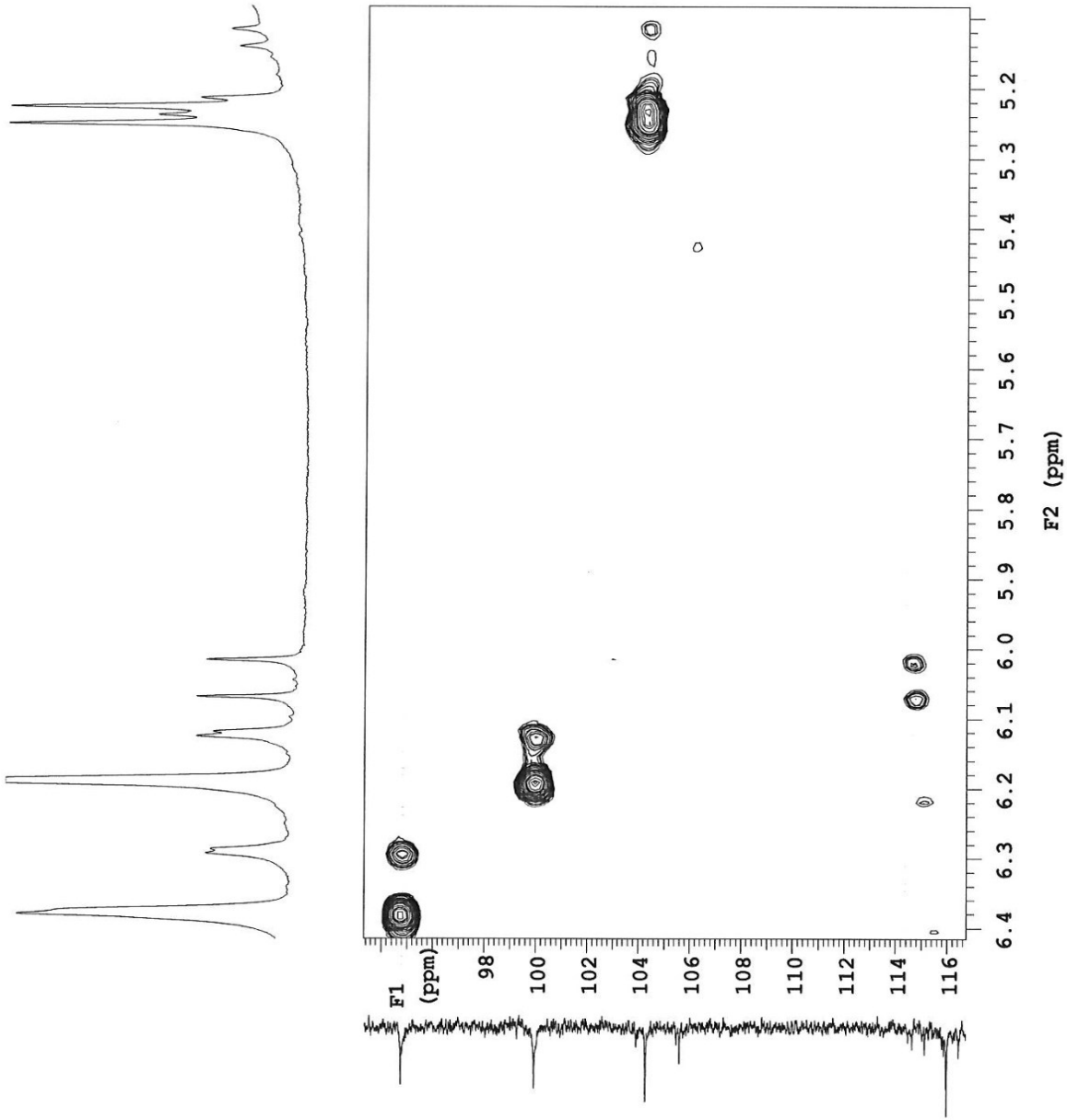
JSFr53234-gHSQC
 Maria Helena-DQI
 File: JSFr53234-gHSQC
 Pulse Sequence: gHSQC
 Solvent: cd3od
 Ambient temperature
 Operator: ivania
 File: JSFr53234-gHSQC
 Mercury-300BB "nem-dqi-rnm"

Relax. delay 1.301 sec
 Acq. time 0.199 sec
 Width 2861.2 Hz
 2D Width 12826.7 Hz
 16 repetitions
 2 x 128 increments
 OBSERVE H1, 300.0581265 MHz
 DECOUPLE C13, 75.4553346 MHz
 Low power 10 dB atten.
 on during acquisition
 off during delay
 GARP-1 modulated
 DATA PROCESSING
 Gauss apodization 0.092 sec
 F1 DATA PROCESSING
 Gauss apodization 0.009 sec
 FT size 2048 x 2048
 Total time 1 hr, 54 min, 1 sec



q) Mapa de contornos HSQC ($^1\text{H} \times ^{13}\text{C}$) dos compostos 2 + 3.

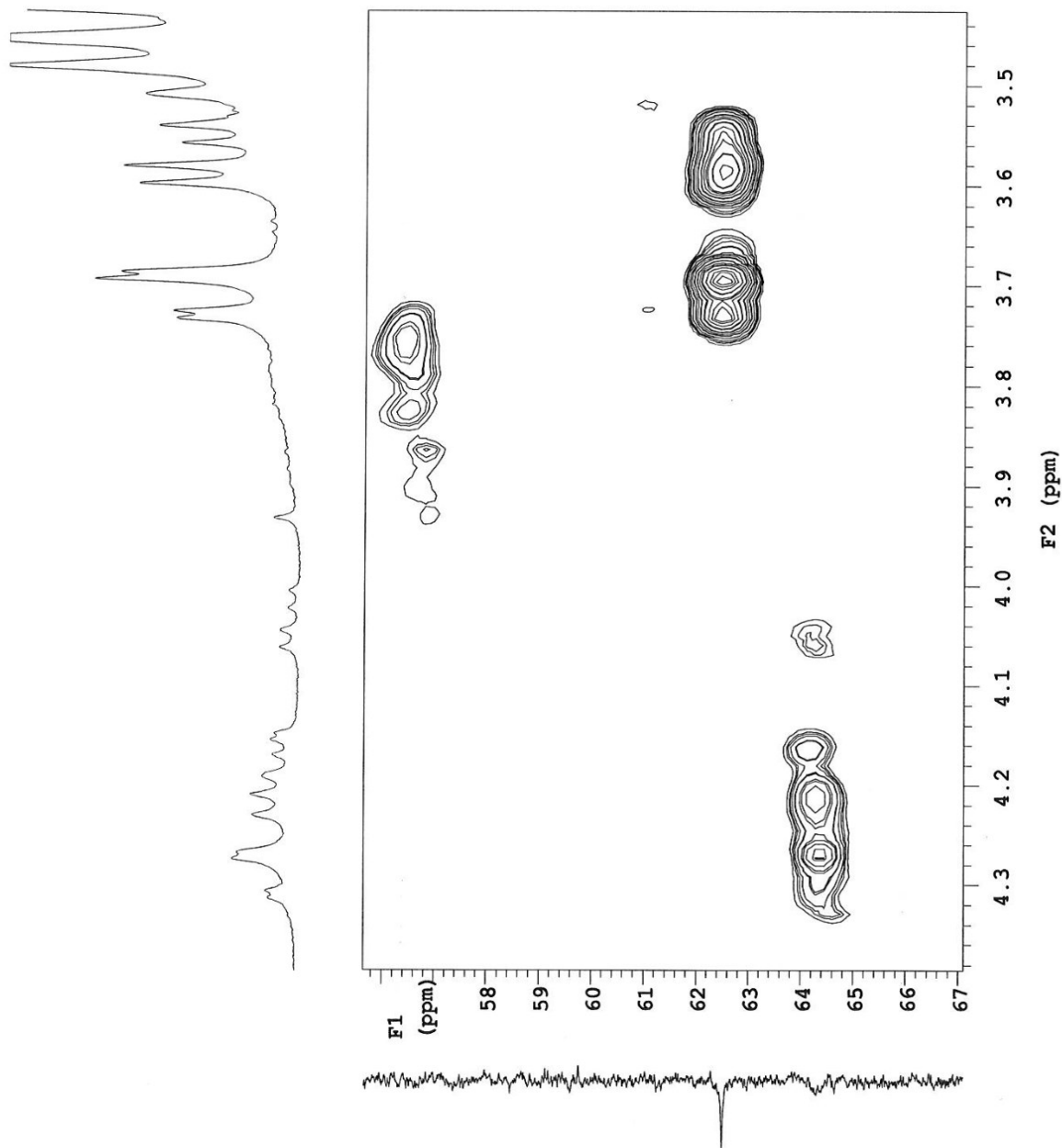
J5F53234-gHSQC
 Maria Helena-DQI
 File: J5F53234-gHSQC
 Pulse Sequence: gHSQC



r) Expansão do mapa de contornos HSQC (região 6,4 a 5,1 ppm) dos compostos 2 + 3.

impresso na UNIVERSIDADE - CATALIA TERRERA

JSFr53234-gHSQC
Maria Helena-DQI
File: JSFr53234-gHSQC
Pulse Sequence: gHSQC



s) Expansão do mapa de contornos HSQC (região 4,3 a 3,5 ppm) dos compostos 2 + 3.