

Supplementary material

Stoichiometry of complex between ligand 1 and TMA maleate

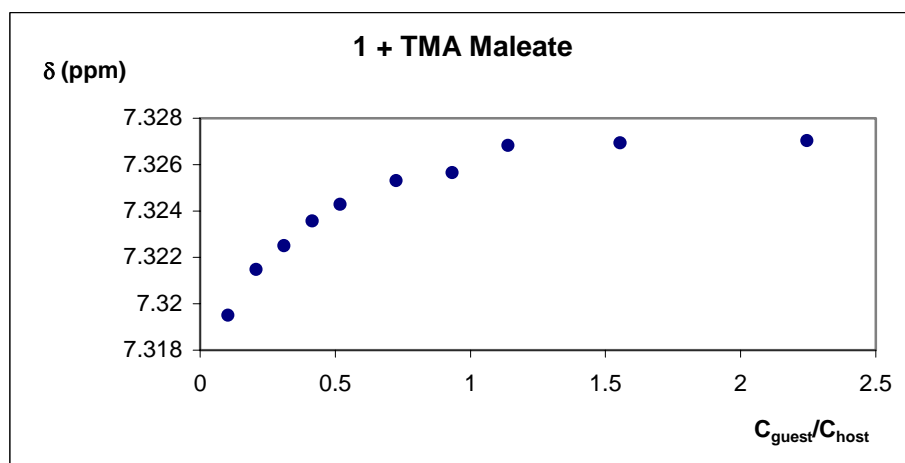
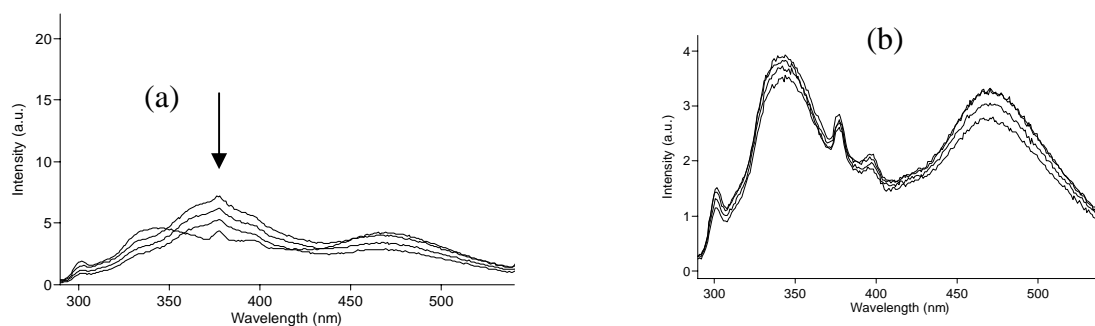


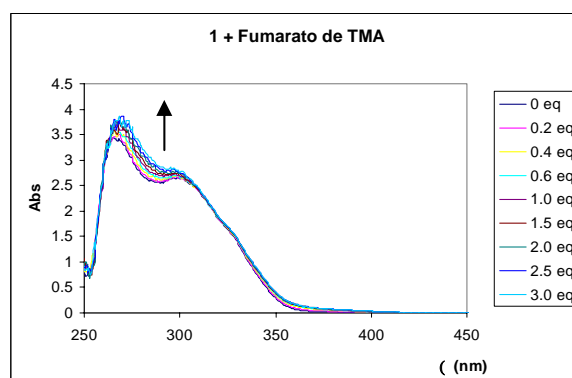
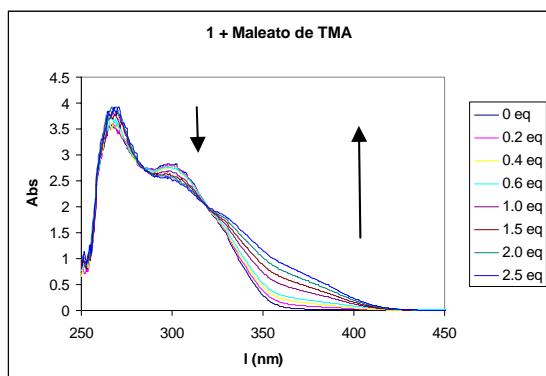
Table 1. Stoichiometry and log K in DMSO for ligands **1** and **2** with TMA fumarate and maleate by using ^1H NMR.

		Ligand 1		Ligand 2	
		TMA fumarate	TMA maleate	TMA fumarate	TMA maleate
^1H RMN	log K	4.39±0.06	5.1±0.9	2.48±0.07	2.88±0.07
	stoichiometry	1:2	1:1	1:2	1:1
UV	log K	5.0±0.3	5.3±0.3	3.0±0.2	2.93±0.16
	stoichiometry	1:2	1:1	1:2	1:1
Fluorescence	log K	4.31±0.02	<i>small modification</i>	2.86±0.15	3.00±0.18
	stoichiometry	1:2		1:2	1:1

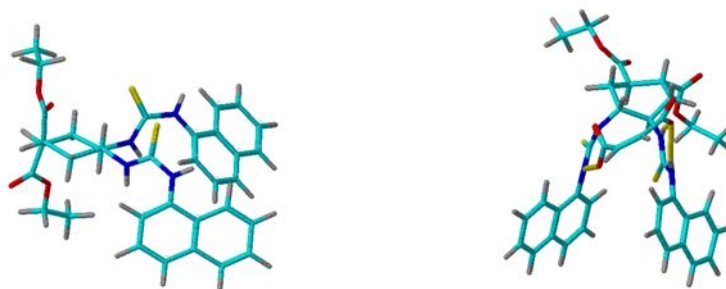
Fluorescence spectra for ligand **2** in DMSO ($\lambda_{\text{exc}} = 275$ nm) (a) in presence of TMA fumarate; (b) in presence of TMA maleate.



UV spectra of ligand **1** in the presence of TMA maleate and TMA fumarate

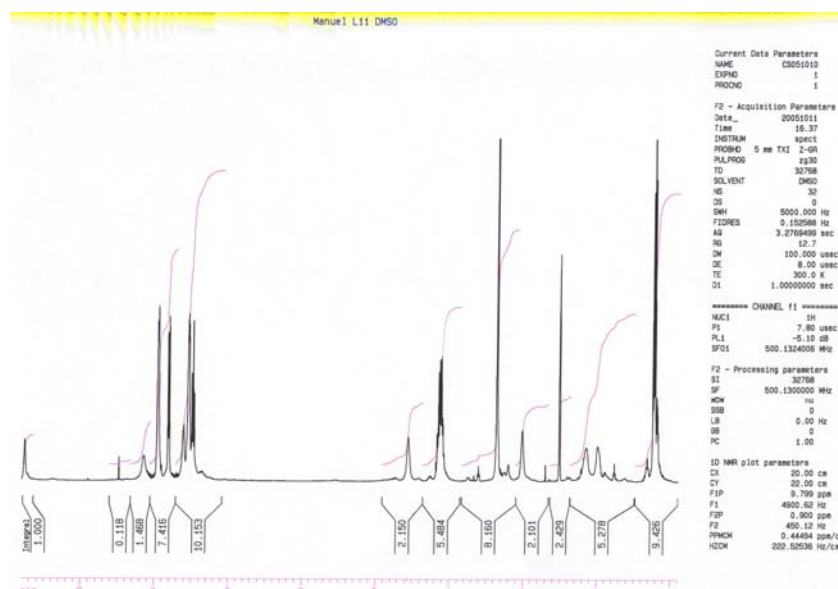


PcModel structures: (a) Ligand **1**, (b) **1**+ TMA maleate.

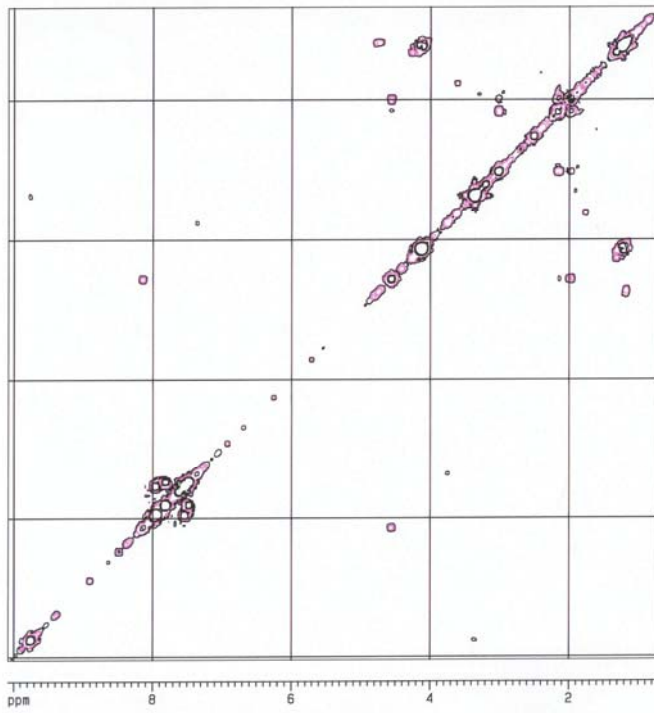


^1H NMR spectra

Ligand **1** in DMSO-d_6



Ligand 1-COSY



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Current Data Parameters
NAME 080510
EXPNO 2
PROCNO 1

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Date_ 20051111
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PULPROG zgpg30
TD 65536
SOLVENT DMS
NS 4
DS 4
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F2RES 0.118623 Hz
AQ 0.001460 sec
RG 32.0
DM 79.800 mm
DE 2.00 mm
TE 300.2 K
AQ 0.000000 sec
SI 1.400000 sec
SFO 500.136000 MHz
SFR 0.000000 MHz
SIR 0.000000 MHz
SDF 0.000000 MHz
SCHM1 0.000000 MHz
KORR 1.400000 MHz

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NUC1 1H
PC 0.00 mm
PI 0.00 mm
PL1 -13.00 dB
PT1 500.131000 MHz

--- BRACKET CHANNEL ---
SFOBRK 836.100
SFRBRK 836.100
SFO1 0.00 MHz
SFR1 0.00 MHz
SFO2 0.00 MHz
SFR2 0.00 MHz
SFO3 40.00 MHz
SFR3 -40.00 MHz
PAB 1000.00 MHz

F1 - Acquisition Parameters
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SWH 800.864 Hz
F2RES 0.118623 Hz
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RG 32.0
DM 79.800 mm
DE 2.00 mm
TE 300.2 K
AQ 0.000000 sec
SI 1.400000 sec
SFO 500.136000 MHz
SFR 0.000000 MHz
SIR 0.000000 MHz
SDF 0.000000 MHz
SCHM1 0.000000 MHz
KORR 1.400000 MHz

--- CHANNEL f1 ---
NUC1 1H
PC 0.00 mm
PI 0.00 mm
PL1 -13.00 dB
PT1 500.131000 MHz

--- BRACKET CHANNEL ---
SFOBRK 836.100
SFRBRK 836.100
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SFR1 0.00 MHz
SFO2 0.00 MHz
SFR2 0.00 MHz
SFO3 40.00 MHz
SFR3 -40.00 MHz
PAB 1000.00 MHz

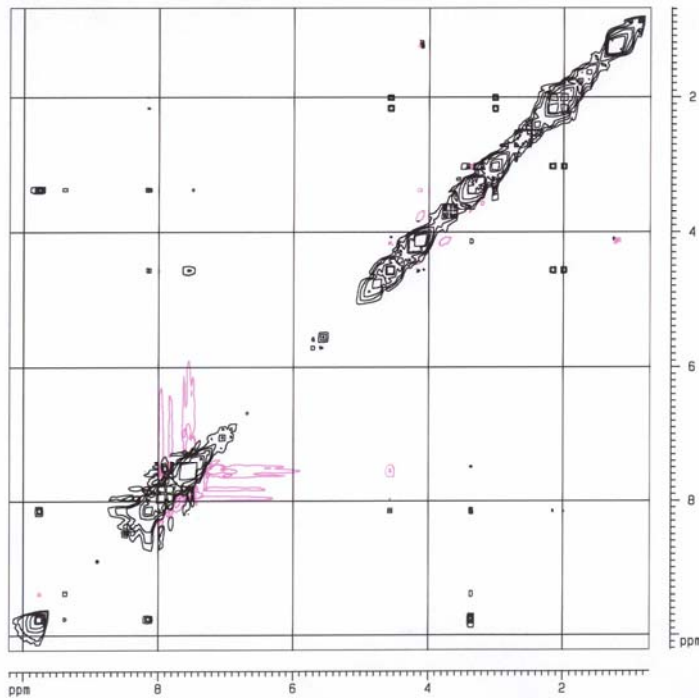
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WDW EM
SSB 0
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PC 1.00

F1 - Processing Parameters
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WDW EM
SSB 0
GB 0
PC 1.00

30 MHz 31P Parameters
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FPL15 15.000000 MHz
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FPL17 15.000000 MHz
FPL18 15.000000 MHz
FPL19 15.000000 MHz
FPL20 15.000000 MHz

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Ligand 1-NOESY



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Current Data Parameters
NAME 080510
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20051111
Time 18.45
INSTRUM spect
PROBHD 5 mm TGI 1-40
PULPROG zgpg30
TD 65536
SOLVENT DMS
NS 4
DS 4
SWH 800.864 Hz
F2RES 0.118623 Hz
AQ 0.001460 sec
RG 32.0
DM 79.800 mm
DE 2.00 mm
TE 300.2 K
AQ 0.000000 sec
SI 1.400000 sec
SFO 500.136000 MHz
SFR 0.000000 MHz
SIR 0.000000 MHz
SDF 0.000000 MHz
SCHM1 0.000000 MHz
KORR 1.400000 MHz

--- CHANNEL f1 ---
NUC1 1H
PC 0.00 mm
PI 0.00 mm
PL1 -13.00 dB
PT1 500.131000 MHz

--- BRACKET CHANNEL ---
SFOBRK 836.100
SFRBRK 836.100
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SFR1 0.00 MHz
SFO2 0.00 MHz
SFR2 0.00 MHz
SFO3 40.00 MHz
SFR3 -40.00 MHz
PAB 1000.00 MHz

F1 - Acquisition Parameters
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DE 2.00 mm
TE 300.2 K
AQ 0.000000 sec
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SFR 0.000000 MHz
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SCHM1 0.000000 MHz
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--- CHANNEL f1 ---
NUC1 1H
PC 0.00 mm
PI 0.00 mm
PL1 -13.00 dB
PT1 500.131000 MHz

--- BRACKET CHANNEL ---
SFOBRK 836.100
SFRBRK 836.100
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SFO2 0.00 MHz
SFR2 0.00 MHz
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SFR3 -40.00 MHz
PAB 1000.00 MHz

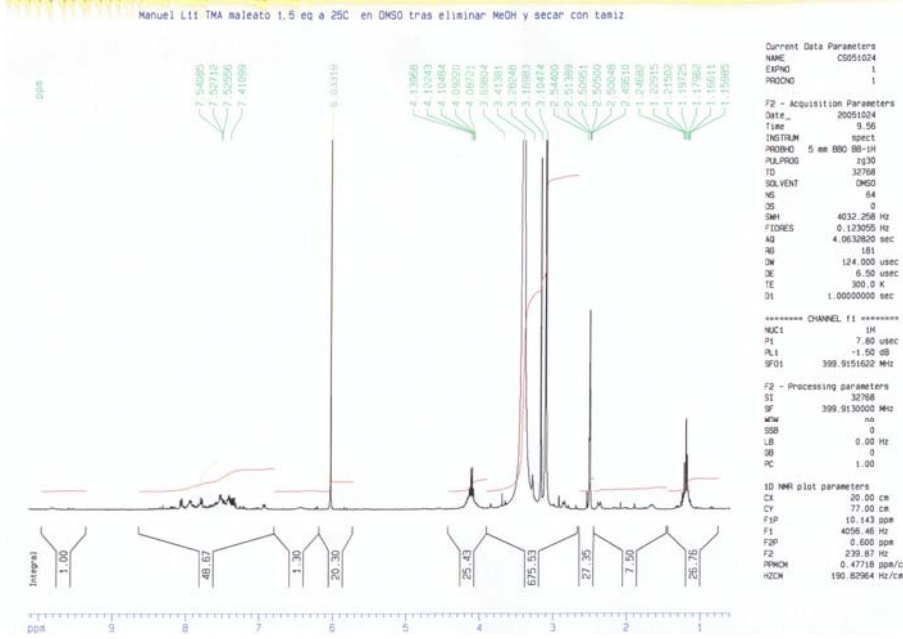
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F1 - Processing Parameters
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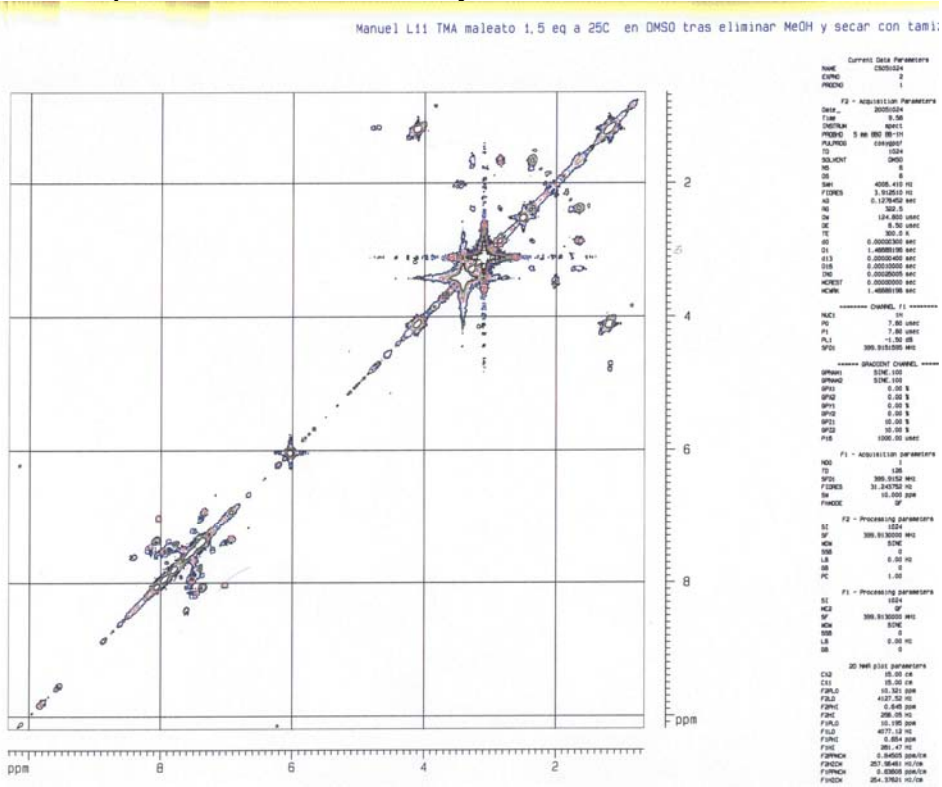
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CQ1 15.00 Hz
FPL1 15.000000 MHz
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FPL12 15.000000 MHz
FPL13 15.000000 MHz
FPL14 15.000000 MHz
FPL15 15.000000 MHz
FPL16 15.000000 MHz
FPL17 15.000000 MHz
FPL18 15.000000 MHz
FPL19 15.000000 MHz
FPL20 15.000000 MHz

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Ligand 1 + 1.5 equiv. of TMA maleate in dry DMSO-d₆

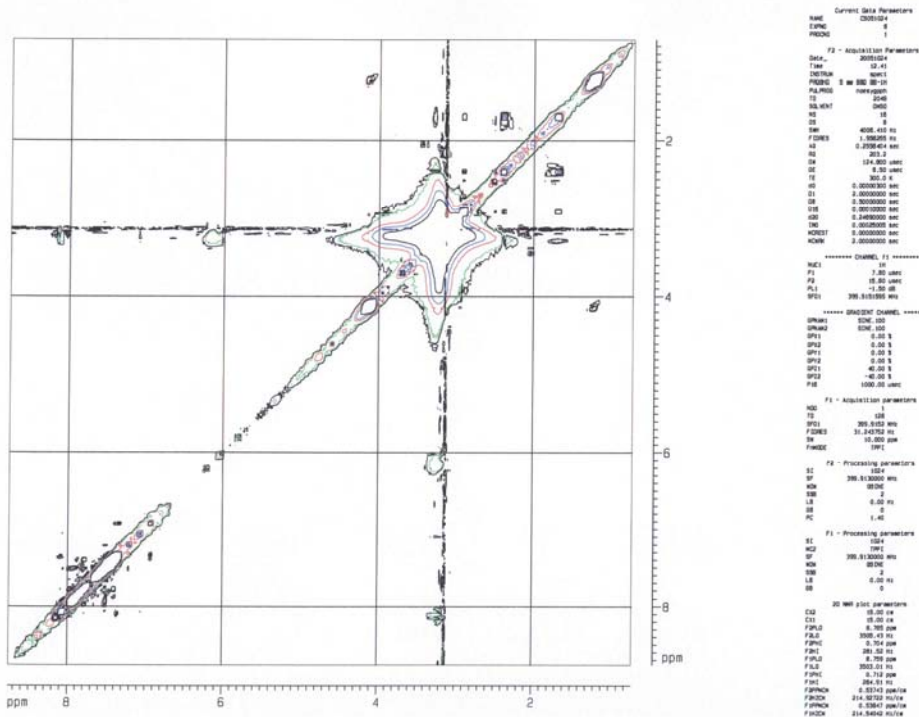


Ligand 1 + 1.5 equiv. of TMA maleate in dry DMSO-d₆-COSY

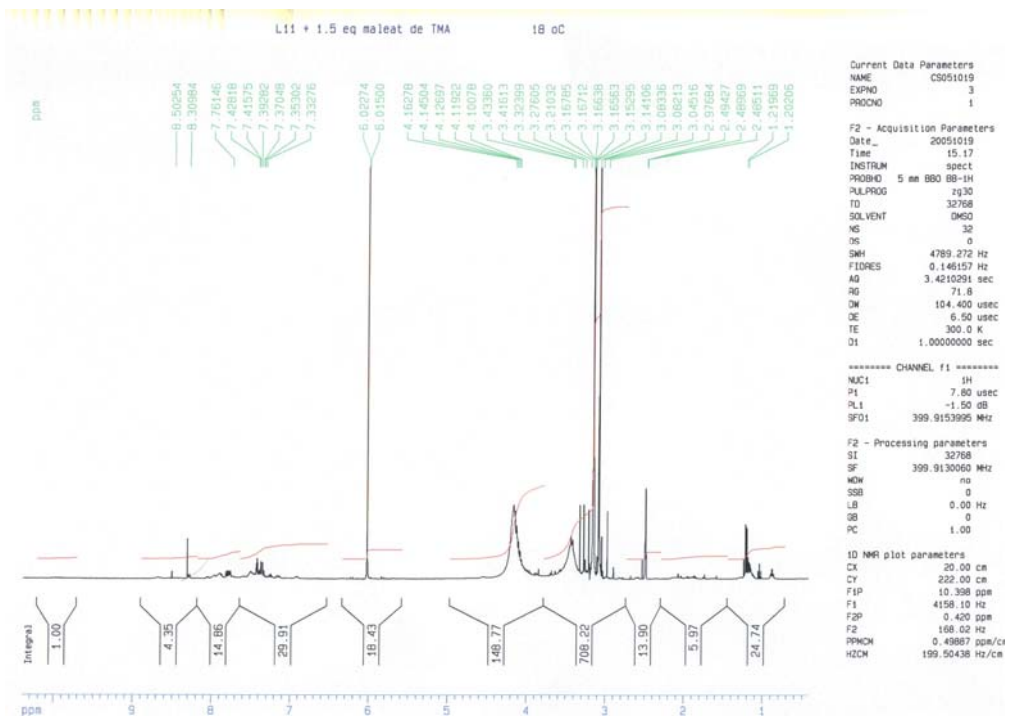


Ligand 1 + 1.5 equiv. of TMA maleate in dry DMSO-d₆-NOESY

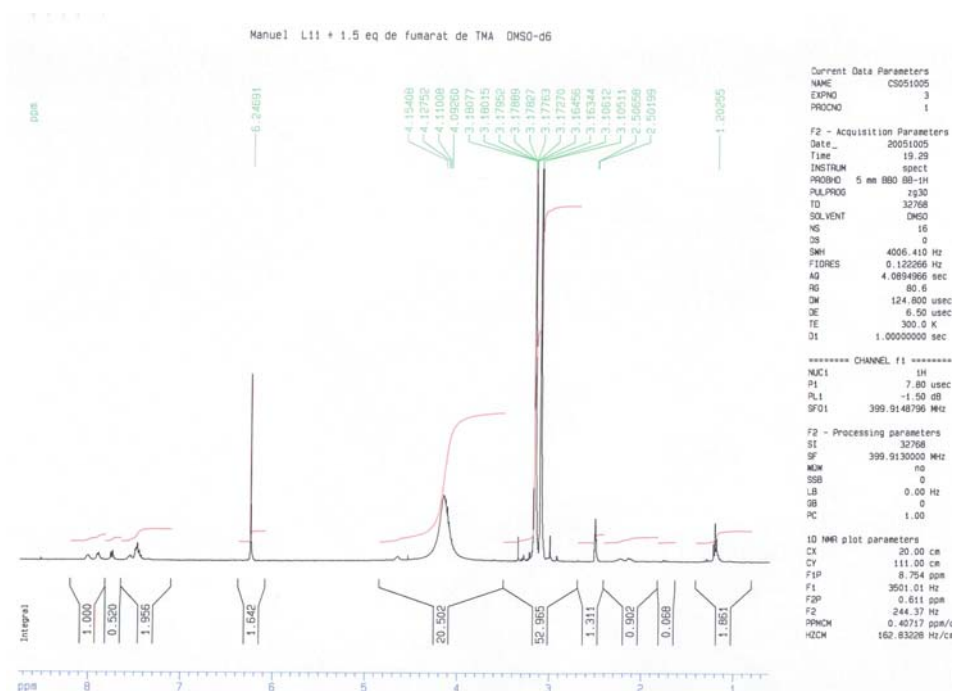
Manuel L11 TMA maleato 1,5 eq a 60C en DMSO tras eliminar MeOH y secar con tamiz



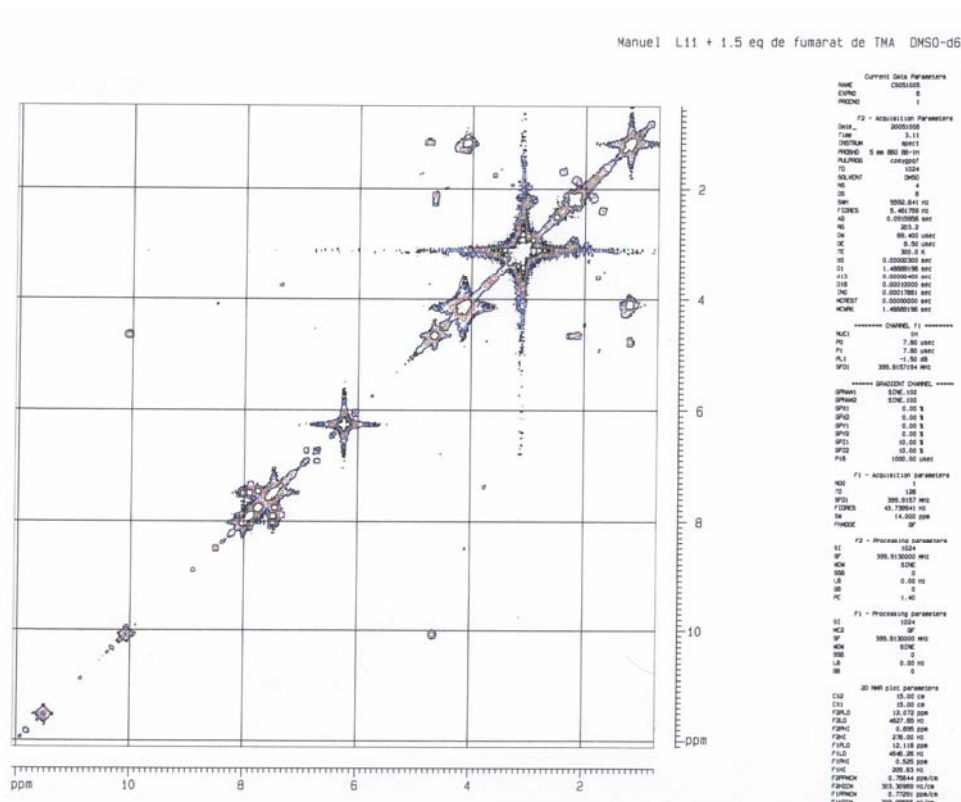
Ligand 1 + 1.5 equiv. of TMA maleate in DMSO/water



Ligand **1** + 1.5 equiv. of TMA fumarate in DMSO



Ligand **1** + 1.5 equiv. of TMA fumarate in DMSO-COSY



Ligand **1** + 1.5 equiv. of TMA fumarate in DMSO-NOESY

