Supporting Information

Contents

Synthesis of the compounds.

Starting materials.

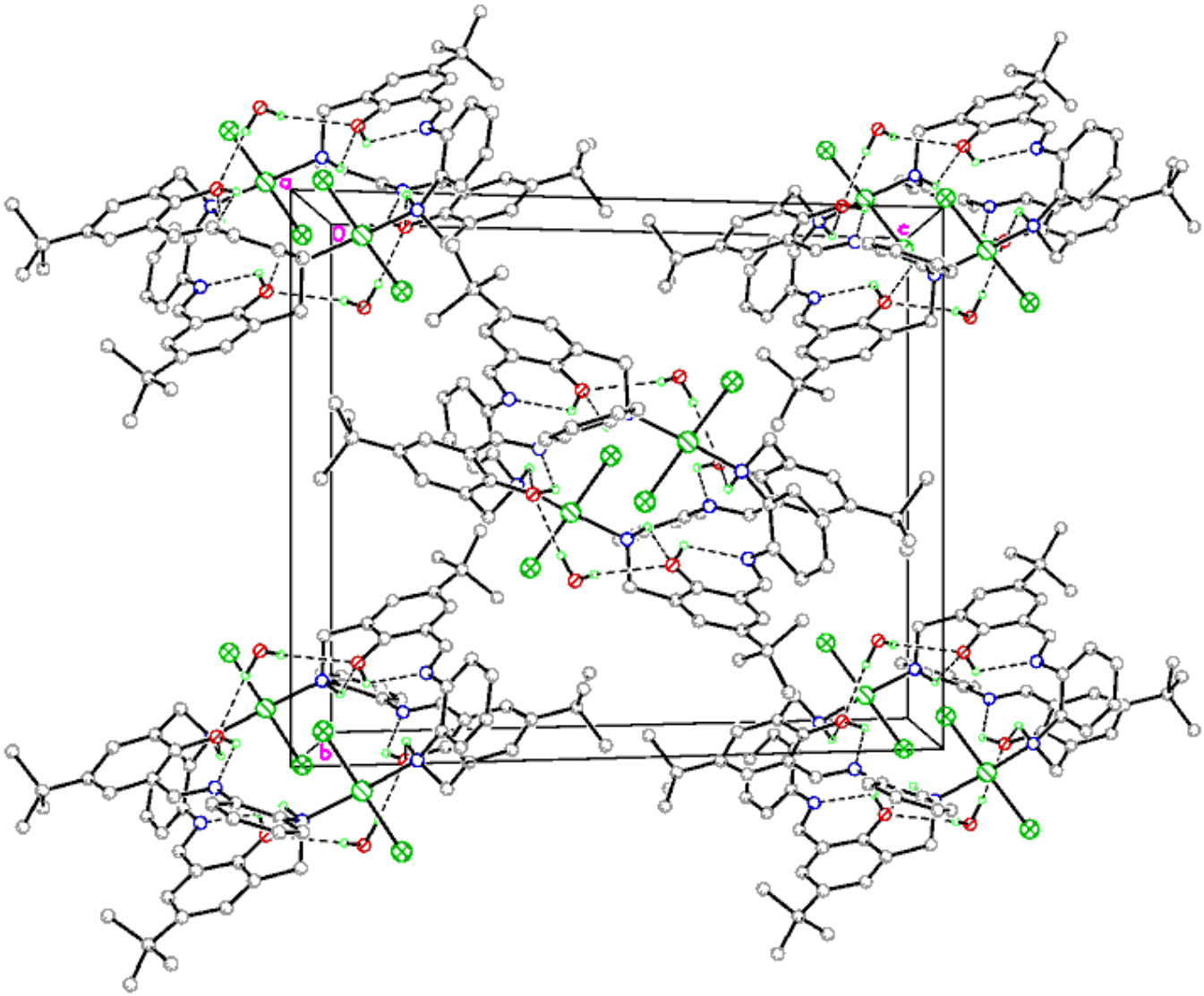
Starting macrocycle **1** were synthesized by literature method[1]. In brief: mixture of 175 mg (0.83 mmol) of 2,6-diformyl-4-*tert*-butylphenol and 91 mg (0.83 mmol) of *o*-phenylenediamine were stirred under reflux for 3 h. Then the mixture was cooled overnight and large dark-red crystals were filtered off, solution evaporated in vacuum to a halve of volume and additional crop of macrocycle **1** were separated after cooling. Others reagents and solvents were obtained from commercial sources.

Instrumentation details.

NMR spectra were measured on a BRUKER AVANCE-400 MHz NMR-spectrometer at 24 ^{o}C. IR spectra were recorded on a Nicolet FT-IR spectrometer in Nujol or KBr. IR spectra measured on Nicolet Protege 460 Fourier spectrometerc with MCT-detector (resolution 4 cm^{-1}, range 4000-400 cm^{-1}) as a KBr pellets. Thermogravimetric and differential thermal analysis were made on a coupled heat-flux DSC-TGA, SDT Q-600 modulus from TA Instruments previously calibrated with zinc. A heating rate of 10 °C/min from 25 to 800°C under flow of dry air (100 mL/min). Relative error were less than 1%.

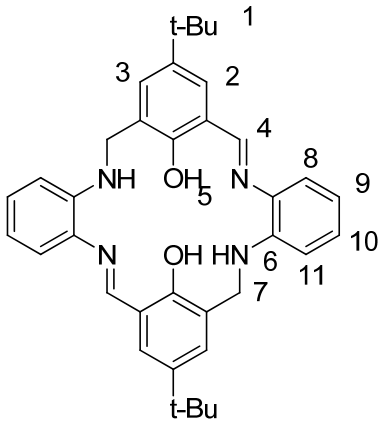
1. Ustynyuk, Y. A.; Borisova, N. E.; Nosova, V. M.; Reshetova, M. D.; Talismanov, S. S.; Nefedov, S. E.; Aleksandrov, G. A.; Eremenko, I. L.; Moiseev, I. I., *Rus Chem Bull* **2002,** *51*, 454-463.

The crystal packing of molecules of 2.



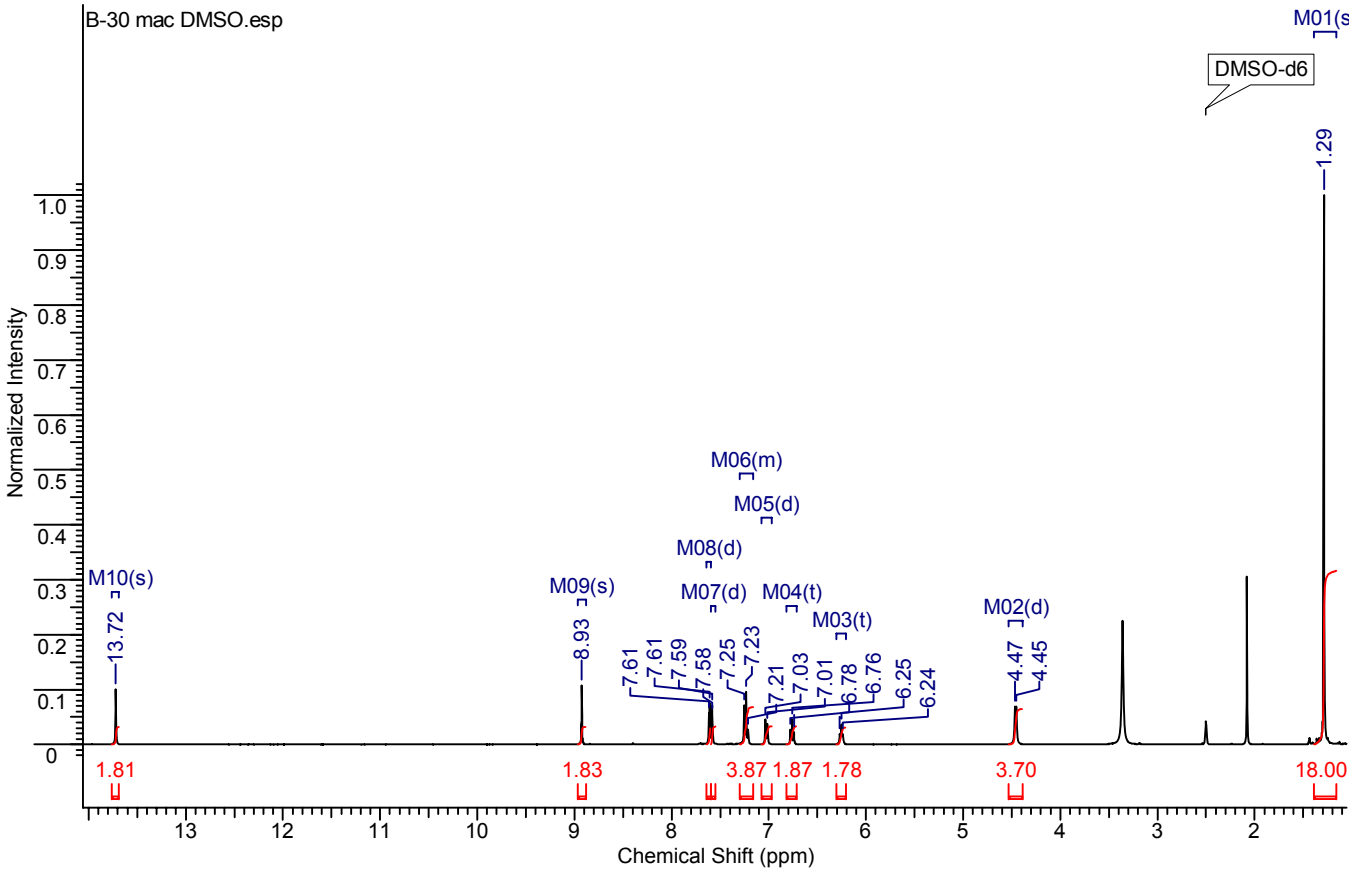
The disordered methylene chloride solvate molecules are not shown.

NMR-Spectra of macrocycle 1 and their palladium complex 2.

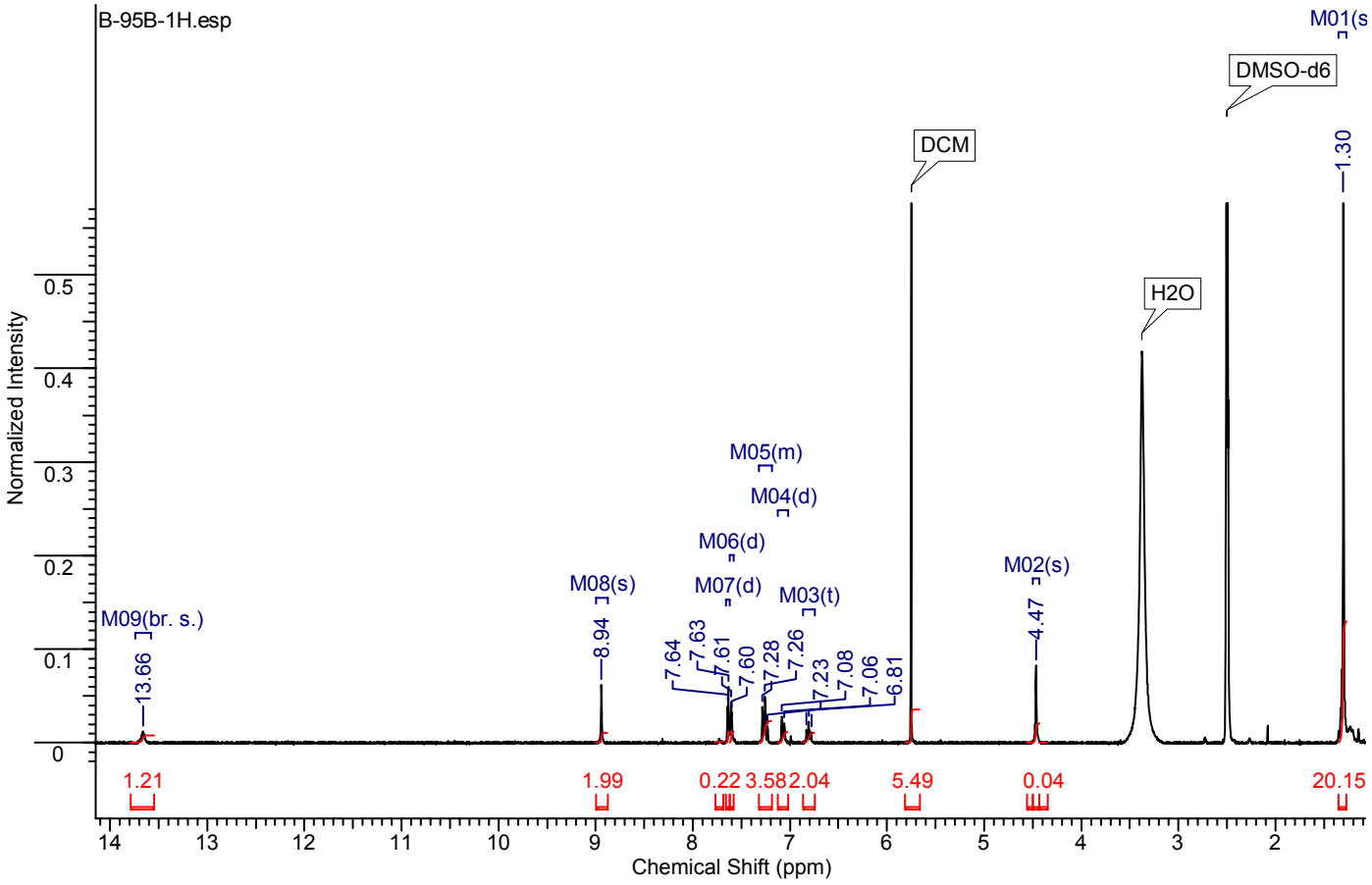


	1	2	3	4	5	6	7	8	9	10	11
1 DMSO-d^6	1.30 s	7.61 d (2.2)	7.63 d (2.2)	8.95 s	13.73 s	6.25 t (5.8)	4.47 d (5.8)	7.26 d (7.58)	6.77 t (7.58)	7.24 t (7.83)	7.03 d (7.83)
1 $CDCl_3$	1.34 s	7.35 d (2.35)	7.43 d (2.35)	8.63 s	13.56 s	6.33 t (5.49)	4.47 d (5.49)	7.07 d	6.79 t	7.25 t	6.96 d
1 acetone-d^6	1.33 s	7.54 s		8.81 s	13.72 s	6.38 br.s	4.49 s	7.19 m	6.75 t	7.19 m	6.98 d
1 CD_2Cl_2	1.32	7.41 d (2.2)	7.46 d (2.2)	8.66 s	13.55 s (free) 4.13 with H_2O	4.13 br.s with H_2O	4.43 s	7.09 dd (7.83, 1.22)	6.81 td (7.83, 1.2)	7.24 td (8.07, 1.47)	6.99 d (8.07)
2 $CDCl_3$	1.12 s	6.84 s	6.51 s	7.51 s	12.14 s	-	3.83 dd (10.45, -12.59) 5.44 d (-12.59)	-	6.92 td (7.09, 3.06)	-	8.46 d (7.09)
2 CD_2Cl_2	1.11 s	6.87 s	6.51 s	7.52 s	12.12 s	7.05 d (9.4)	3.83 dd (9.4, -13.45) 5.36 d (-13.45)	6.73 d (7.56)	7.26 t (7.56)	7.47 dd (7.56, 8.14)	8.43 d (8.14)
2 CD_2Cl_2 (600 µl)–D_2O (50 µl) (to a solution of **2** in DCM add D_2O and shake vigorously)	1.12 s	6.74 s	6.50 s	7.52 s	absent due to exchange with D_2O	7.05 d (9.78)	3.84 dd (9.78, -12.29)	6.74 d (7.34)	7.26 td (8.04, 1.41)	7.48 td (8.16, 1.16)	8.44 dd (7.76, 0.92)
2 DMSO-d^6	1.30 s	7.60 d (2.0)	7.64 d (2.0)	8.94 s	13.66 s	-	4.47 s	7.26 m	6.80 t (7.35)	7.26 m	7.07 d (7.64)

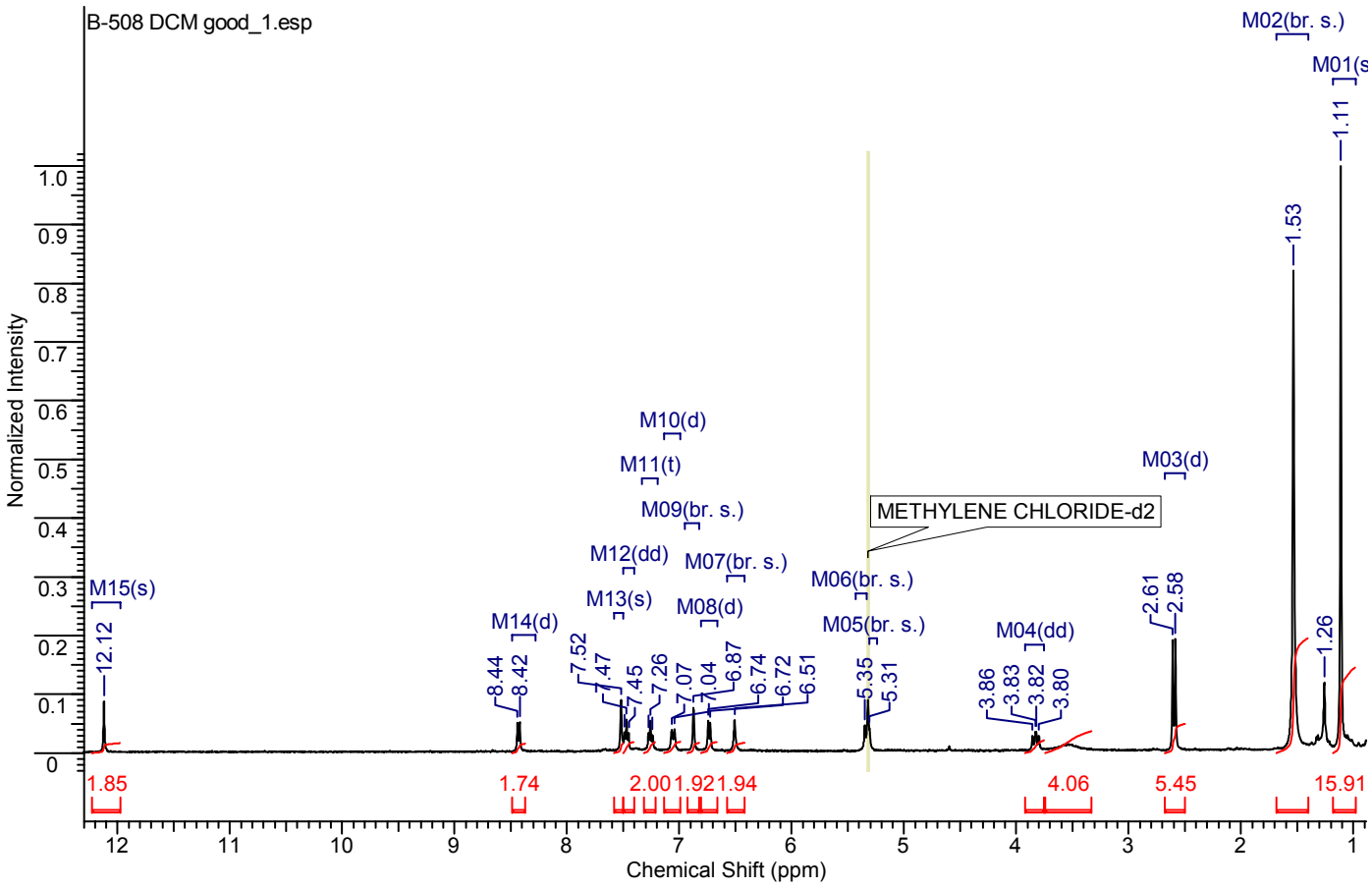
1 (DMSO-d^6)



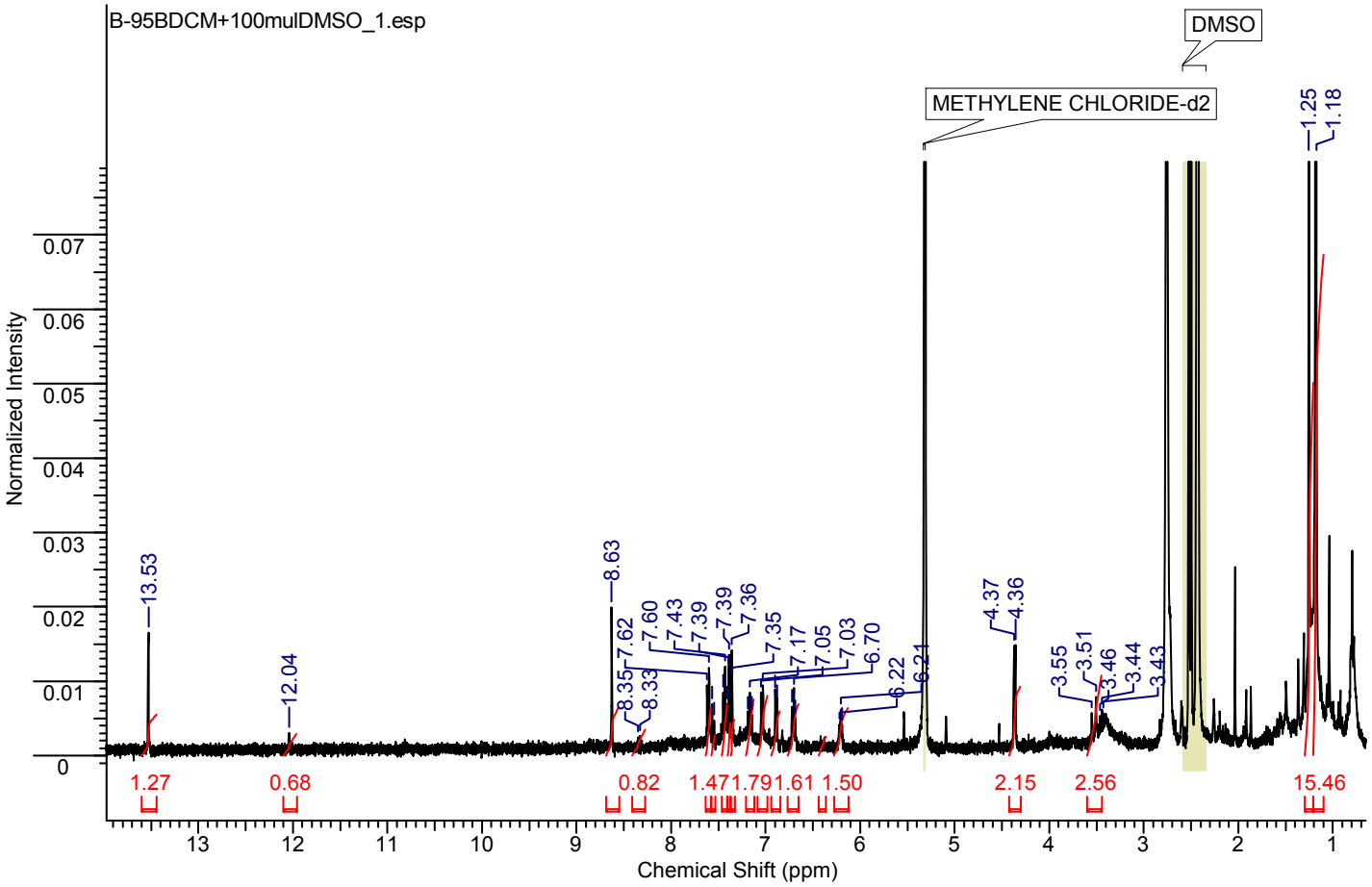
2 DMSO-d^6



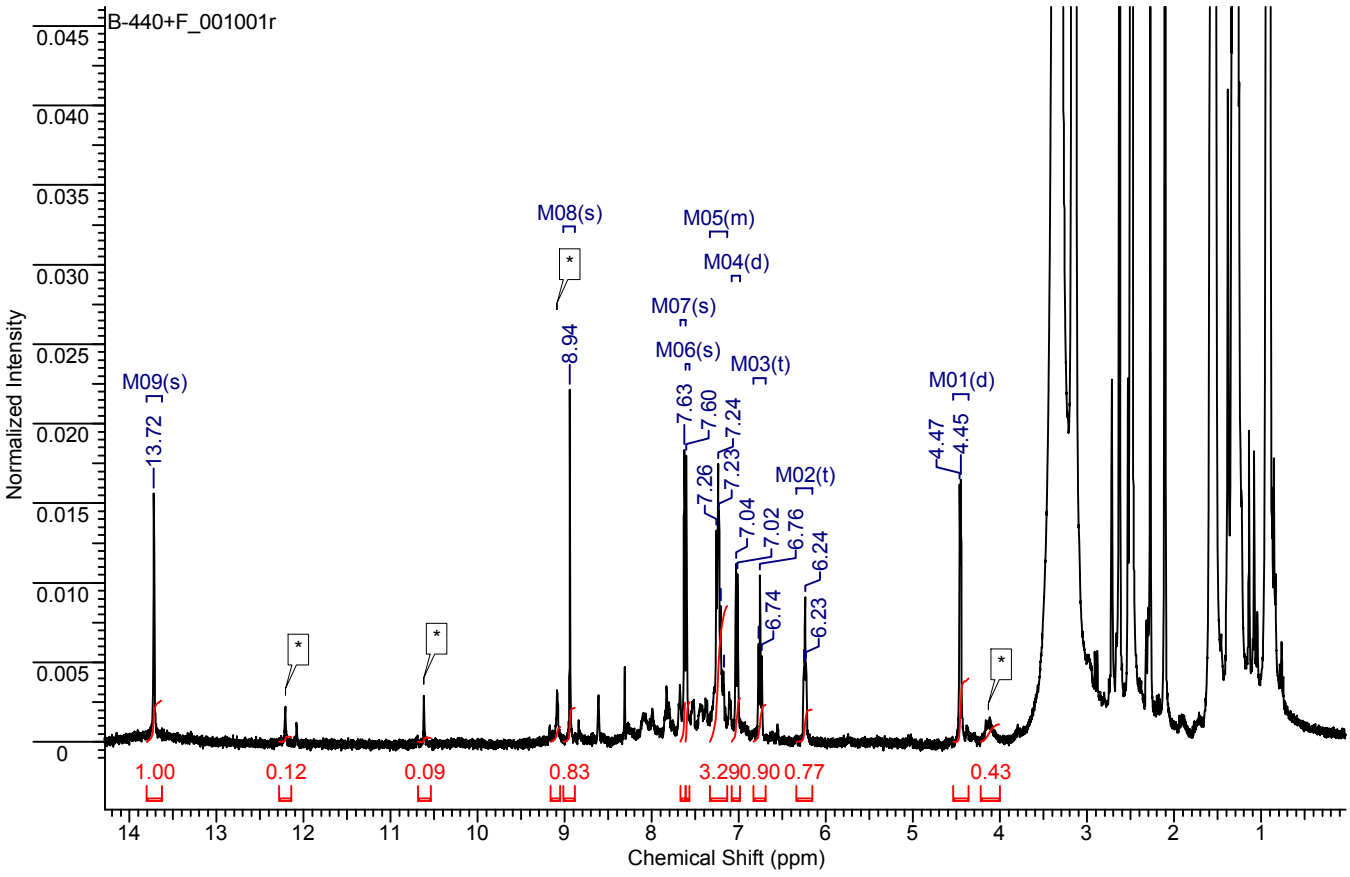
2 CD_2Cl_2



2 15% DMSO in CD_2Cl_2

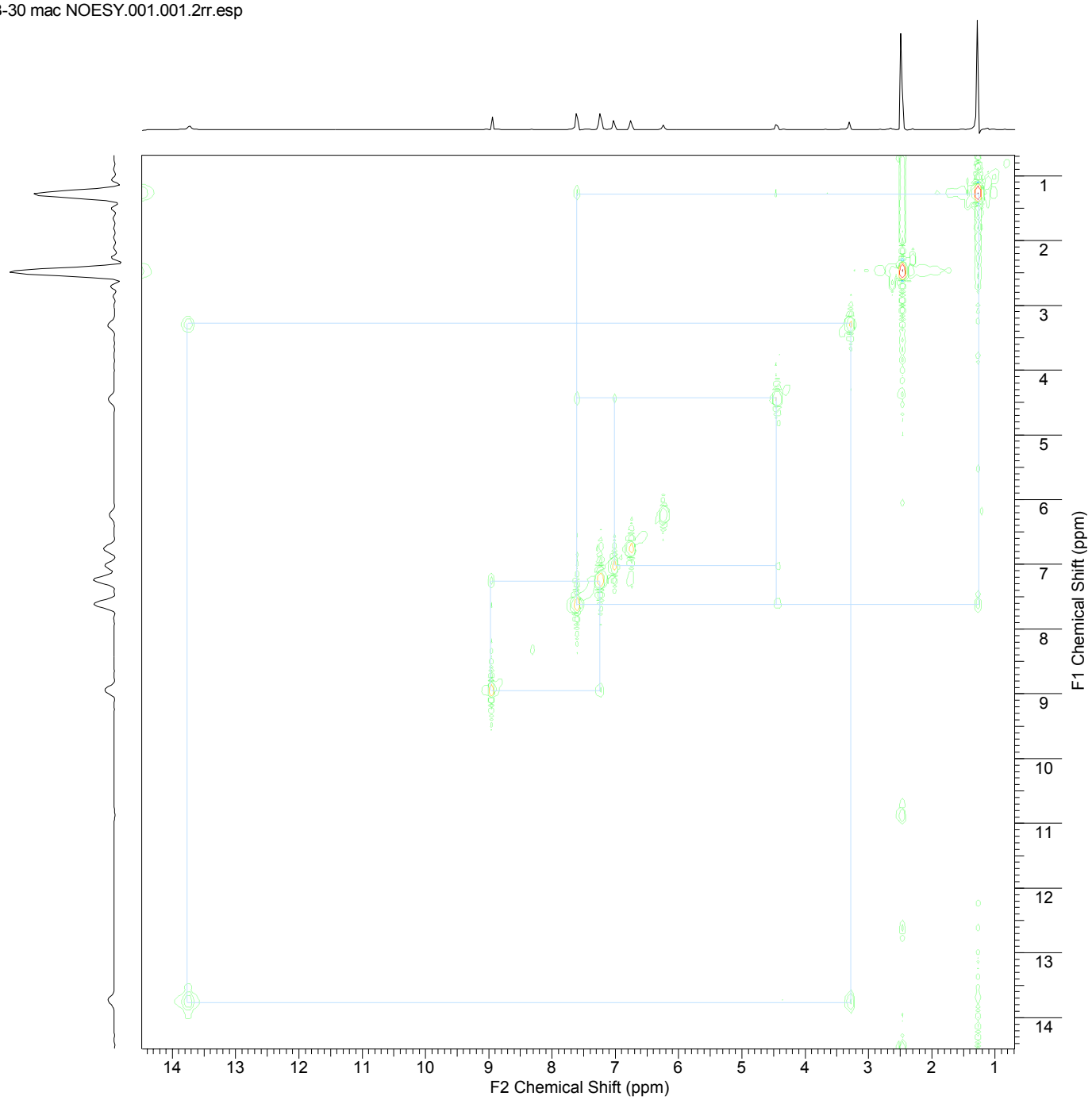


2 +Bu_4F (Peaks marked with * correspond to macrocycle **1** degradation product.)



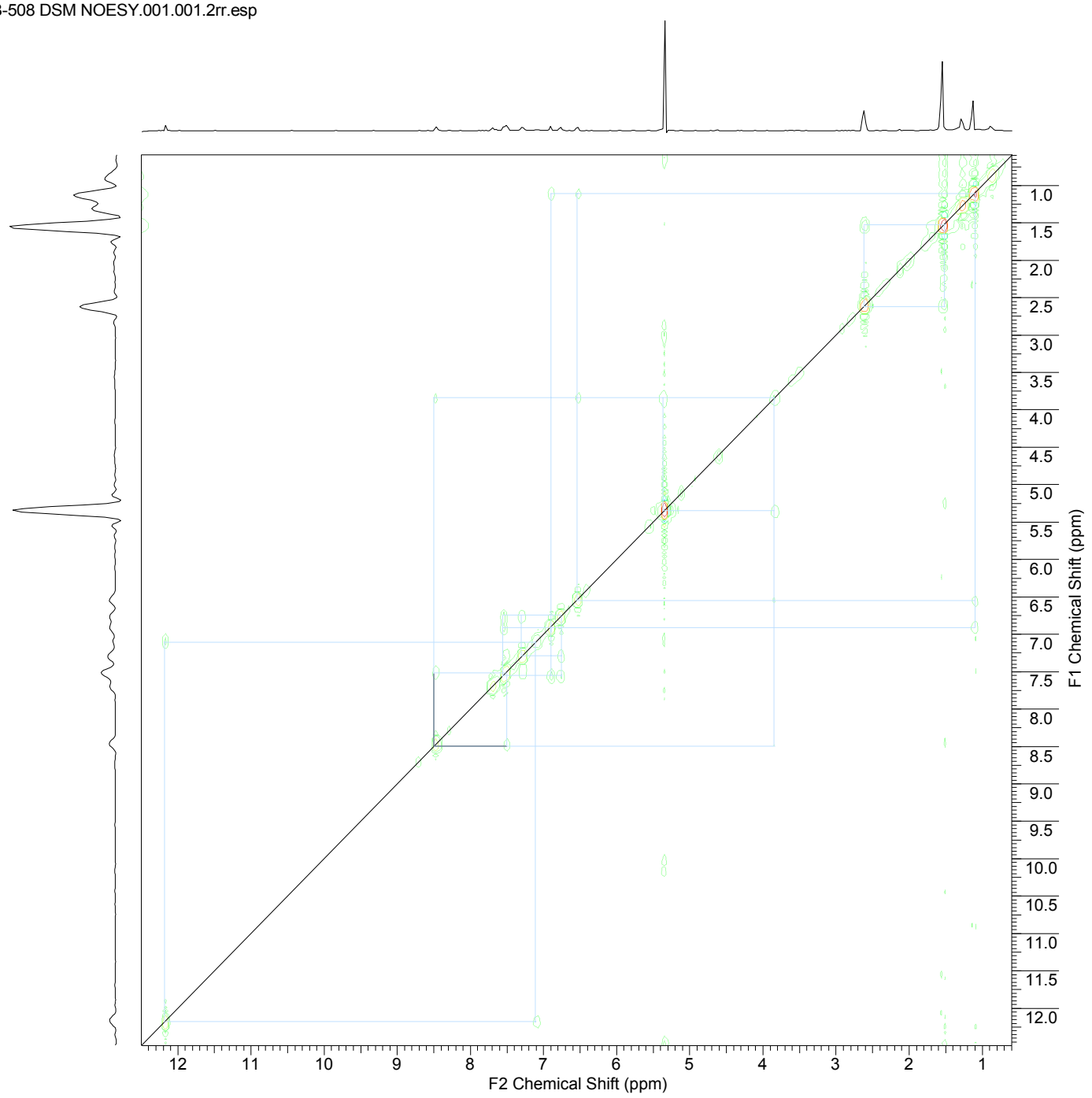
Macrocycle **1** in DMSO-d^6 NOESY

B-30 mac NOESY.001.001.2rr.esp

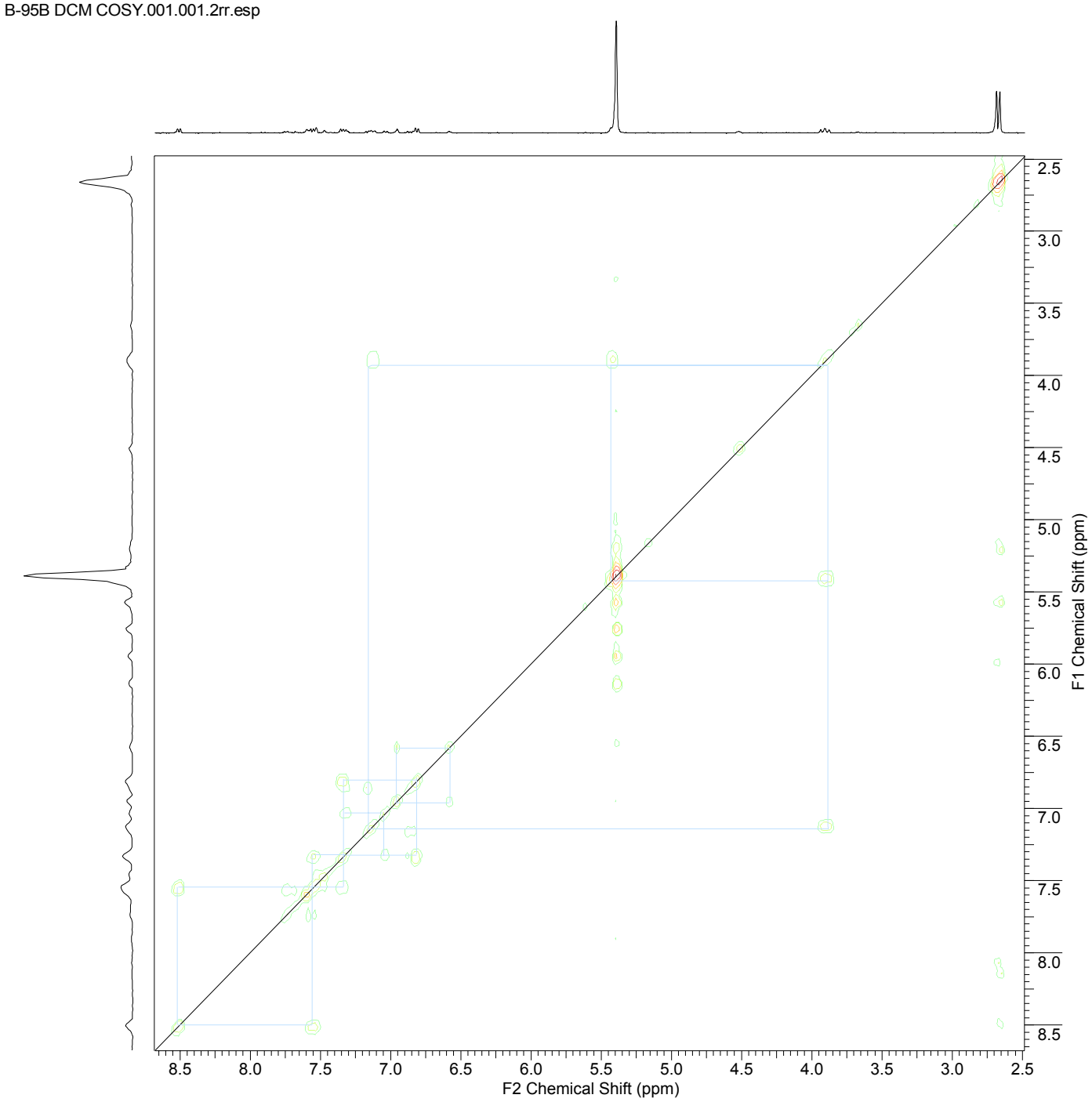


Complex **2** in DCM NOESY

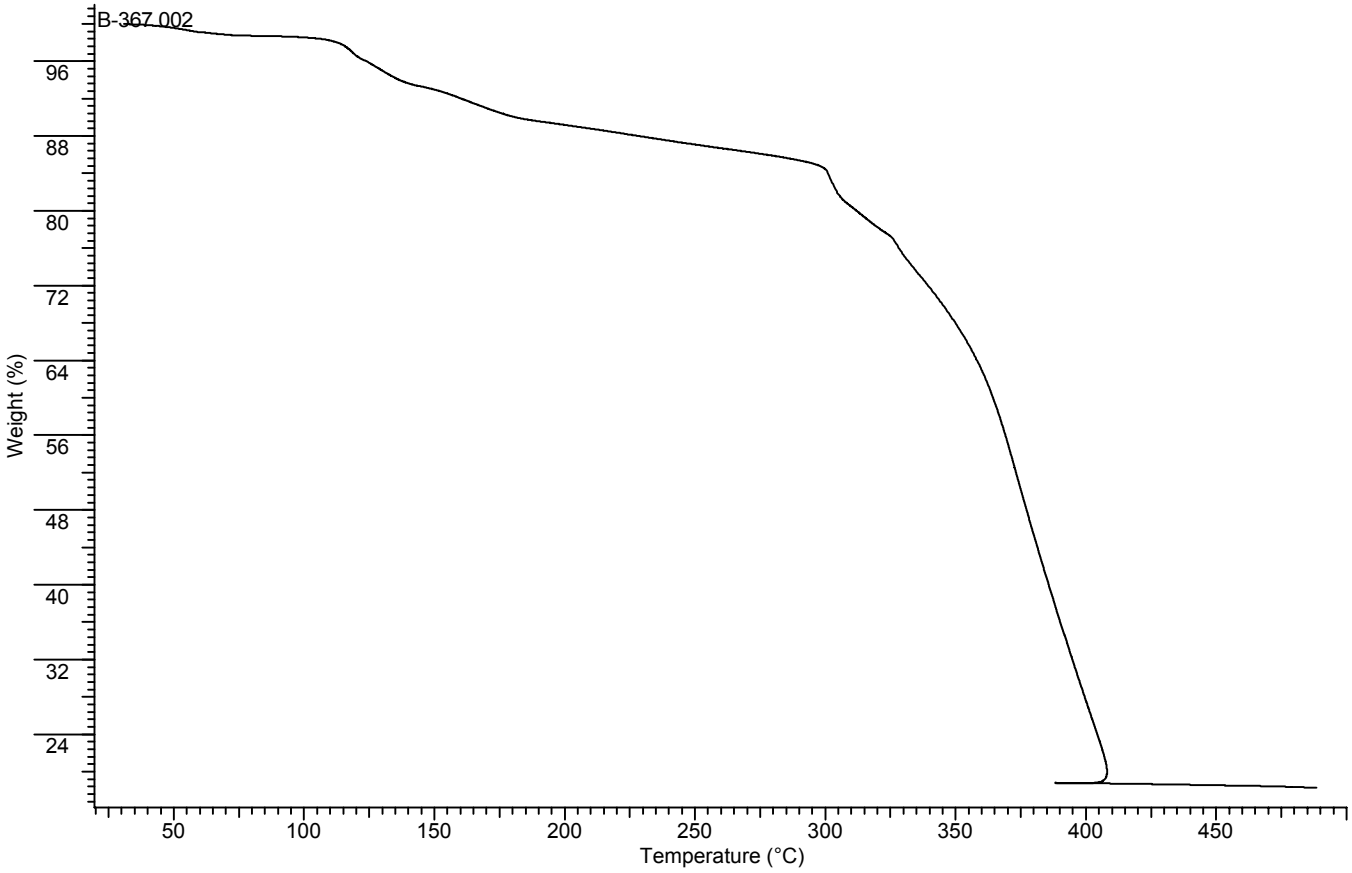
B-508 DSM NOESY.001.001.2rr.esp



Complex **2** in DCM COSY



TGA Data for palladium complex 2.



DSC data for complex **2**.