

ELECTRONIC SUPPLEMENTARY MATERIAL

Ferrocenyl-bis-(1-(4-benzyl-5-morpholinooxazol-2-yl)-N-(4-(trifluoro-methyl)benzyl)methanamine)

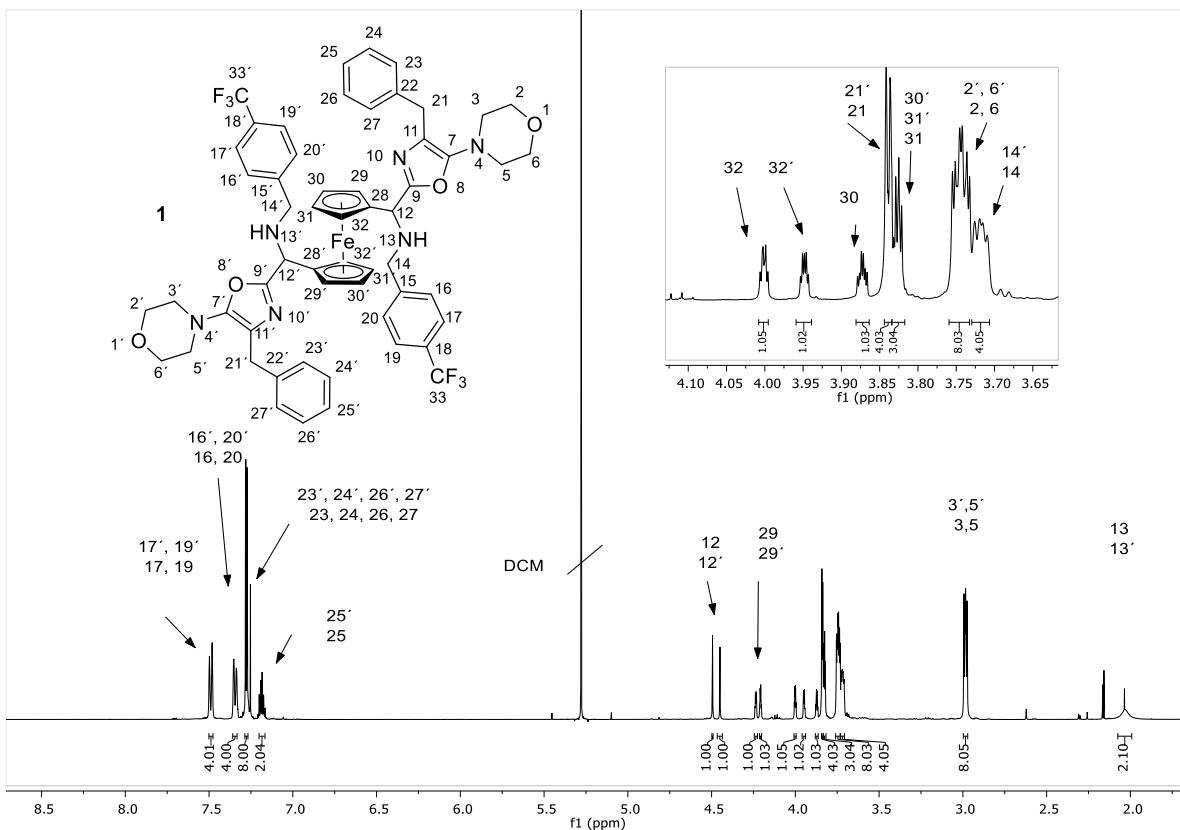
Roberto E. Blanco-Carapia¹, Enrique A. Aguilar-Rangel¹, Alejandro Islas-Jácome^{1,*} and Eduardo González-Zamora^{1,*}

¹ Departamento de Química, Universidad Autónoma Metropolitana-Iztapalapa, Av. Ferrocarril San Rafael Atlixco 186, Col. Leyes de Reforma 1A Sección, Iztapalapa, Ciudad de Mexico C.P. 09310, Mexico

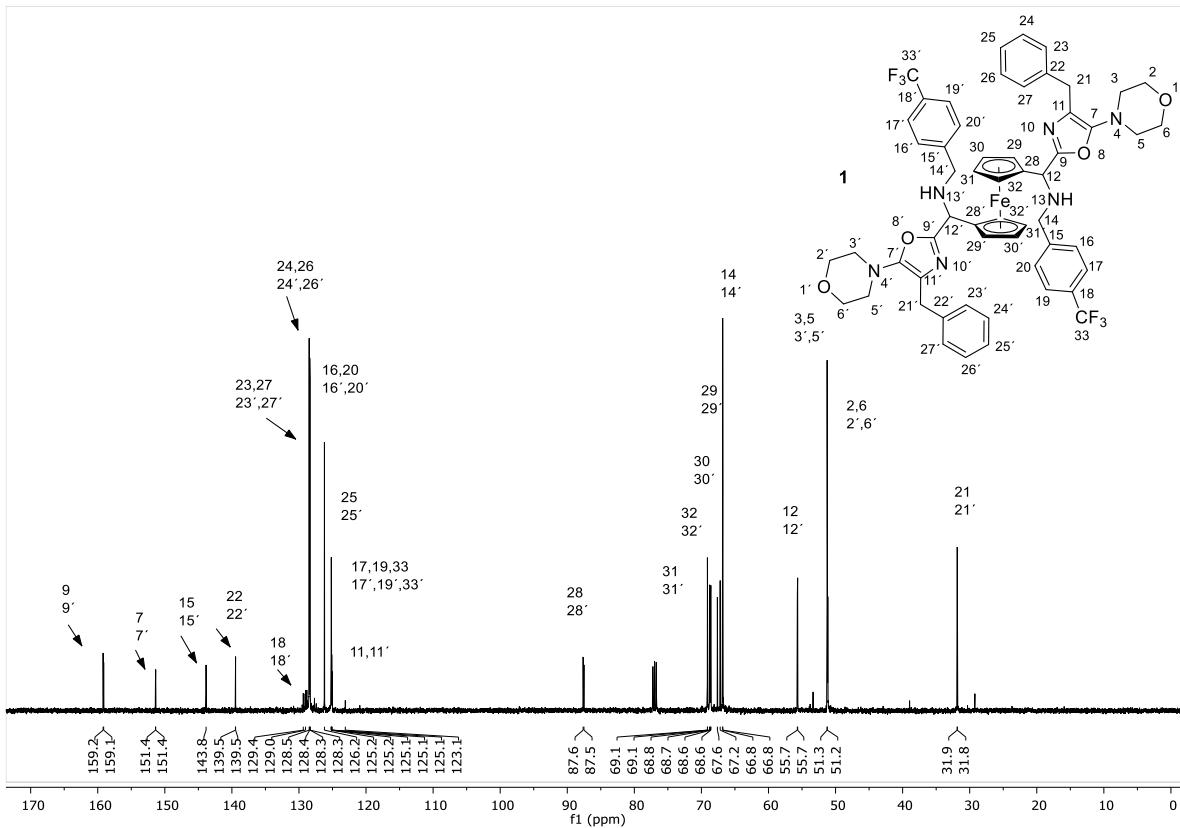
* Correspondence: aij@xanum.uam.mx (A.I.-J); egz@xanum.uam.mx (E.G.-Z.)

TABLE OF CONTENTS

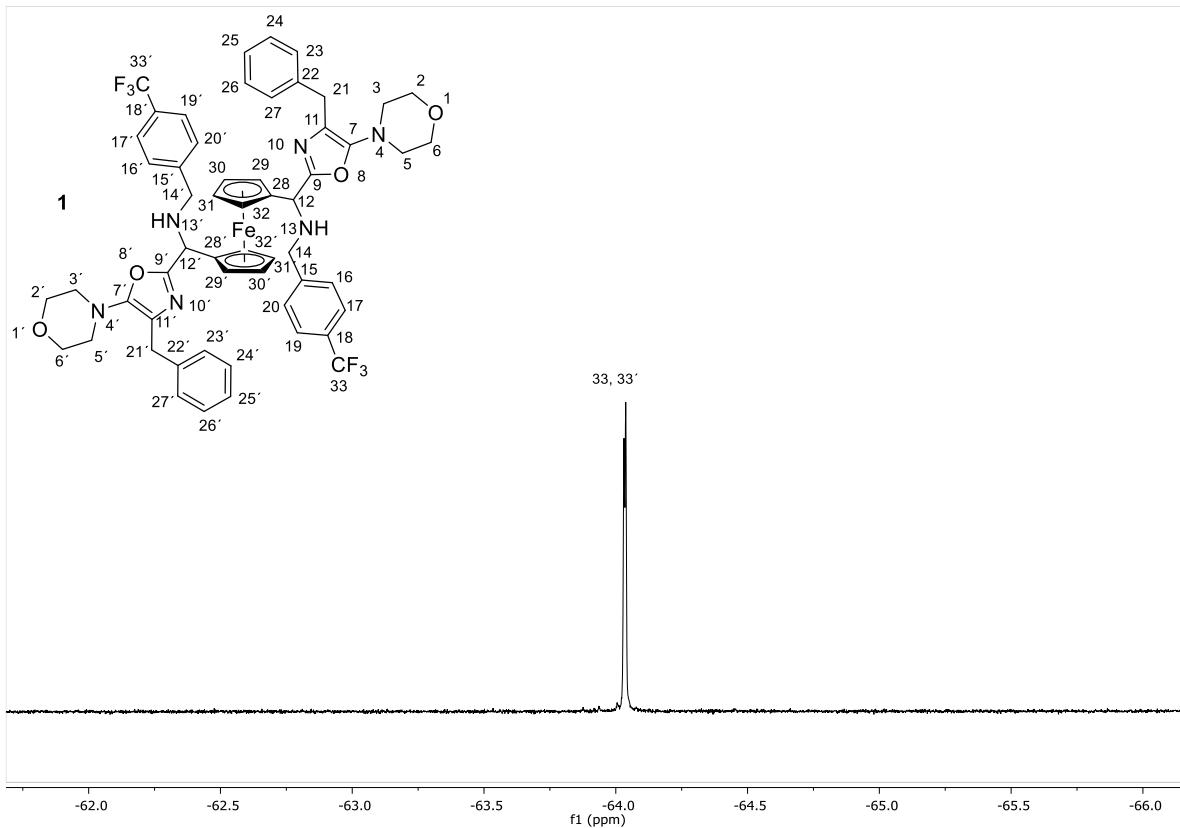
Spectra of compound 1	Page
¹ H-NMR	S2
¹³ C-NMR	S3
¹⁹ F-NMR	S4
2D-NMR (COSY).....	S5
2D-NMR (HSQC).....	S6
2D-NMR (HMBC-part I)	S7
2D-NMR (HMBC-part II)	S8
HRMS	S9
FT-IR	S10



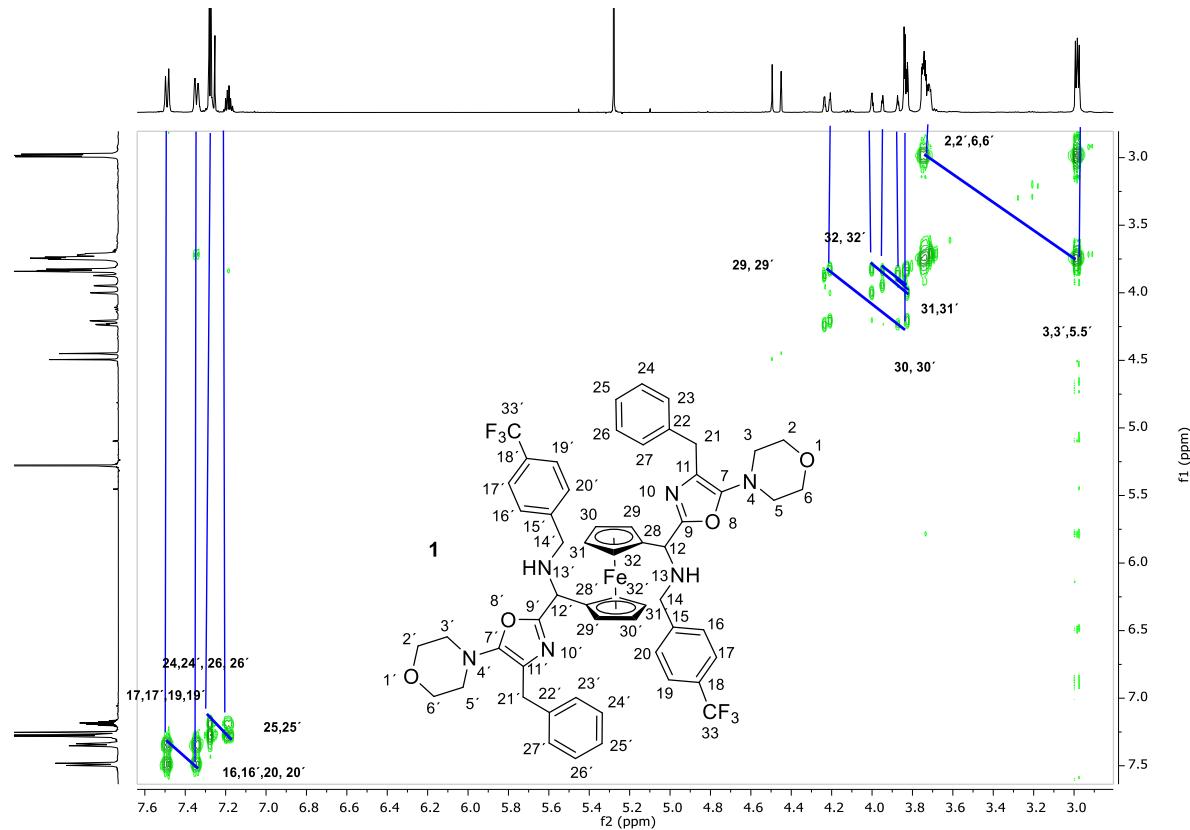
¹H-NMR (500 MHz, CDCl₃) spectrum of compound **1**



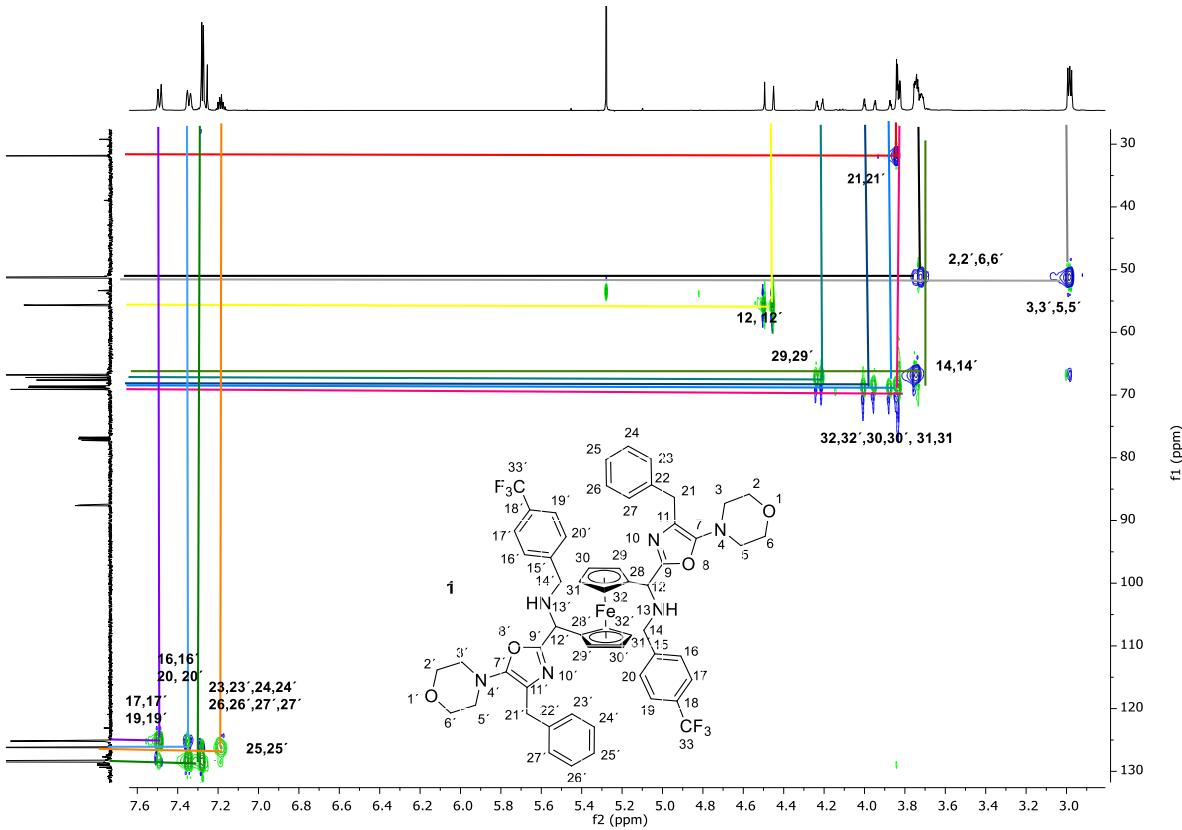
^{13}C -NMR (125 MHz, CDCl_3) spectrum of compound **1**



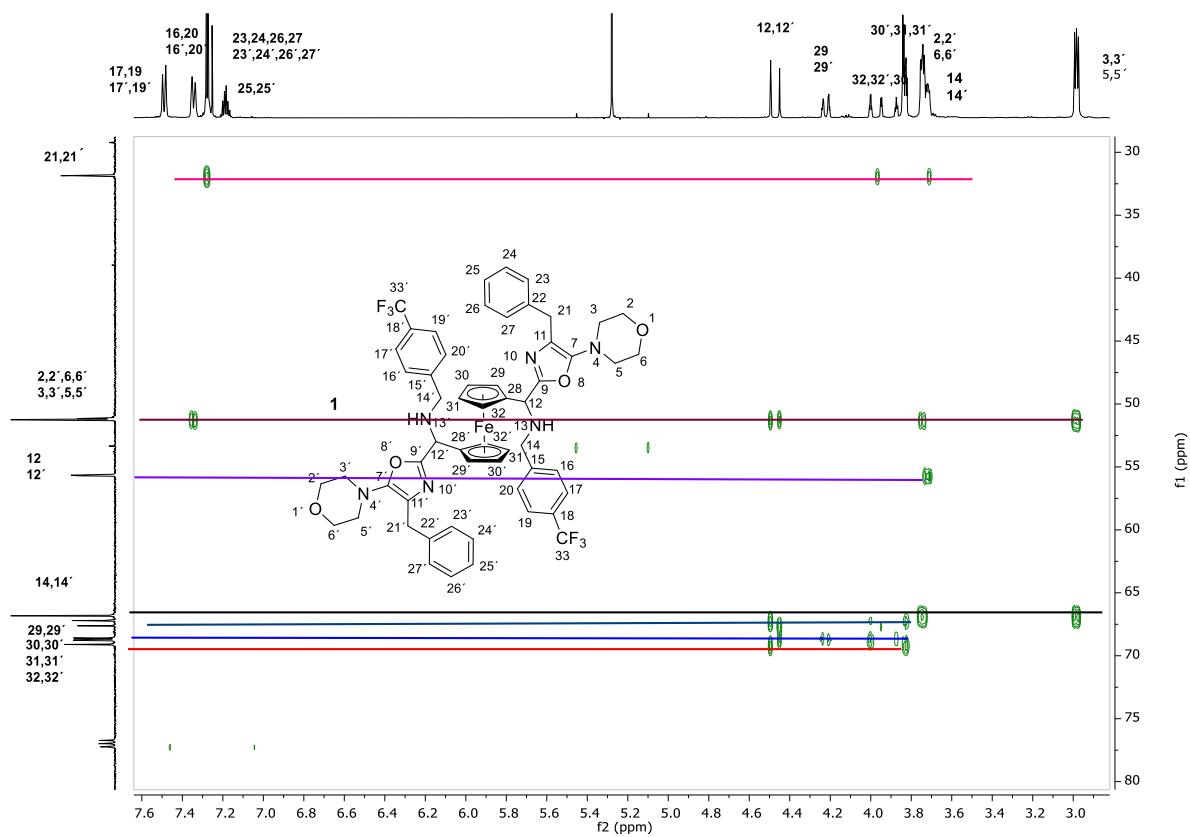
^{19}F -NMR (468.6 MHz, CDCl_3) spectrum of compound **1**



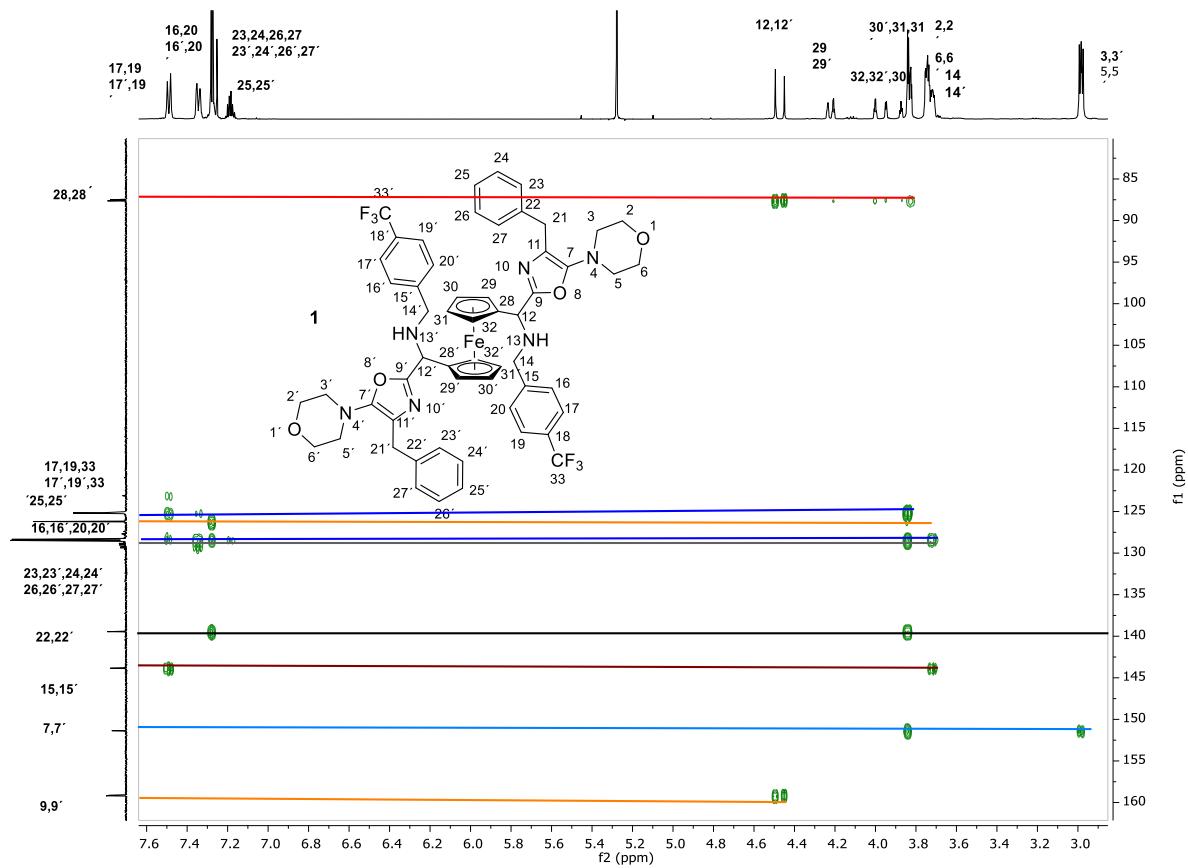
2D-NMR (COSY) spectrum of compound **1**



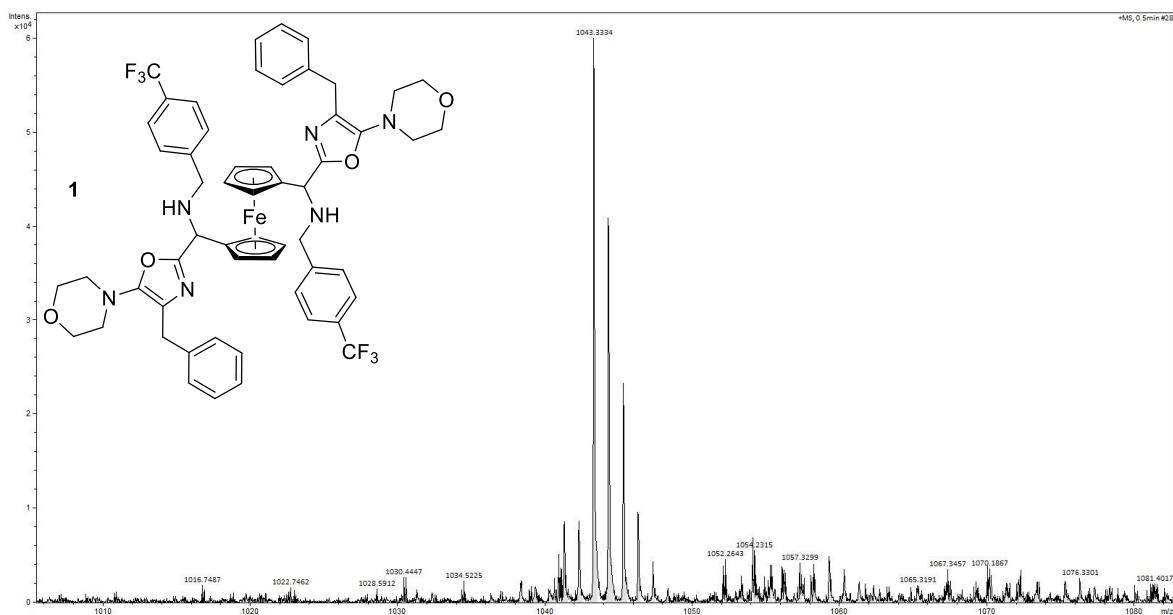
2D-NMR (HSQC) spectrum of compound 5



2D-NMR (HMBC-part I) spectrum of compound **1**



2D-NMR (HMBC-part II) spectrum of compound 5

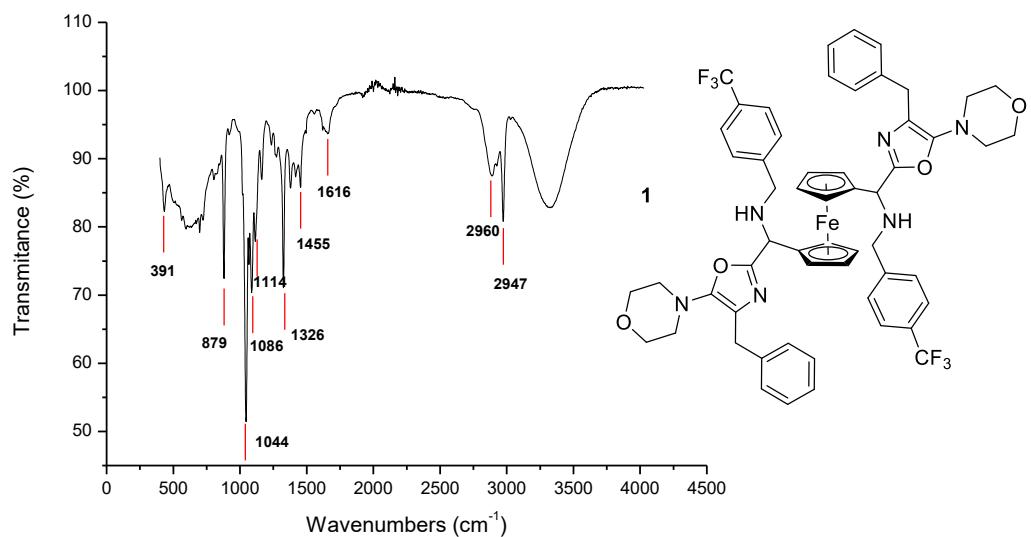


Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

Meas. m/z	#	Ion Formula	Sum Formula	m/z	err [ppm]	mSigma	# Sigma	rdb	e ⁻ Conf
1043.3334	1	C56H53F6FeN6O4	C56 H53 F6 Fe N6 O4	1043.3383	4.6	93.1		1	30.5 even

HRMS (ESI⁺-TOF) spectrum of compound 1



FT-IR (ATR) spectrum of compound **1**