Electronic Supporting Information (ESI) for New Journal of Chemistry 2021:

Evaluation of cyrhetrenyl and ferrocenyl precursors as 5-lipoxygenase inhibitors. Biological and computational studies.

Michelle Muñoz-Osses[a], Javiera Quiroz[b], Yesseny Vásquez-Martínez[c], Erick Flores[a], Elizabeth Navarrete[b], Fernando Godoy[a], Claudia Torrent[b], Marcelo Cortez-San Martín[d], Alejandra Gómez[a*], Carolina Mascayano[b*]

[a.] *Departamento Química de los Materiales, Universidad de Santiago de Chile, Chile.*
[b.] *Departamento Ciencias del Ambiente, Universidad de Santiago de Chile, Chile.*
[c.] *Programa Centro de Investigaciones Biomédicas y Aplicadas (CIBAP), Escuela de Medicina, Facultad de Ciencias Médicas, Universidad de Santiago de Chile, Chile.*
[d.] *Departamento Biología, Universidad de Santiago de Chile, Chile.*

Index

Experimental Section:
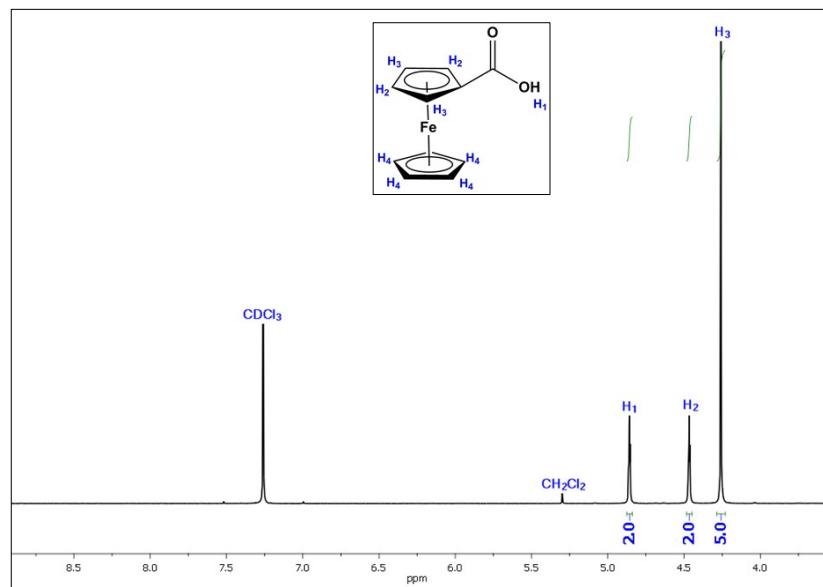
Figure S1. ^{1}H-NMR of **1c** in CDCl$_3$.
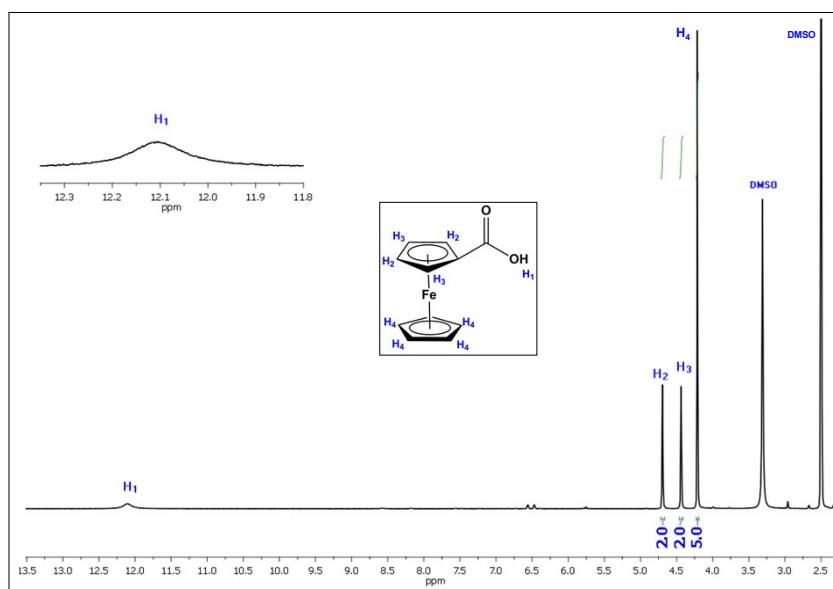
Figure S2. ^{1}H-NMR of **1c** in DMSO-d$_6$.
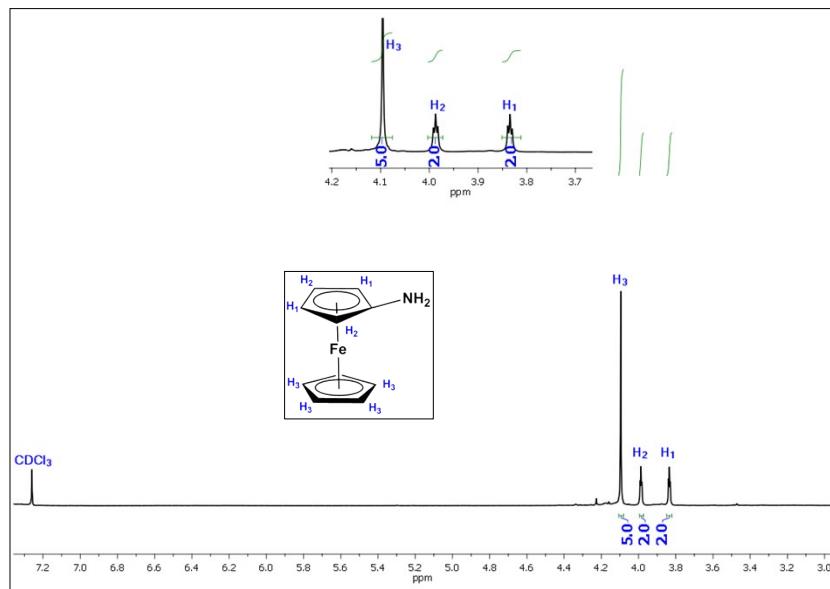
Figure S3. ^{1}H-NMR of **1d** in CDCl$_3$.
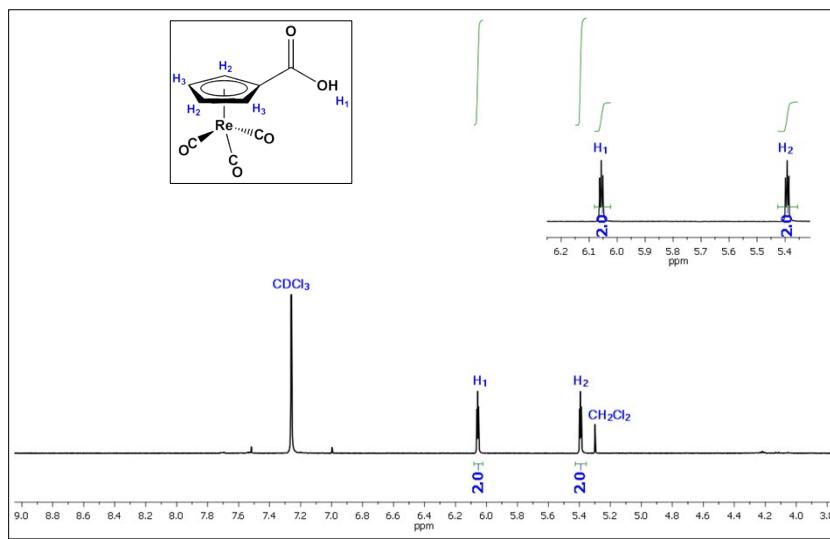
**Figure S4.** ^{1}H-NMR of **2c** in CDCl$_3$
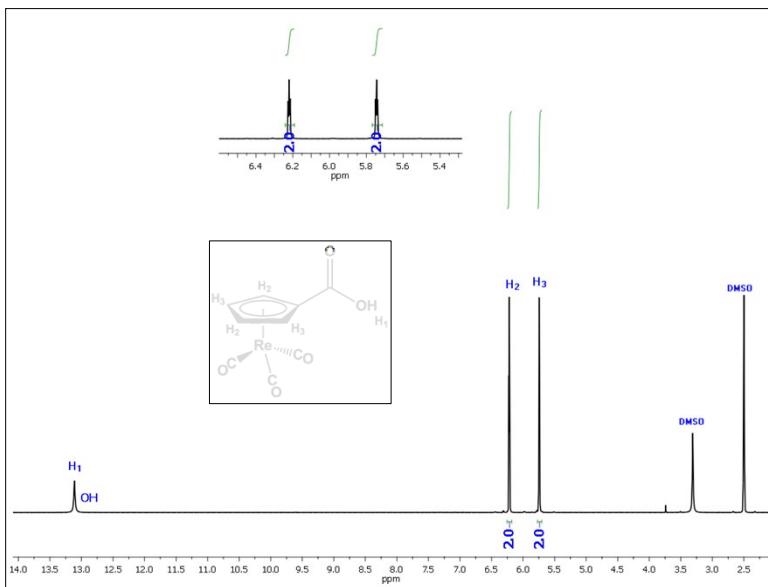
Figure S5. ^{1}H-NMR of **2c** DMSO-d$_6$.
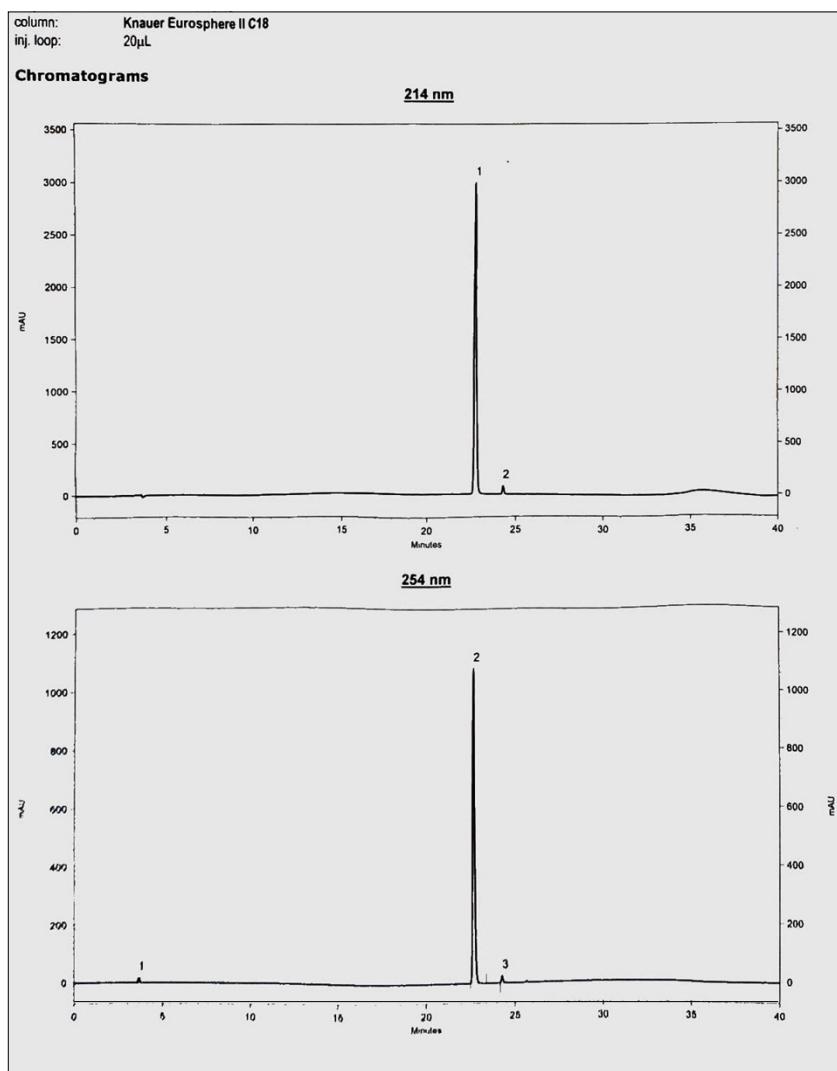
Integration Table

UV-Detektor S
2550 [Channel
1] Results

Pk #	Retention Time	Area	Area %
1	22,717	24240191	97,95
2	24,283	506903	2,05

Totals			
		24747094	100,00

UV-Detektor S
2550 [Channel
2] Results

Pk #	Retention Time	Area	Area %
1	3,617	61894	0,73
2	22,683	8290719	97,51
3	24,267	149953	1,76

Totals			
		8502566	100,00

Figure S6. HPLC (H_2O:CH_3CN) of **2c**. Retention time: 22.68 minutes (254nm), 97% purity.
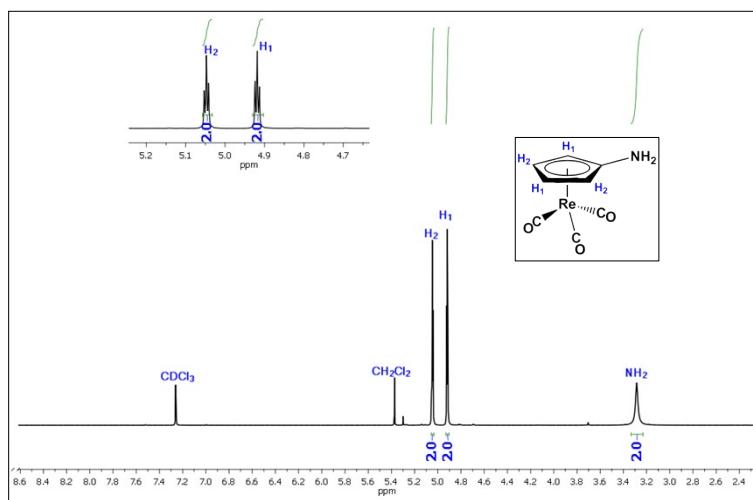

**Figure S7.** ^{1}H-NMR of **2d** in $CDCl_3$.
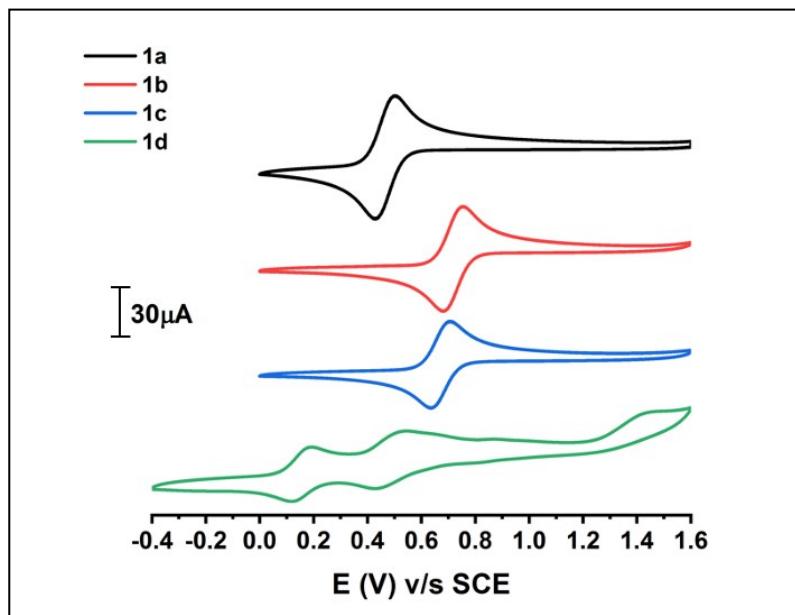
Figure S8. Cyclic voltammetry of ferrocenyl derivatives **1a-d** (1 mM) in dry CH_3CN using $(Bu_4N)[PF_6]$ (0.1 M) as the supporting electrolyte.
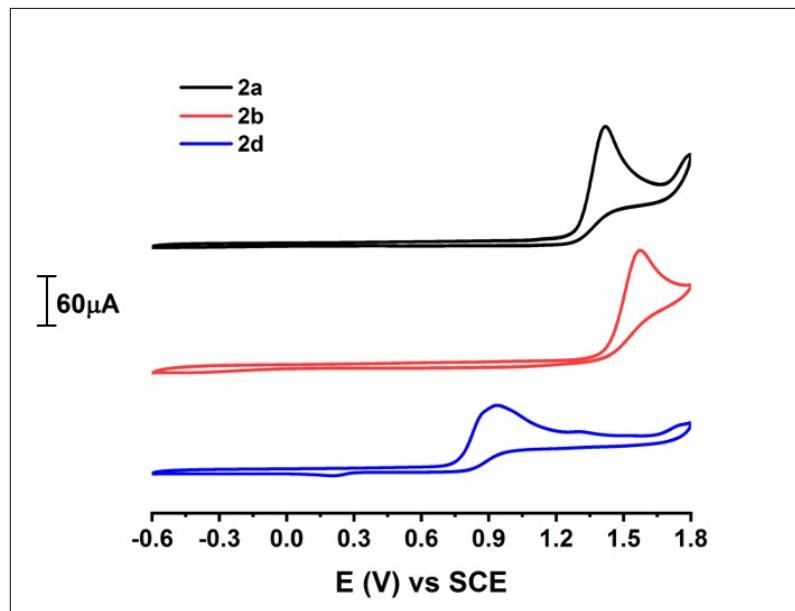

Figure S9. Cyclic voltammetry of cyrhetrenyl complexes **2a,b,d** (1 mM) in dry CH_3CN using $(Bu_4N)[PF_6]$ (0.1 M) as the supporting electrolyte.
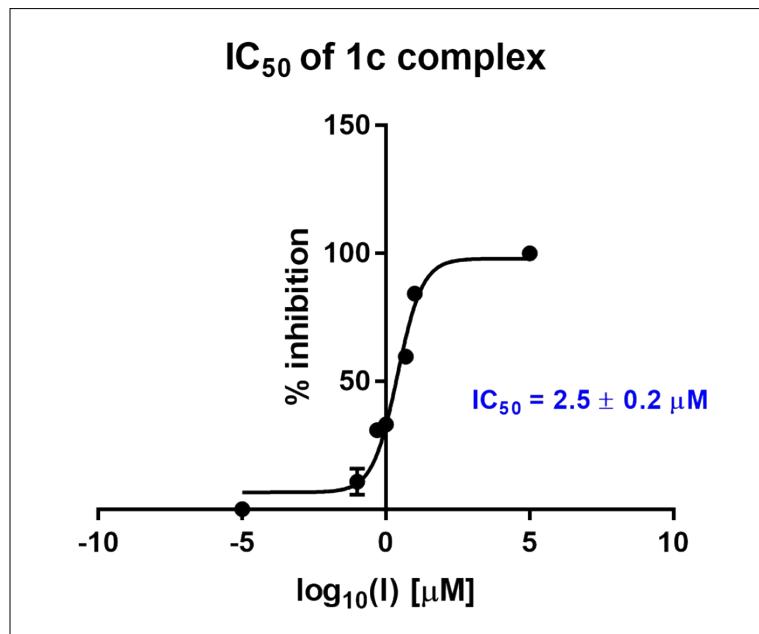
Figure S10. IC_{50} (μM) of ferrocenyl carboxylic acid complex (**1c**) in 5-hLOX.
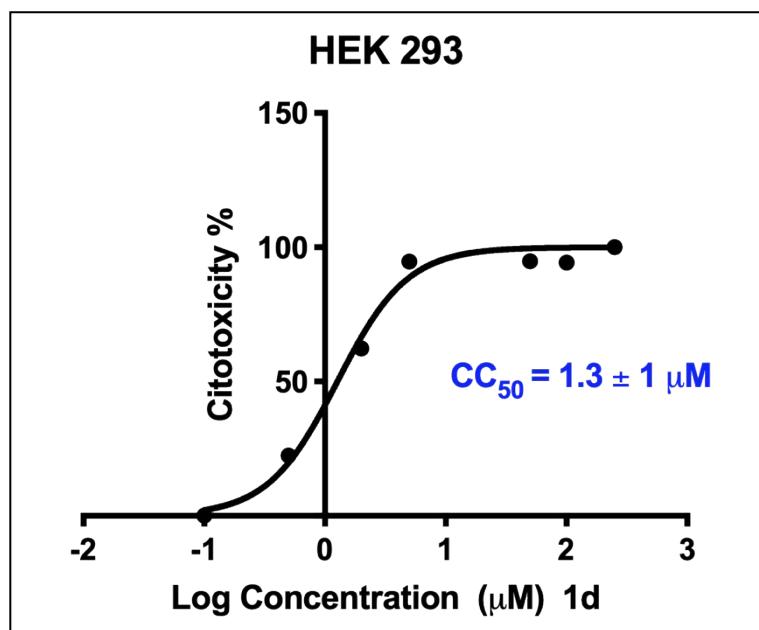

Figure S11. CC_{50} (μM) of aminoferrocene complex (**1d**) in HEK293 cell.

Table S1. *In vitro* antibacterial assay. The expressed values are the percent inhibition of bacterial growth achieved by compounds at a concentration of 100 µg/mL and Minimum inhibitory concentration (MIC; µg /mL)

| Compounds	*S. aureus* ATCC 6538	Compounds	*S. aureus* ATCC 6538	Compounds	*S. aureus* ATCC 6538
1a	0 (>100 µg/mL) > 537 µM	**1c**	6 (>100 µg/mL) > 434 µM	***Ciprofloxacin** (MIC)	100 (2 µg/mL) 6.03 µM
2a	23 (>100 µg/mL) > 298 µM	**2c**	37 (>100 µg/mL) > 264 µM	***Vancomycin** (MIC)	100 (5 µg/mL) 3.45 µM
1b	16 (>100 µg/mL) > 467 µM	**1d**	40 (>100 µg/mL) > 498 µM	***Meticillin** (MIC)	100 (5 µg/mL) 13.14 µM
2b	38 (>100 µg/mL) > 275 µM	**2d**	35 (>100 µg/mL) > 286 µM	***Ampicillin** (MIC)	-
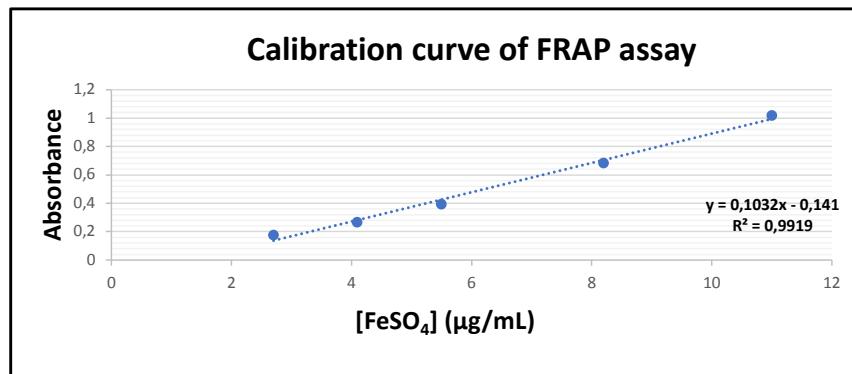
Figure S12. Calibration curve for the FRAP assay.