Novel Homo- (Fe_2) and Heterobimetallic [(Fe,M) with M = Re or Mn] Sulfonyl Hydrazones.

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Supplementary Materials

(33 pages)

CONTENTS

1.- Supplementary Figures

Figure S11. ^{1}H-NMR spectrum of a solution of compound [Fe(η^5-C_5H_5){[(η^5-C_5H_4)-S(O)$_2$-NH-N=CH-(η^5-C_5H_4)]Fe(η^5-C_5H_5)}] (**4**) in a mixture DMSO-d_6:D_2O (1:1) at 298 K.

Figure S12. Partial views of the ^{1}H-NMR spectrum of a solution of compound [Fe(η^5-C_5H_5){[(η^5-C_5H_4)-S(O)$_2$-NH-N=CH-(η^5-C_5H_4)]Re(CO)$_3$}] (**5a**) in a mixture DMSO-d_6:D_2O (1:1) at 298 K.

Figure S13. Partial views of the ^{1}H-NMR spectra of a freshly prepared solution of compound [Fe(η^5-C_5H_5){[(η^5-C_5H_4)-S(O)$_2$-NH-N=CH-(η^5-C_5H_4)]Mn(CO)$_3$}] (**5b**) in a mixture DMSO-d_6:D_2O (1:1) and after different periods of storage (*t*) at 298 K.

Figure S14. The cyclic voltammograms for compound **4**, at scan rates of 50, 100, 250 mV s^{-1}.

Figure S15. The cyclic voltammograms for compound **5a**, at scan rates of 50, 100, 250 mV s^{-1}.

Figure S16. The cyclic voltammograms for compound **5b**, at scan rates of 50, 100, 250 mV s^{-1}.

Figure S17. BJ Inhibition of cell growth proliferation in the normal and non-tumoral BJ cell line after 72 h of exposure to compounds **2**, **4**, **5a**, **5b** and cisplatin.

2.- Supplementary Tables

Table S1. Crystal data and details of the refinement of the crystal structures of compounds: [Fe(η^5-C_5H_5){(η^5-C_5H_4)-SO_2-NH-N=CMe_2}] (**3**) and [Fe(η^5-C_5H_5){[(η^5-C_5H_4)-S(O)$_2$-NH-N=CH-(η^5-C_5H_4)]M(CO)$_3$}] with M = Re (**5a**) or Mn (**5b**).

Table S2. Final atomic coordinates for the optimized geometry of compound [Fe(η^5-C_5H_5){(η^5-C_5H_4)-S(O)$_2$-NH-NH_2}] (**2**)

Table S3. Final atomic coordinates for the optimized geometry of compound [Fe(η^5-C_5H_5){(η^5-C_5H_4)-S(O)$_2$-NH=CMe_2}] (**3**).

Table S4. Final atomic coordinates for the optimized geometry of compound [Fe(η^5-C_5H_5){[(η^5-C_5H_4)-S(O)$_2$-NH-N=CH-(η^5-C_5H_4)]Fe(η^5-C_5H_5)}] (**4**).

Table S5. Final atomic coordinates for the optimized geometry of compound [Fe(η^5-C_5H_5){[(η^5-C_5H_4)-S(O)$_2$-NH-N=CH-(η^5-C_5H_4)]Re(CO)$_3$}] (**5a**).

Table S6. Final atomic coordinates for the optimized geometry of compound [Fe(η^5-C_5H_5){[(η^5-C_5H_4)-S(O)$_2$-NH-N=CH-(η^5-C_5H_4)]Mn(CO)$_3$}] (**5b**).

Table S7. Summary of experimental ultraviolet data [position of the bands (wavelengths λ_i (in nm)) and logarithms of the molar extinction coefficients, (log ε_i, in parenthesis)] and computational studies [Monoelectronic transitions with greater contributions ($\geq$ 15%)) to the absorption bands detected in the UV-vis spectra of compounds **2**-**4**, **5a** and **5b**, calculated position of the bands λ_i (calc) in nm and oscillator strengths (*f*)].

1.- Supplementary Figures

Figure S1. Schematic view of: **A**) the assembly of a molecule of **3**, sited at (*x*, *y*, *z*) and another unit at (*−1+x*, *y*, *1/2-z*) by cooperative N-H···O intermolecular interactions (blue dotted line) and **B**) simplified view of the CH···π short contact between: a) the H13 atom of a molecule at (*x*, *y*, *z*) and the C_5H_5 of the vicinal molecule sited at (*x*, *-y*, *1/2+z*) (green dotted line) [the distance H13B···centroid of this ring is 2.995 Å]; and b) the hydrogen H8B of a molecule at (*x*, *y*, *z*) and the C_5H_5 ring of a close unit located at (*x*, *-y*, *1/2-z*) (purple dotted lines) [the separation between the H8B atom and the centroid of this ring is 3.459 Å]. In this figure, the intermolecular N-H···O interactions shown in **A**) appear as a dotted blue line). In both cases the labels of most of the atoms have been omitted for clarity.

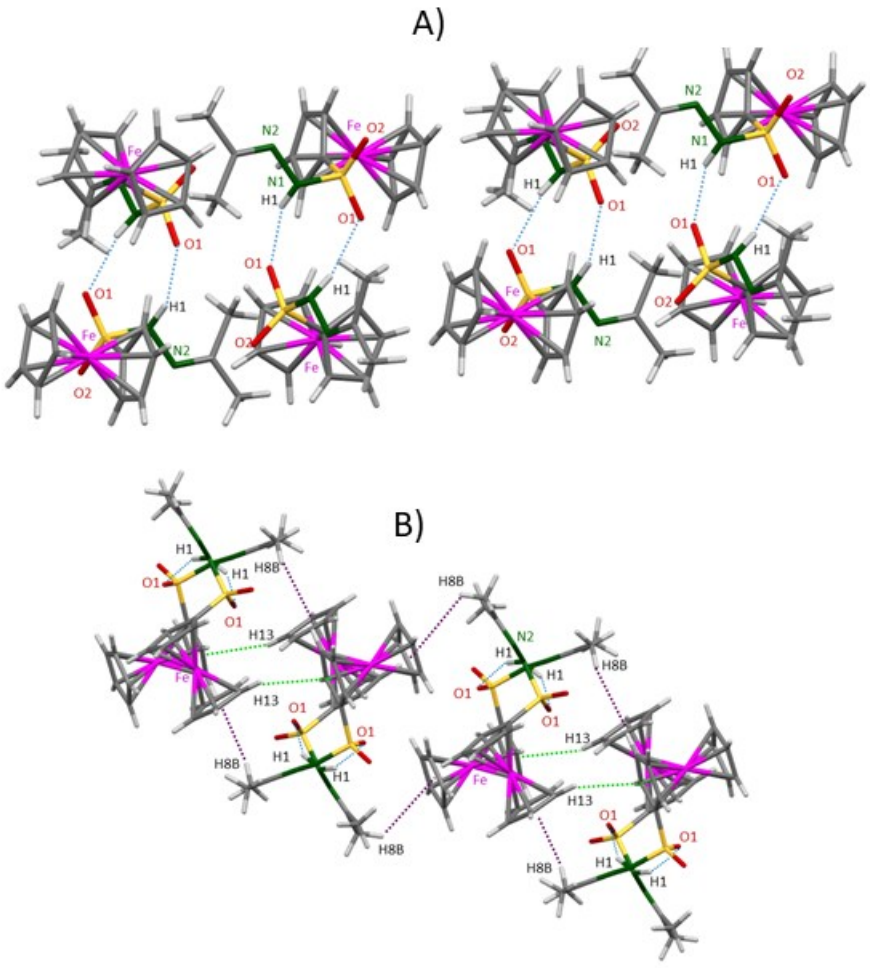


Figure S2. Simplified view of the assembly of the molecules of **5a** in the crystal through C-H···O interactions involving the hydrogen atoms H12 and H13 of a molecule at (*x*, *y*, *z*) and oxygen atoms of the sulfonyl unit (O4 and O5, respectively) of a vicinal unit sited at (*x*, *-1+y*, *z*) (blue dotted line) giving chains. These structural units are connected by the C-H···π interactions the H3 atom of a molecule and the C_5H_5 ring of the ferrocenyl unit belonging to a different chain (purple dotted line) and C-H···O short contacts (red dotted line)involving the oxygen O2 of one of the CO ligands of each cyrhetrenyl unit. Labels of most of the atoms have been omitted for clarity.

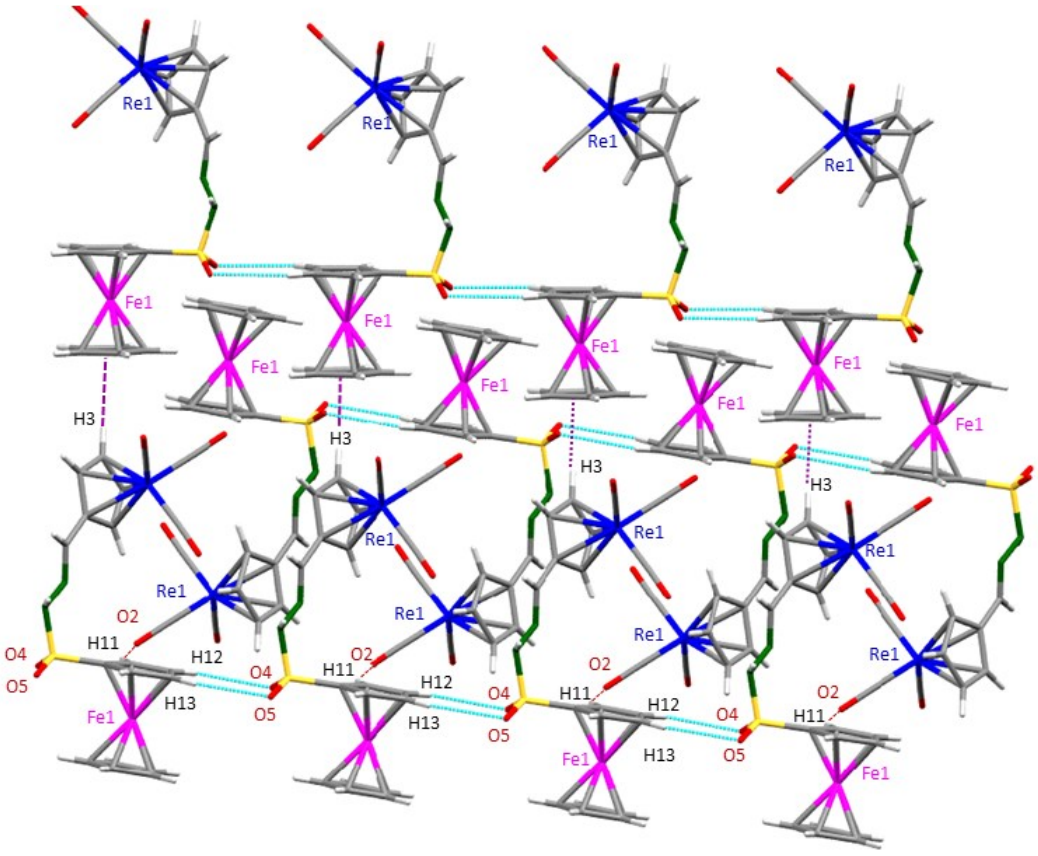


Figure S3. Schematic view of the connectivity between molecules **A** and **B** present in the crystals of **5b** through intermolecular N-H···O interactions (N2A-H2A ···O5B (in purple) and N2B-H2B···O5A (in red). Labels of most of the atoms have been omitted for clarity.

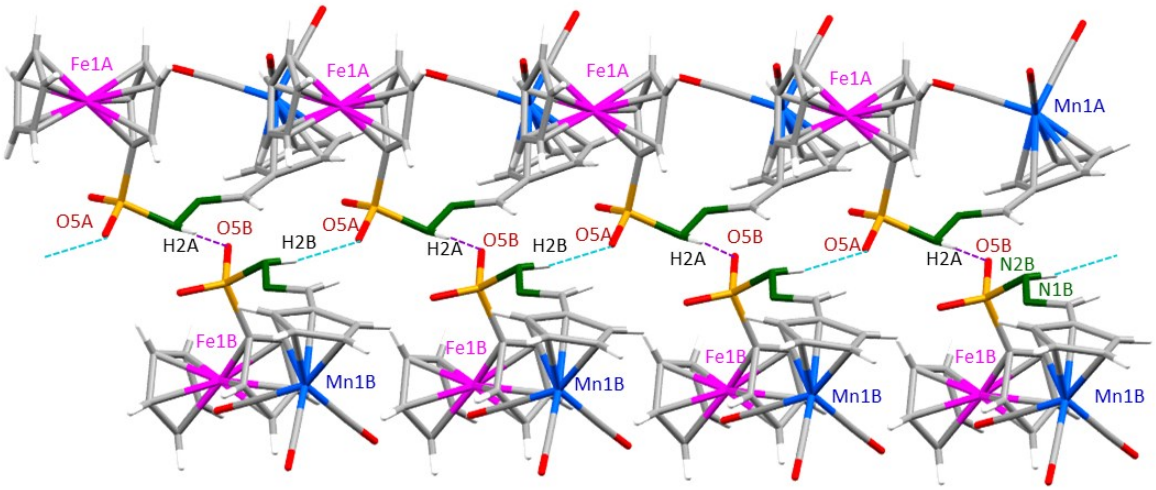


Figure S4. ^{1}H-NMR spectra of a freshly prepared solution of compound [Fe(η^5-C_5H_5){(η^5-C_5H_4)-S(O)$_2$-NH-NH$_2$}] (**2**) in CD_3CN at 298K.

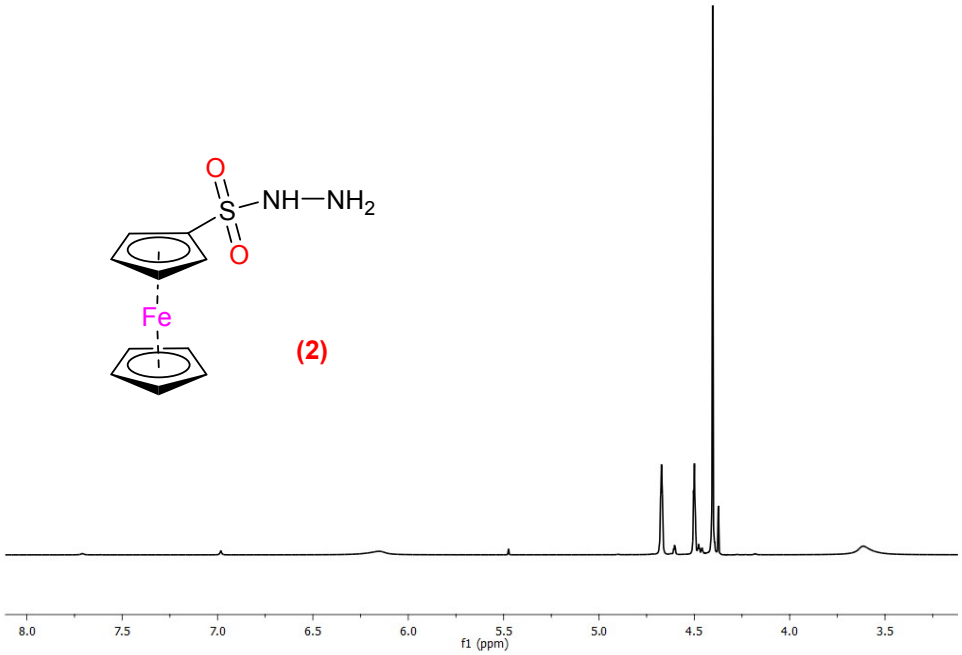
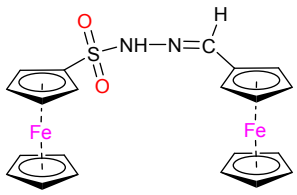


Figure S5. ^{1}H-NMR spectra of a freshly prepared solution of compound [Fe(η^5-C_5H_5){[(η^5-C_5H_4)-S(O)$_2$-NH-N=CH-(η^5-C_5H_4)]Fe(η^5-C_5H_5)}] (**4**) in CD_3CN at 298 K.



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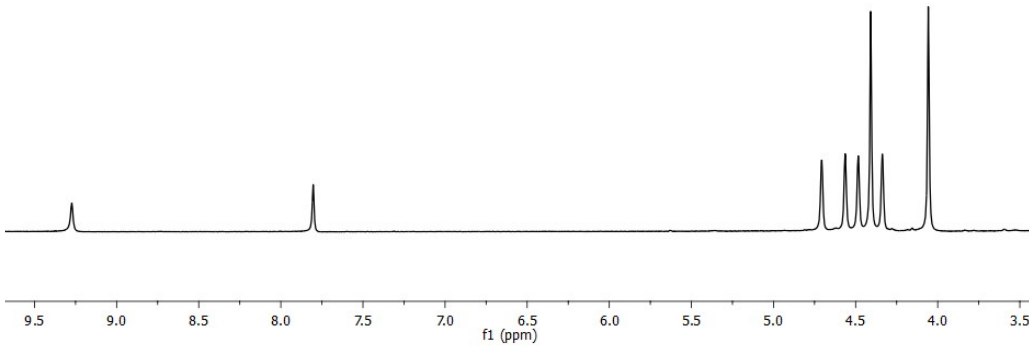


Figure S6. ^{1}H-NMR spectra of a freshly prepared solution of compound [Fe(η^5-C_5H_5){[(η^5-C_5H_4)-S(O)$_2$-NH-N=CH-(η^5-C_5H_4)]Re(CO)$_3$}] (**5a**) in CD_3CN at 298 K.

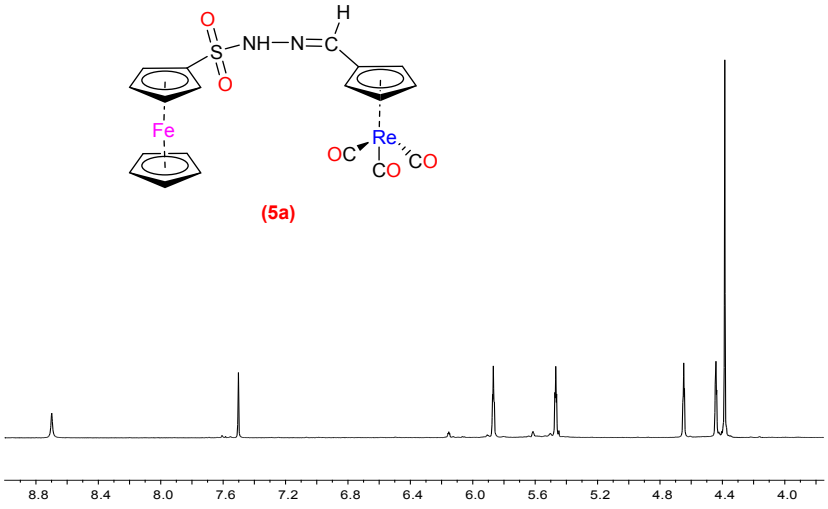


Figure S7. ^{1}H-NMR spectra of a freshly prepared solution of compound [Fe(η^5-C_5H_5){[(η^5-C_5H_4)-S(O)$_2$-NH-N=CH-(η^5-C_5H_4)]Mn(CO)$_3$}] (**5b**) in CD_3CN at 298 K.

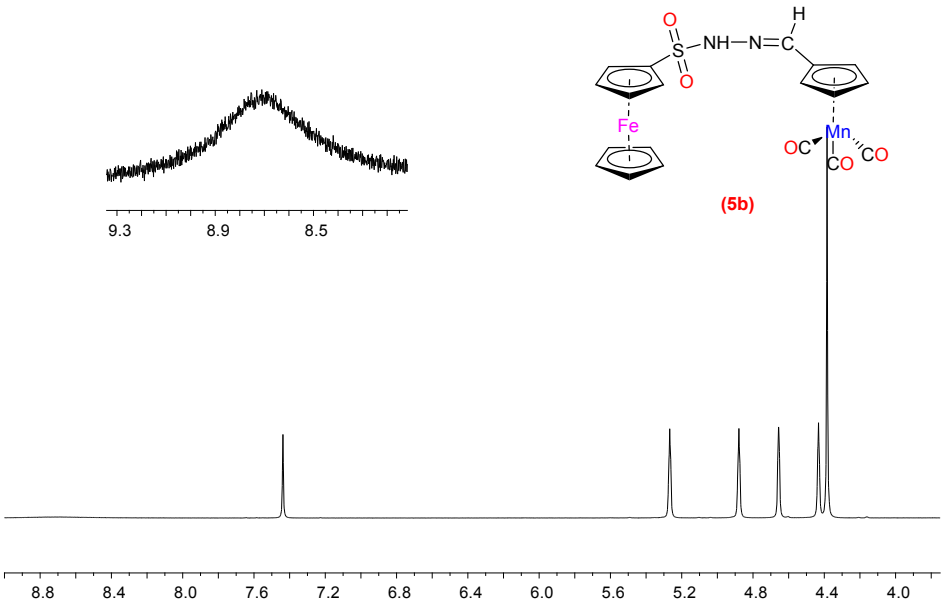


Figure S8. ^{1}H-NMR spectra of a freshly prepared solution of compound [Fe(η^5-C_5H_5){[(η^5-C_5H_4)-$S(O)_2$-NH-N=CH-(η^5-C_5H_4)]Fe(η^5-C_5H_5)}] (**4**) in DMSO-d_6 and after different periods of storage (*t*) at 298 K.

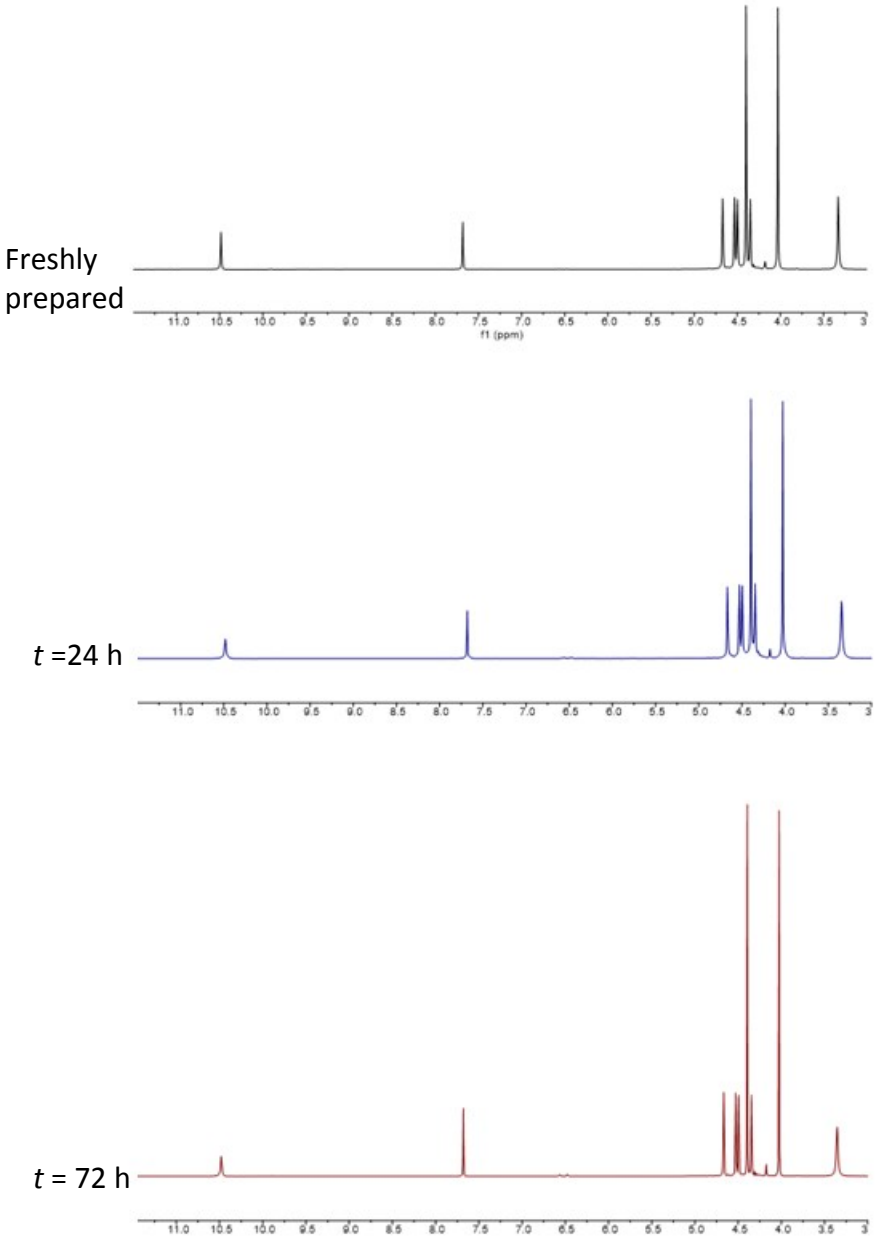


Figure S9. ^{1}H-NMR spectra of a freshly prepared solution of compound [Fe(η^5-C_5H_5){[(η^5-C_5H_4)-S(O)$_2$-NH-N=CH-(η^5-C_5H_4)]Re(CO)$_3$}] (**5a**) in DMSO-d_6 and after different periods of storage at 298 K.

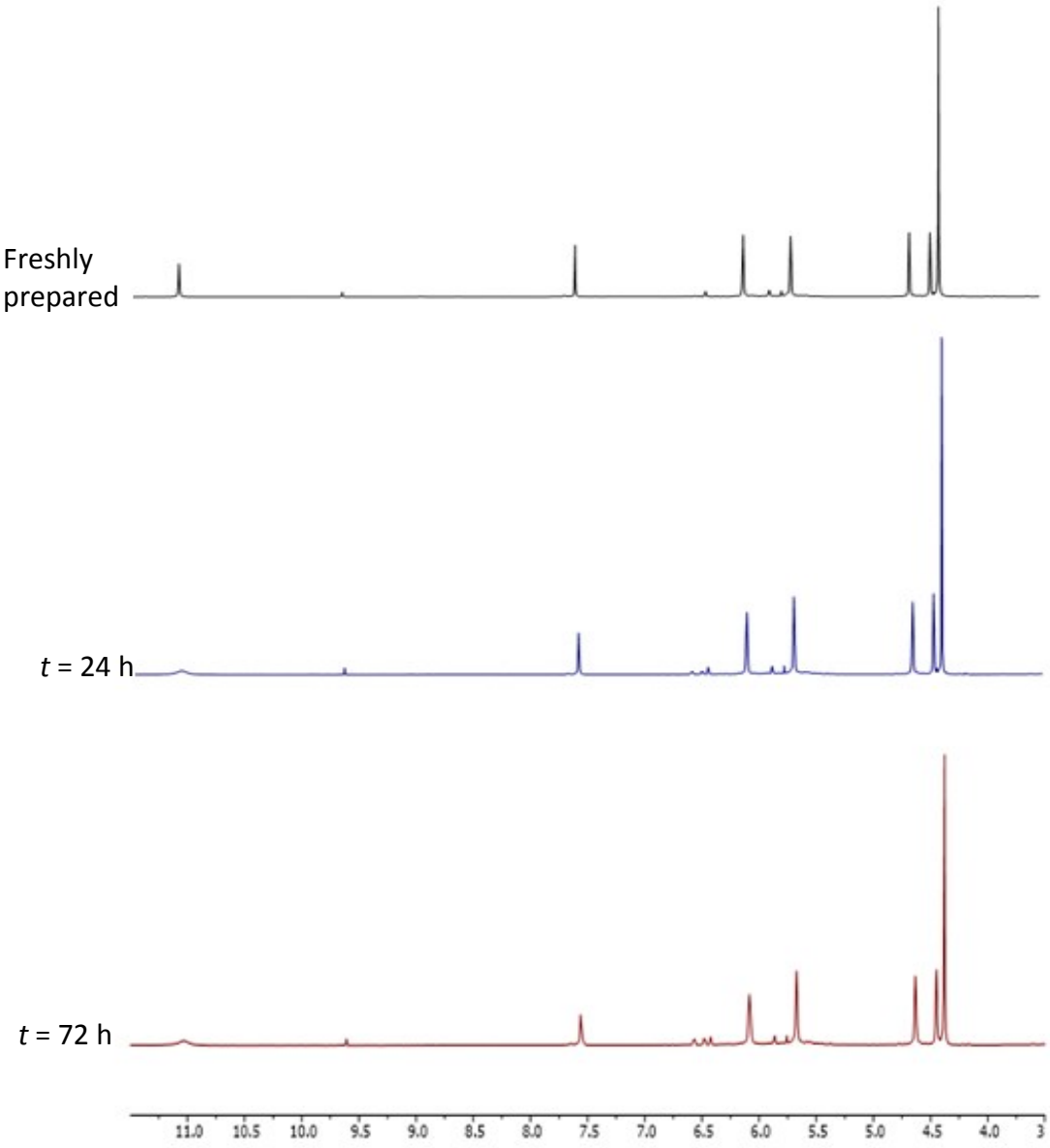
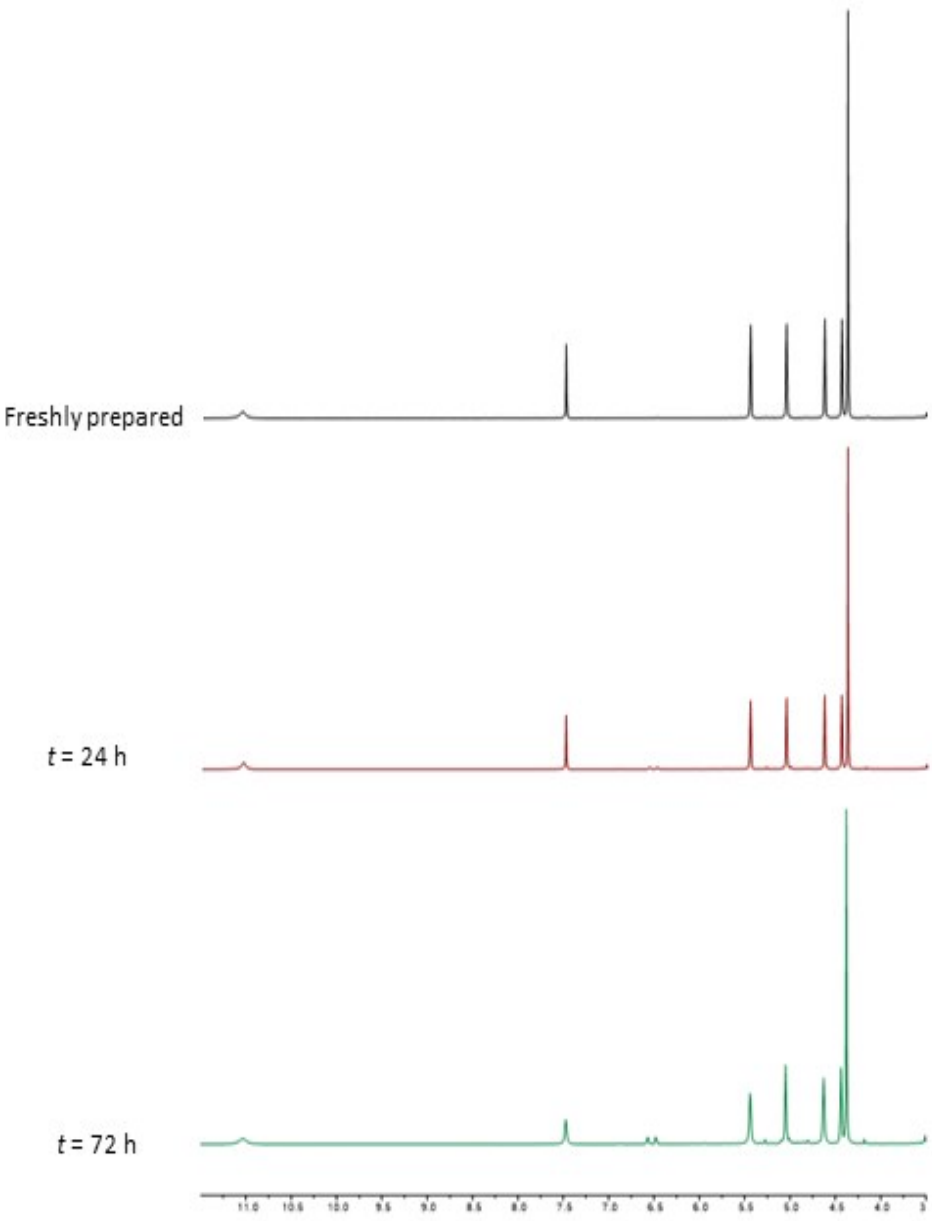


Figure S10. ^{1}H-NMR spectra of a freshly prepared solution of compound [Fe(η^5-C_5H_5){[(η^5-C_5H_4)-$S(O)_2$-NH-N=CH-(η^5-C_5H_4)]Mn$(CO)_3$}] (**5b**) in DMSO-d_6 and after different periods of storage (*t*) at 298 K.



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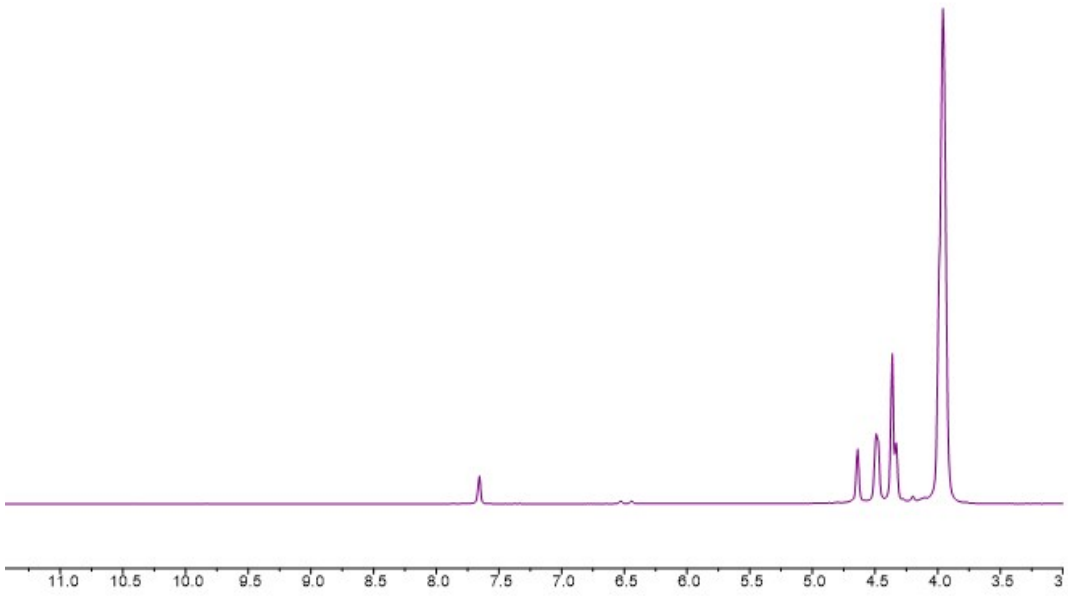


Figure S12. Partial views of the ^{1}H-NMR spectrum of a solution of compound [Fe(η^5-C_5H_5){[(η^5-C_5H_4)-$S(O)_2$-NH-N=CH-(η^5-C_5H_4)]Re$(CO)_3$}] (**5a**) in a mixture DMSO-d_6:D_2O (1:1) at 298 K.

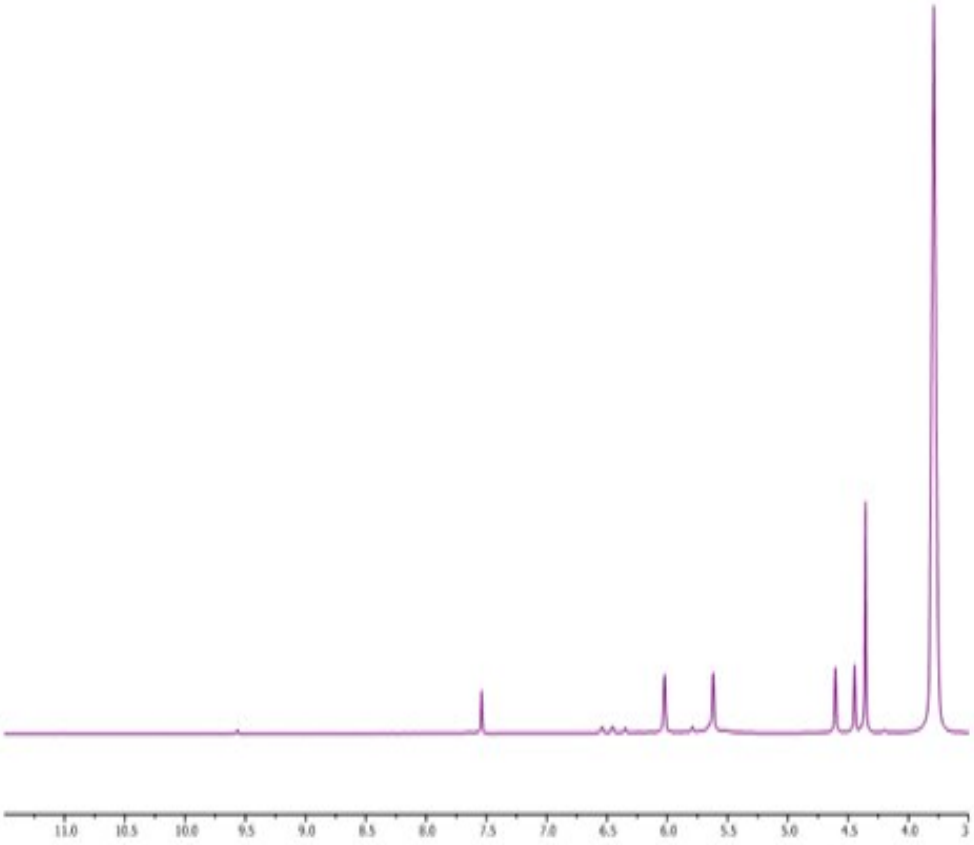


Figure S13. Partial views of the ^{1}H-NMR spectra of a freshly prepared solution of compound [Fe(η^5-C_5H_5){[(η^5-C_5H_4)-S(O)$_2$-NH-N=CH-(η^5-C_5H_4)]Mn(CO)$_3$}] (**5b**) in a mixture DMSO-d_6:D_2O (1:1) and after different periods of storage (*t*) at 298 K.

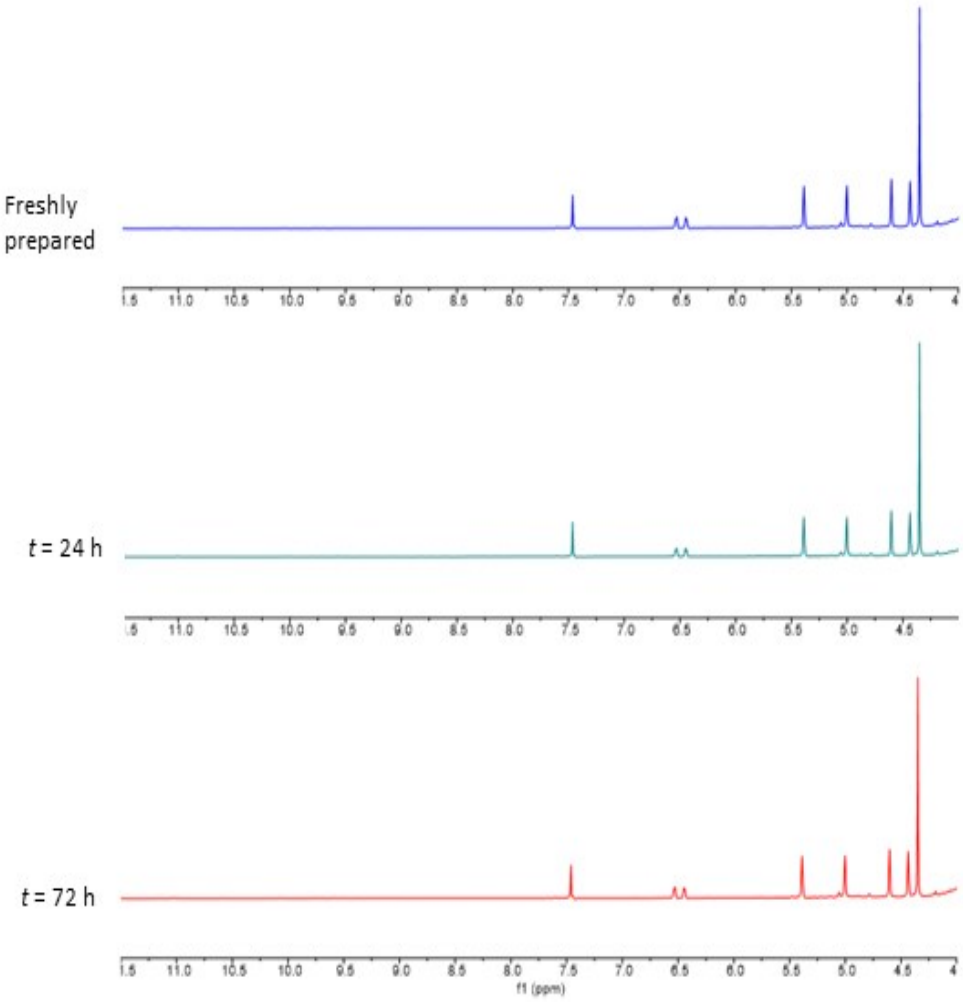


Figure S14. The cyclic voltammograms for compound **4**, at a scan rate of 50, 100, 250 mV s^{-1}.

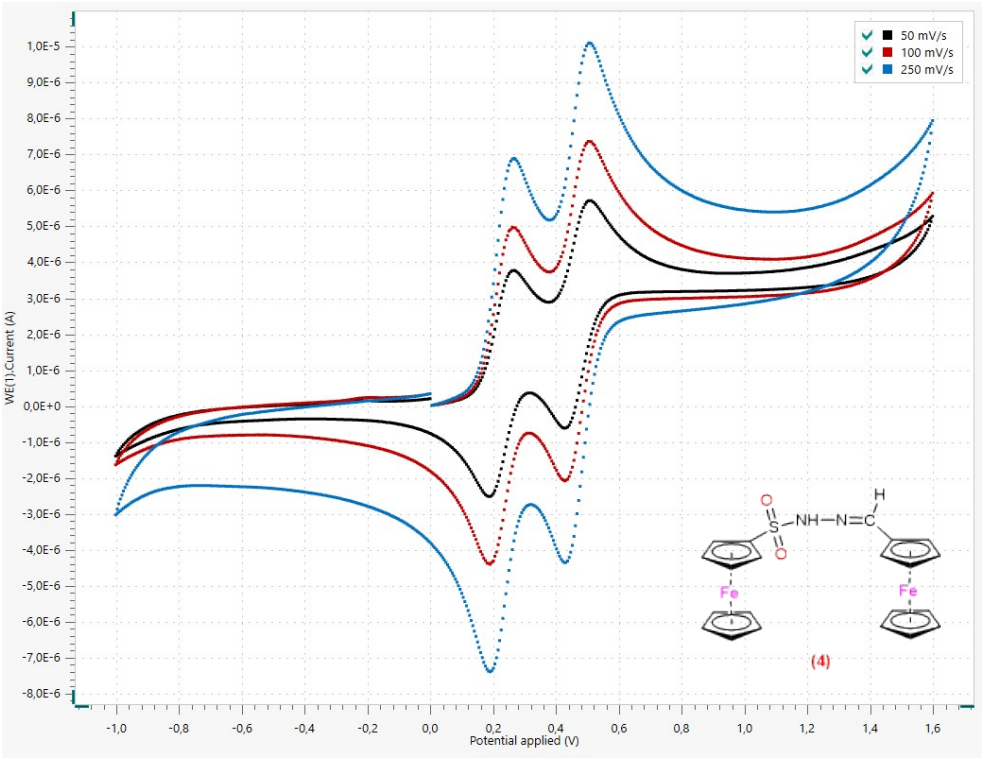


Figure S15. The cyclic voltammograms for compound **5a**, at scan rates of 50, 100, 250 mV s^{-1}.

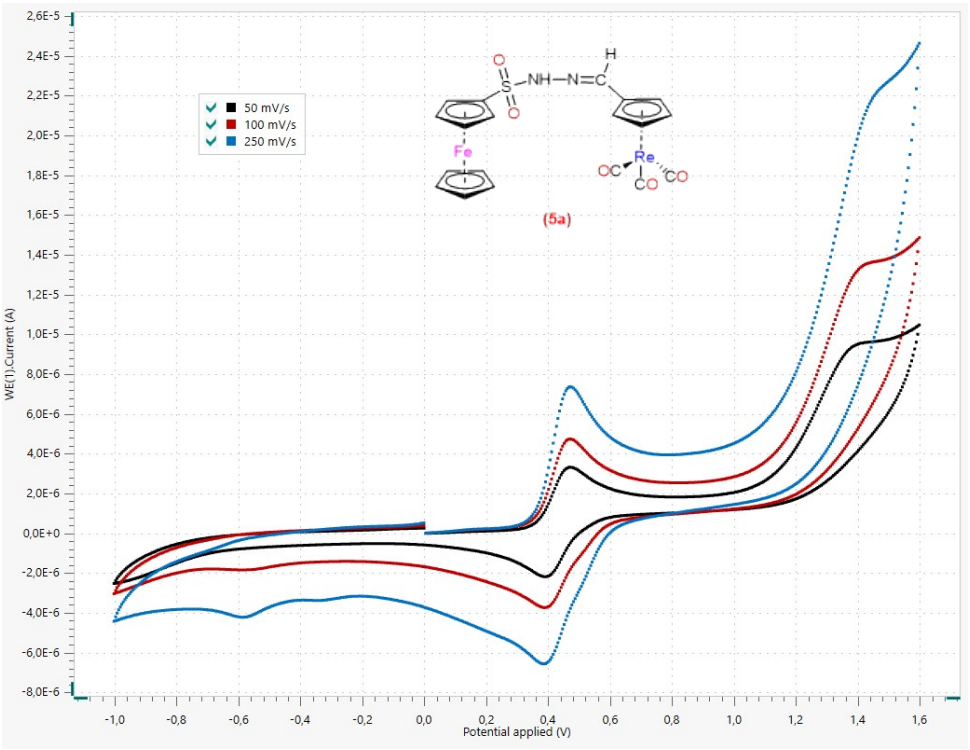


Figure S16. The cyclic voltammograms for compound **5b**, at scan rates of 50, 100, 250 mV s^{-1}.

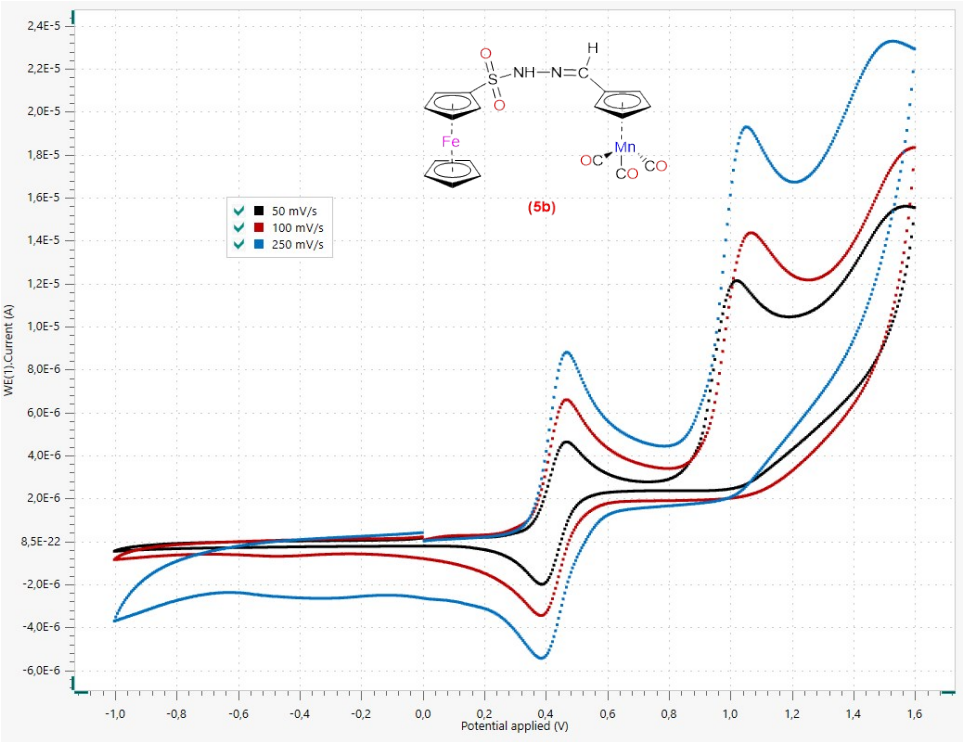
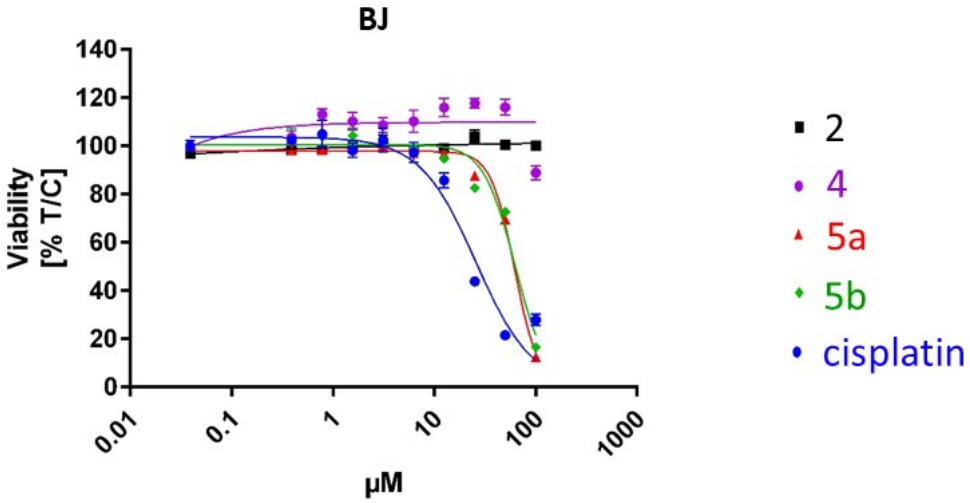


Figure S17. BJ Inhibition of cell growth proliferation in the normal and non-tumoral BJ cell line after 72 h of exposure to compounds **2**, **4**, **5a**, **5b** and cisplatin.



2. Supplementary Tables

Table S1. Crystal data and details of the refinement of the crystal structures of compounds: [Fe(η^5-C_5H_5){(η^5-C_5H_4)-$SO_2NHN{=}CMe_2$}] (**3**) and [Fe(η^5-C_5H_5){[(η^5-C_5H_4)-$S(O)_2$-NH-N=CH-(η^5-C_5H_4)]$M(CO)_3$}] with M = Re (**5a**) or Mn (**5b**).

	3	**5a**	**5b**
Crystal size (mm × mm × mm)	0.18 × 0.15 × 0.12	0.155 × 0.134 × 0.088	0.18 × 0.05 × 0.012
Empirical formula	$C_{13}H_{16}FeN_2O_2S$	$C_{19}H_{15}FeN_2O_5ReS$	$C_{19}H_{15}FeN_2O_5MnS$
Formula weight	320.20	625.44	494.18
T(K)	298	298	298
λ(Å)	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Triclinic
Space group	C2/c	$P2_1/n$	P-1
a (Å)	20.8459(10)	12.6127(8)	7.1339(3)
b (Å)	9.8908(5)	7.7038(5)	15.3593(6)
c (Å)	13.3379(7)	22.0 053(15)	18.4395(7)
α (deg)	90	90	80.8480(19)
β (deg.)	95.843(3)	99.323(2)	84.4154(17)
γ (deg)	90	90	81.2946(17)
V ($Å^3$)	2735.8(2)	2109.9(2)	1996.19(14)
Z	8	4	4
$D_{calc.}$ (Mg × m^{-3})	1.555	1.969	1.669
μ (mm^{-1})	1.253	6.550	1.520
F(000)	1328	1200	1000
Θ Range for data collec. (deg.)	from 2.281 to 29.853	from 1.749 to 27.504	from 1.356 to 29.259
Index ranges	$-27 \le h \le 28$ $-13 \le k \le 13$ $-18 \le l \le 18$	$-16 \le h \le 16$ $-9 \le k \le 10$ $-28 \le l \le 27$	$-19 \le h \le 9$ $-21 \le k \le 21$ $-25 \le l \le 25$

N. of collected reflections	45313	48431	38060
N. Independent. reflec. [R_{int}]	3863 [0.0252]	4843 [0.0309]	10926(0.0255)
Completeness to Θ = 25.242	98.75	100 %	99.9 %
Absorption correction	← Semiempirical from equivalents →		
Refinement method	← Full- matrix least- squares on F^2 →		
N. of parameters	174	266	523
Goodness of fit on F^2	1.080	1.071	1.027
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.0406	R_1 = 0.0250,	R_1 = 0.0327,
	wR_2 = 0.1059	wR_2 = 0.0544	wR_2 = 0.0832
Final R indices (all data)	R_1 = 0.0486,	R_1 = 0.0301,	R_1 = 0.0426,
	wR_2 = 0.1117	wR_2 = 0.0562	wR_2 = 0.0898

Table S2. Final atomic coordinates for the optimized geometry of compound [Fe(η^5-C_5H_5){(η^5-C_5H_4)-$S(O)_2$-NH-NH_2}] (**2**).

Atom	*x*	*y*	*z*
Fe	-0.461474	0.4704	0.797537
H	0.522196	3.037422	0.088060
C	0.207536	2.082250	-0.311543
C	-1.122335	1.735429	-0.701013
H	2.099966	0.868002	-0.278181
H	-1.987302	2.383469	-0.646130
C	-1.127747	0.380885	-1.137185
H	-1.978816	-0.192466	-1.477778
C	0.216708	-0.108948	-1.015715
C	1.045996	0.947577	-0.505862
H	-1.572306	2.005503	2.903990
C	-1.196412	1.023709	2.646172
C	0.158206	0.587512	2.759995
H	-3.020294	-0.033458	1.885878
H	0.988812	1.182932	3.116718
C	0.229782	-0.758164	2.292889
H	1.124933	-1.360093	2.208789
C	-1.081865	-1.155941	1.891270
H	-1.347535	-2.109599	1.454650
C	-1.961963	-0.055644	2.111748
S	0.746996	-1.752111	-1.408698
O	1.992471	-1.992576	-0.675471
O	-0.414070	-2.641423	-1.319125
N	1.177611	-1.747426	-3.060233
H	0.350161	-1.683117	-3.649014
N	2.194846	-0.869186	-3.489248
H	2.070258	0.069606	-3.100008
H	3.075404	-1.243146	-3.144078

Table S3. Final atomic coordinates for the optimized geometry of compound [Fe(η^5-C_5H_5){(η^5-C_5H_4)-S(O)$_2$-NH=CMe$_2$}] (**3**).

Atom	*x*	*y*	*z*
Fe	1.472446	-1.086039	1.452730
H	0.717492	-3.529735	0.214624
C	0.824982	-2.465176	0.052510
C	2.003326	-1.804693	-0.413592
H	-1.179785	-1.645280	0.662363
H	2.941159	-2.283352	-0.663967
C	1.749596	-0.405668	-0.461213
H	2.437040	0.372631	-0.761140
C	0.399622	-0.211298	-0.020235
C	-0.175098	-1.484396	0.299446
H	3.194589	-2.842318	2.857382
C	2.628961	-1.923594	2.943944
C	1.272209	-1.810480	3.373060
H	4.084803	-0.365302	2.253156
H	0.626681	-0.433263	3.317870
C	0.904543	-0.433263	3.317870
H	-0.071086	-0.022167	3.541787
C	2.034802	0.307186	2.855093
H	2.054302	1.371656	2.663639
C	3.099533	-0.613560	2.626152
S	-0.397565	1.342020	0.192094
O	-1.530637	1.151131	1.100265
O	0.596912	2.393330	0.440053
N	-0.922114	1.708226	-1.404187
H	-0.976926	2.727693	-1.489177
N	-2.010013	0.963980	-1.824330
C	-2.722942	1.438995	-2.779753
C	-2.473244	2.776726	-3.440899
H	-2.610446	3.607815	-2.733481
H	-1.447102	2.840820	-3.825323
H	-3.162115	2.941108	-4.272995
C	-3.872014	0.599439	-3.266009
H	-3.923009	-0.335717	-2.704343
H	-3.763141	0.370018	-4.334524
H	-4.822548	1.137337	-3.150449

Table S4. Final atomic coordinates for the optimized geometry of compound [Fe(η^5-C_5H_5){[(η^5-C_5H_4)-S(O)$_2$-NH-N=CH-(η^5-C_5H_4)]Fe(η^5-C_5H_5)}] (**4**).

Atom	*x*	*y*	*z*
Fe	4.132666	-0.160446	-1.253812
H	2.579396	0.849272	-3.408863
C	2.690532	0.859473	-2.332470
C	3.487302	1.778791	-1.582783
H	1.438994	-0.888991	-1.672082
H	4.086171	2.580635	-1.994621
C	3.393987	1.437035	-0.204384
H	3.889787	1.918626	0.626727
C	2.530482	0.294083	-0.113286
C	2.092350	-0.063401	-1.429925
H	4.380372	-2.277665	-3.105590
C	4.886617	-1.77368	-2.292399
C	4.764814	-2.087434	-0.906522
H	6.046952	-0.167580	-3.342242
H	4.136045	-2.855164	-0.475626
C	5.56696	-1.160634	-0.173120
H	5.653999	-1.115653	0.904543
C	6.185239	-0.277323	-1.107304
H	6.838558	0.550486	-0.863692
C	5.763252	-0.653851	-2.417730
S	2.105277	-0.537512	1.383469
O	1.825163	-1.935131	1.074371
O	3.057621	-0.131756	2.420289
N	0.635431	0.163840	1.914882
H	0.806757	1.066299	2.370426
N	-0.403472	0.095491	1.016707
C	-1.339880	0.964499	1.134948
H	-1.292610	1.759127	1.893305
Fe	-4.334649	0.094939	0.764460
H	-2.299521	-0.975879	-0.865525
C	-2.875176	-0.082683	-0.667117

C	-2.517579	0.934423	0.280112
H	-4.643420	-0.274563	-2.023775
C	-3.558632	1.924559	0.262764
H	-3.592584	2.815401	0.877259
C	-4.532419	1.529400	-0.698415
C	-4.107023	0.293519	-1.274788
H	-3.975390	0.385711	3.554147
C	-4.534567	-0.151514	2.798933
C	-4.144761	-1.380706	2.184348
H	-6.324220	1.157351	2.469229
H	-3.232815	-1.929092	2.381901
C	-5.150548	-1.734670	1.236293
H	-5.137980	-2.605838	0.594083
C	-6.157491	-0.723114	1.259381
H	-7.045157	-0.694329	0.640823
C	-5.776494	0.256227	2.225546
H	-5.442796	2.063271	-0.937553

Table S5. Final atomic coordinates for the optimized geometry of compound [Fe(η^5-C_5H_5){[(η^5-C_5H_4)-$S(O)_2$-NH-N=CH-(η^5-C_5H_4)]Re$(CO)_3$}] (**5a**).

Atom	*x*	*y*	*z*
Re	2.083289	-0.618959	-3.537940
Fe	-1.650293	-0.764982	2.821387
S	-1.224626	2.158707	1.253237
O	-0.423734	-1.110935	-5.261039
O	-2.632827	2.557318	1.317623
C	2.896425	0.970535	-1.983952
H	2.925710	0.765436	-0.922787
O	-0.214376	2.684264	2.164086
C	0.524781	-0.969718	-4.606216
N	-0.784593	2.640676	-0.339234
C	-1.119525	0.401697	1.265653
N	0.393758	2.135521	-0.810965
C	-2.158641	-0.500271	0.855651
H	-3.139590	-0.216699	0.500392
O	3.670874	-2.842166	-4.959000
C	3.931830	0.719771	-2.923405
H	4.900677	0.292892	-2.702775
C	0.015336	-0.361821	1.695321
H	0.941393	0.049442	2.070284
C	1.791091	1.585106	-2.667210
C	0.553168	2.088195	-2.082431
H	-0.222881	2.429203	-2.779657
C	3.039547	-2.030562	-4.420435
O	1.131540	-2.581492	-1.357086
C	-2.115982	-1.947882	4.444051
H	-1.990790	-3.021905	4.491140
C	-1.138925	-0.971564	4.805935
H	-0.140965	-1.176772	5.170910
C	-3.018802	0.143279	4.057103
H	-3.685609	0.936111	3.744756

C	2.161398	1.675516	-4.056432
H	1.548916	2.099026	-4.842385
C	3.474621	1.157270	-4.214079
H	4.035348	1.117595	-5.137814
C	-1.657874	-1.819657	1.038287
H	-2.204137	-2.733934	0.847285
C	-0.328359	-1.733661	1.552534
H	0.305657	-2.571754	1.808677
C	-1.695965	0.319740	4.567867
H	-1.189936	1.267479	4.697772
C	-3.277510	-1.257820	3.982283
H	-4.185628	-1.718072	3.614856
C	1.474027	-1.861636	-2.200148
H	-1.597819	2.617483	-0.962102

Table S6. Final atomic coordinates for the optimized geometry of compound [Fe(η^5-C_5H_5){[(η^5-C_5H_4)-$S(O)_2$-NH-N=CH-(η^5-C_5H_4)]Mn$(CO)_3$}] (**5b**).

Atom	*x*	*y*	*z*
Mn	2.325962	-0.511826	-3.190907
Fe	-1.754080	-0.807672	2.685664
S	-1.266774	2.153589	1.166558
O	-0.254496	-1.500961	-4.226089
O	-2.603755	2.725119	1.334275
C	2.935474	1.244100	-2.067163
H	3.053715	1.275452	-0.992647
O	-0.138279	2.512190	2.016312
C	0.767293	-1.148439	-3.814035
N	-0.849582	2.625977	-0.435972
C	-1.412674	0.400100	1.107852
N	0.325445	2.119416	-0.912133
C	-2.637739	-0.321317	0.903768
H	-3.618189	0.120046	0.792592
O	3.955171	-2.591769	-4.499931
C	3.938563	0.928253	-3.017209
H	4.966687	0.674381	-2.797476
C	-0.335516	-0.538277	1.231953
H	0.702381	-0.290195	1.397289
C	1.722306	1.548530	-2.760865
C	0.462625	2.004487	-2.181803
H	-0.342892	2.267088	-2.880255
C	3.291821	-1.801562	-3.977201
O	2.154674	-1.974618	-0.635146
C	-2.053300	-2.042452	4.309831
H	-2.109715	-3.122717	4.273819
C	-0.866355	-1.268932	4.487084
H	0.136257	-1.661210	4.598057
C	-2.638730	0.191288	4.248469
H	-3.210484	1.103973	4.142121

C	1.997206	1.398839	-4.163087
H	1.286921	1.563582	-4.963512
C	3.352892	1.025546	-4.319612
H	3.858460	0.850335	-5.259963
C	-2.308104	-1.705866	0.905264
H	-3.011777	-2.521977	0.804219
C	-0.899580	-1.837693	1.104863
H	-0.351019	-2.767467	1.174028
C	-1.226360	0.110350	4.448135
H	-0.547894	0.951179	4.507252
C	-3.148889	-1.138576	4.166465
H	-4.181561	-1.413558	3.995468
C	2.201066	-1.424855	-1.651996
H	-1.667175	2.598116	-1.054335

Table S7. Summary of experimental ultraviolet data [position of the bands (wavelengths λ_i (in nm) and logarithms of the molar extinction coefficients, (log ε_i , in parenthesis] and computational studies [Monoelectronic transitions with greater contributions (≥ 15%) to the absorption bands detected in the UV- vis spectra of compounds **2**-**4**, **5a** and **5b**, calculated position of the bands λ_i (calc) in nm and oscillator strengths (*f*)].

Compound	**Experimental data**	**Computational studies**		
	λ_i (log ε_i)	Assignment	λ_i(calc.)	*f*
2	228 (3.9)	HOMO-3 → LUMO (34 %) HOMO-4 → LUMO+1 (27 %)	230.5	0.0076
	262 (3.6)	HOMO → LUMO+2 (91 %)	264.2	0.0013
		HOMO-1 → LUMO+2 (78 %)	248.6	0.0193
3	228 (4.1)	HOMO-3 → LUMO (39 %) HOMO-2 → LUMO+3 (35 %)	226.0	0.0057
		HOMO-3 → LUMO (30 %) HOMO-5 → LUMO (29 %) HOMO-4 → LUMO+1 (24 %)	230.1	0.0158
	262 (4.9)	HOMO-1 → LUMO+3 (54 %) HOMO-1 → LUMO+2 (28 %)	251.5	0.0173
		HOMO → LUMO+3 (84 %)	266.4	0.0110
4	228(4.2)	HOMO-4 → LUMO+4 (31 %)	223.9	0.0369
		HOMO → LUMO+5 (37 %)	225.8	0.0027
		HOMO-4 → LUMO+1 (16 %)	227.7	0.0023
		HOMO-2 → LUMO+4 (73 %)	228.5	0.0023
		HOMO-10 → LUMO (27 %)	229.2	0.0411
	261[a]	HOMO → LUMO+2 (90 %)	259.2	0.0362
		HOMO-4 → LUMO (57 %) HOMO → LUMO+1(15 %)	260.9	0.4555

		HOMO-2 → LUMO+5 (79 %)	261.1	0.0202
		HOMO-1→ LUMO+1 (96 %)	262.1	0.0025
		HOMO-2 → LUMO+5 (79 %)	262.6	0.0085
		HOMO → LUMO+1 (76 %)	267.5	0.1270
	294 (4.0)	HOMO-3 → LUMO+4 (88 %)	295.3	0.0426
		HOMO →LUMO+4 (54 %) HOMO→ LUMO (34 %)	305.2	0.0703
5a	228 (4.2)	HOMO-4 → LUMO+5 (69 %)	226.9	0.0062
		HOMO-1 → LUMO+6 (28 %)	229.3	0.0020
	244 (4.2)	HOMO-2 → LUMO+3 (41%)	236.0	0.0229
		HOMO-2 → LUMO+3 (33 %) HOMO-8 → LUMO (35 %)	238.1	0.0103
		HOMO-5 → LUMO+2 (58 %)	243.2	0.0040
		HOMO-6 → LUMO (48 %) HOMO-7→ LUMO (16 %)	250.6	0.0746
	286 (4.0)	HOMO-2 → LUMO+2 (24%) HOMO-3 → LUMO (24 %)	272.7	0.0859
		HOMO-5 → LUMO (31 %) HOMO-3 → LUMO (27 %)	276.9	0.0625
		HOMO-1 → LUMO+2(70%) HOMO → LUMO+2 (22 %)	282.3	0.0125
		HOMO → LUMO+2 (72 %) HOMO-1 → LUMO+2 (19 %)	283.1	0.0171
		HOMO-2 → LUMO (81 %)	302.3	0.1838
	347(3.2)	HOMO → LUMO (83 %)	340.1	0.0017
5b	228 (4.3)	HOMO-4 → LUMO+9 (33 %)	228.8	0.0091
		HOMO-3 → LUMO+2 (24 %) HOMO-3 → LUMO+11 (15 %)	229.2	0.0071

		HOMO-2 →LUMO+5 (43 %)	231.2	0.0036
	260 (4.0)	HOMO-1→ LUMO+3 (49 %) HOMO-1→ LUMO+4 (31 %)	257.2	0.0031
		HOMO-5 → LUMO (26 %)	261.7	0.1019
		HOMO-1→ LUMO+2 (60 %)	267.8	0.0111
	327 (2.7)	HOMO-1 → LUMO (79 %)	334.4	0.0143
		HOMO → LUMO (75 %)	337.3	0.0009
	451 (2.5)	HOMO-3 → LUMO+4 (25 %) HOMO → LUMO+5 (22 %) HOMO-3 → LUMO+3 (18 %)	464.1	0.0007

[a]As shown in **Figure 8**, the position of this band was not clearly identified.