Supplementary Material

The study of regioselectivity of ferrocenylalkylation of N,S-heterocycles in aqueous-organic media

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Figure S1. ^{1}H NMR spectrum of 1-(1-ferrocenylpropyl)pyrrolidine-2-thione **5c**

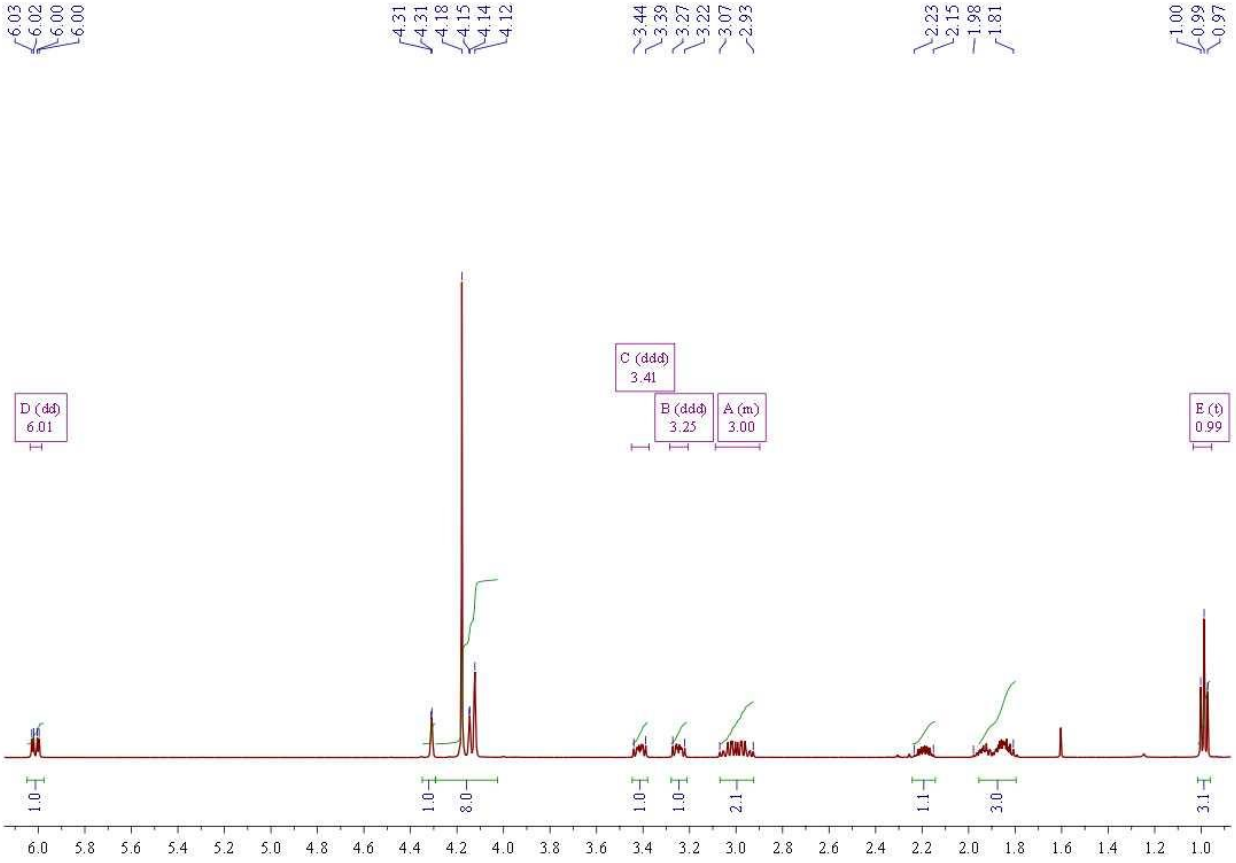

Figure S2. ^{13}C NMR spectrum of 1-(1-ferrocenylpropyl)pyrrolidine-2-thione **5c**

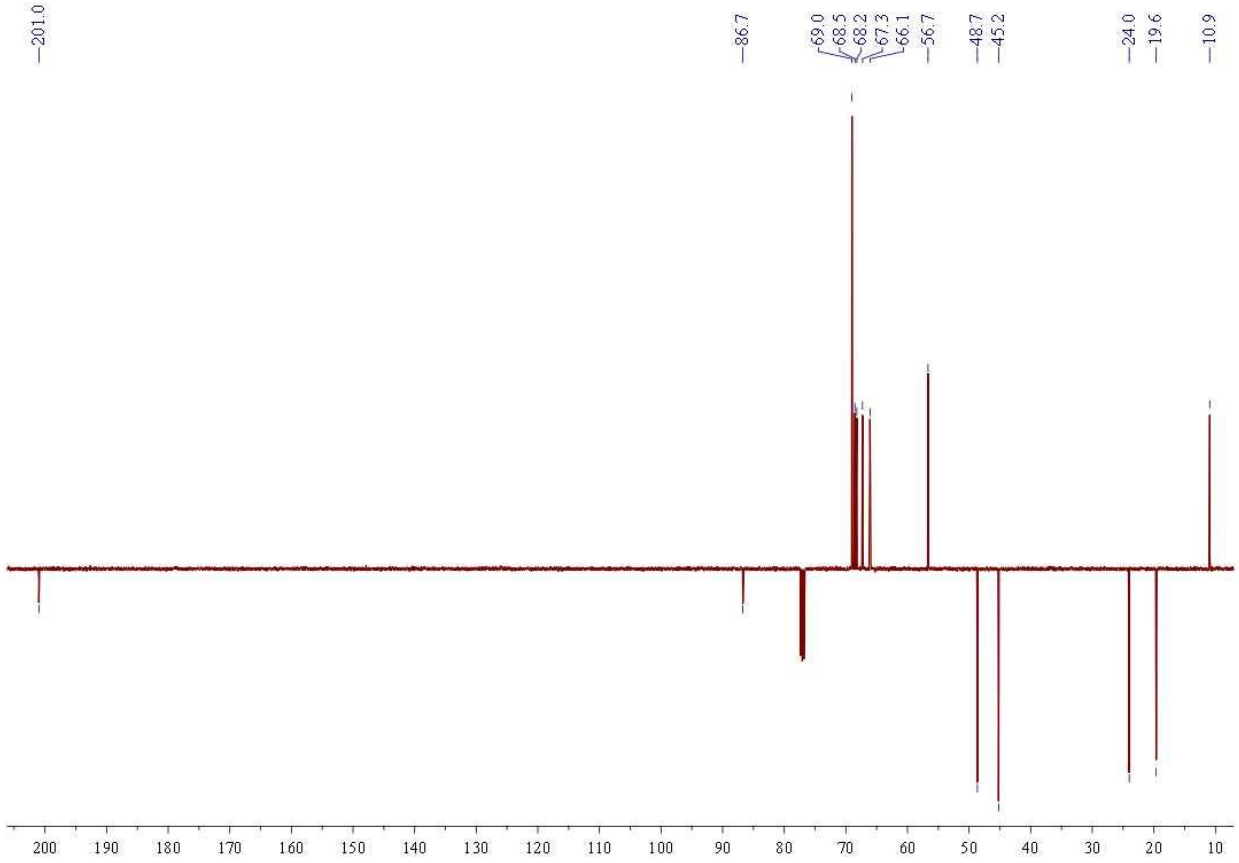

Figure S3. COSY NMR spectrum of 1-(1-ferrocenylpropyl)pyrrolidine-2-thione **5c**

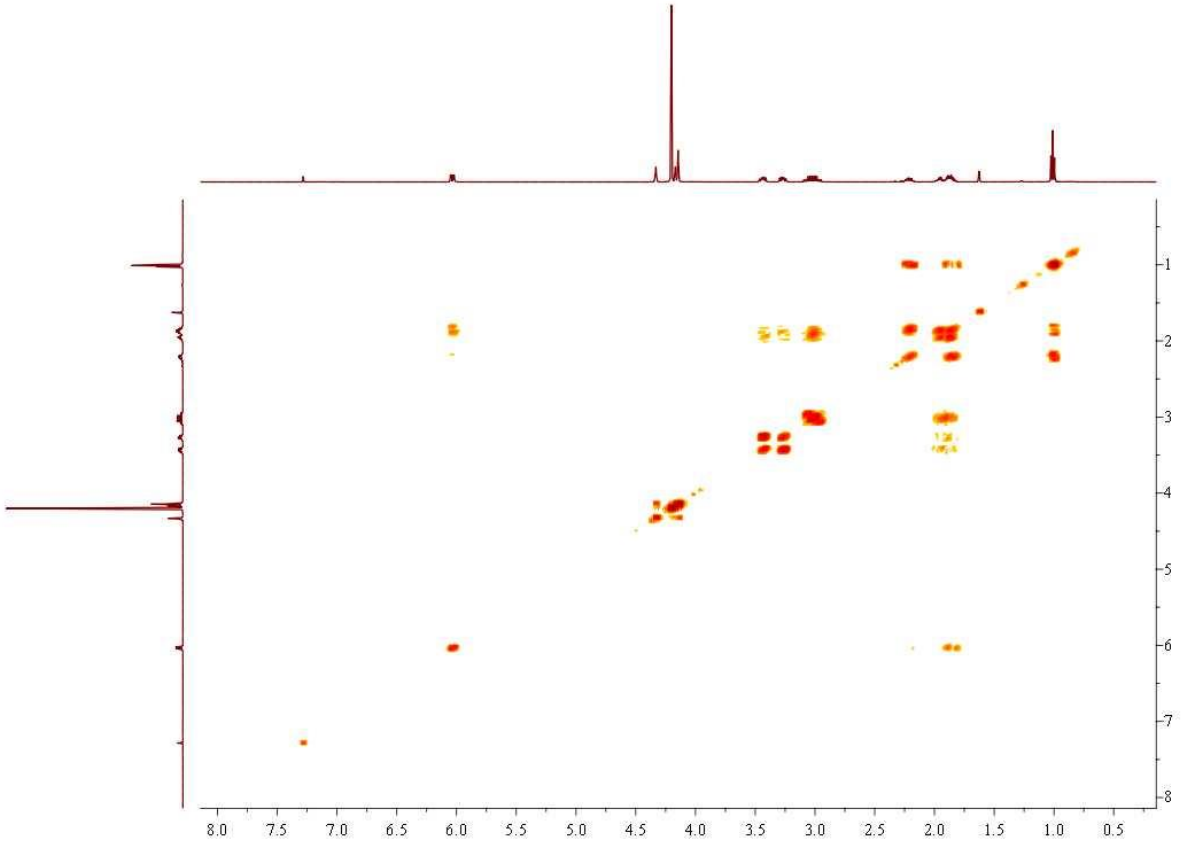

Figure S4. 2D NMR spectra of 1-(1-ferrocenylpropyl)pyrrolidine-2-thione **5c**

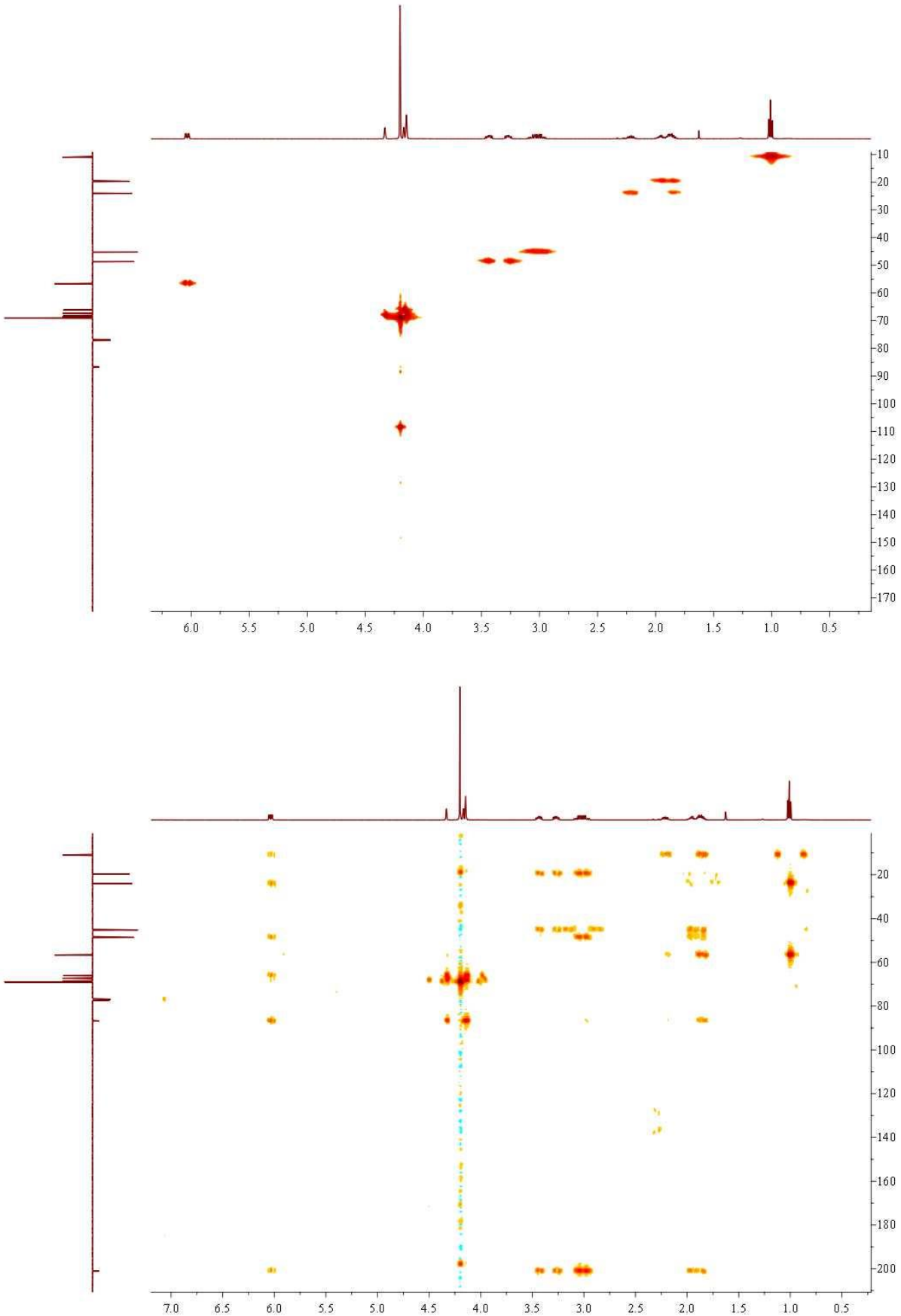

Figure S5. General view of molecule of 1-(ferrocenyl(phenyl)methyl)pyrrolidine-2-thione **5f**

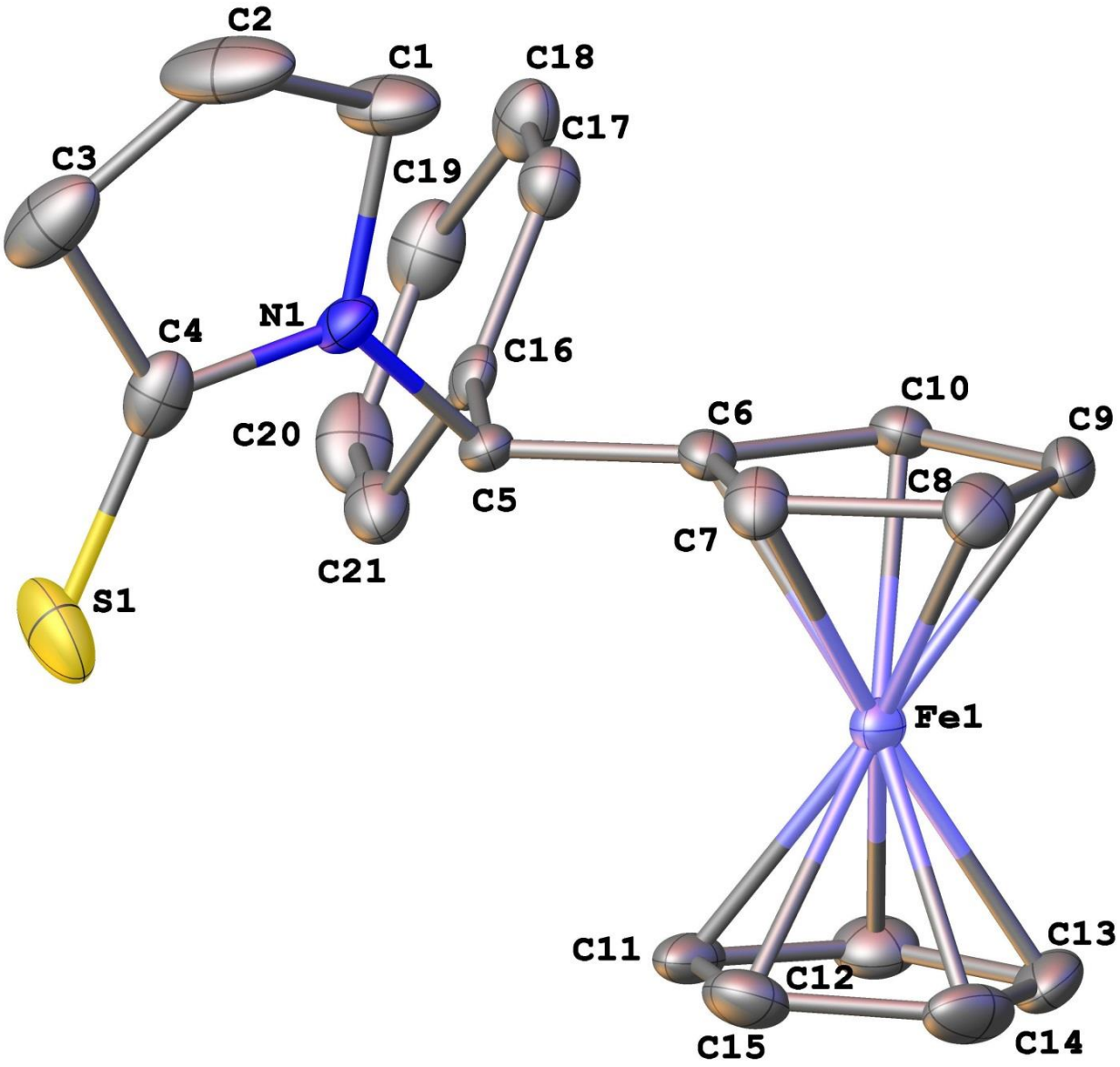

Figure S6. General view of 4,5-dihydro-1-(1-ferrocenyl(phenyl)methyl)-1H-imidazole-2-thiol **7e**

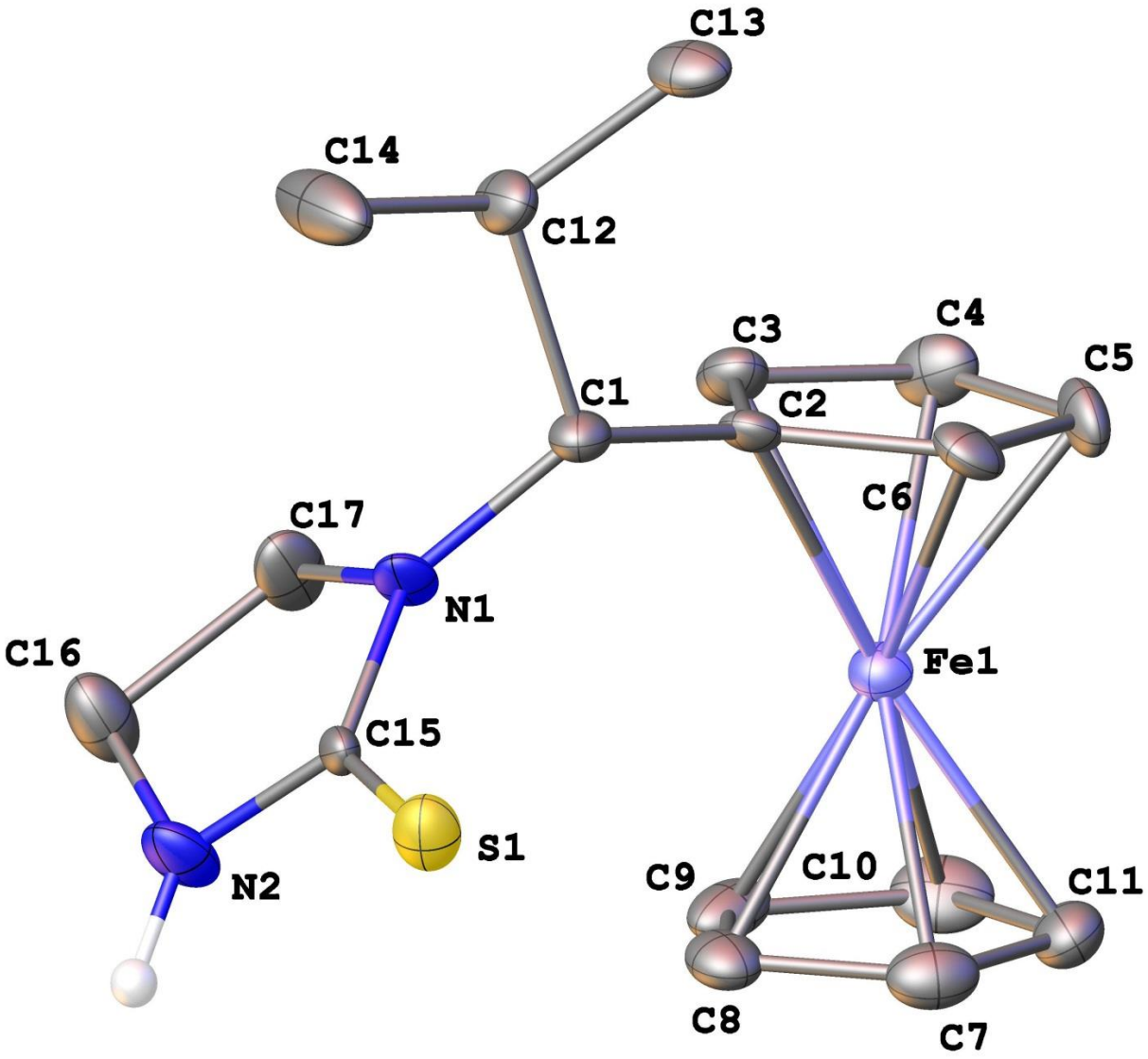

Figure S7. General view of 4,5-dihydro-1-(1-ferrocenylmethyl)-1H-imidazole-2-thiol **7a**

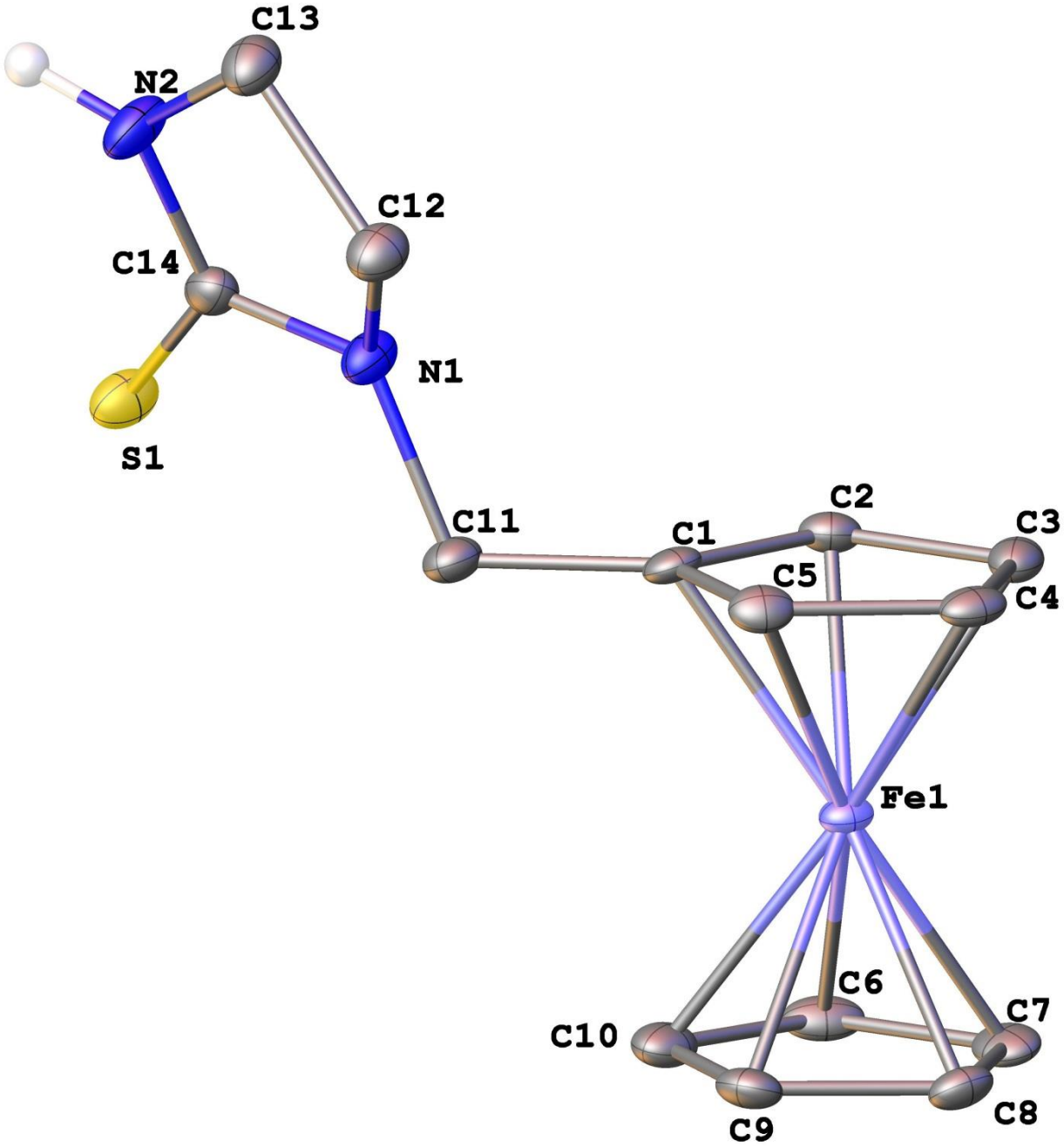

Figure S8. The dimers in crystal packing of 4,5-dihydro-1-(1-ferrocenylmethyl)-1H-imidazole-2-thiol **7a**. The S1_$1 atoms was generated by 1-X, 3-Y, -Z symmetry transformation

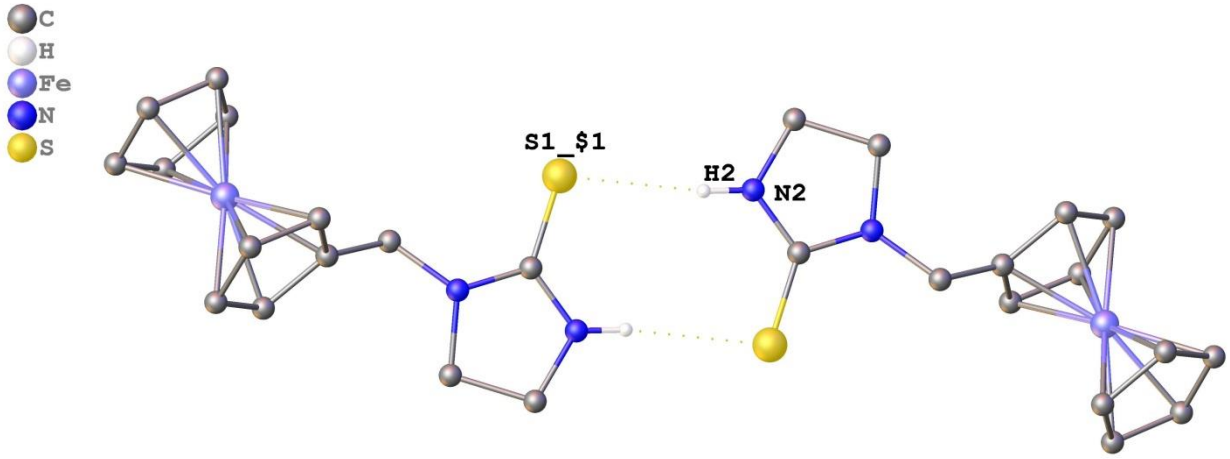

Figure S9. The chains in crystal packing of 4,5-dihydro-1-(1-ferrocenyl(phenyl)methyl)-1H-imidazole-2-thiol **7e**

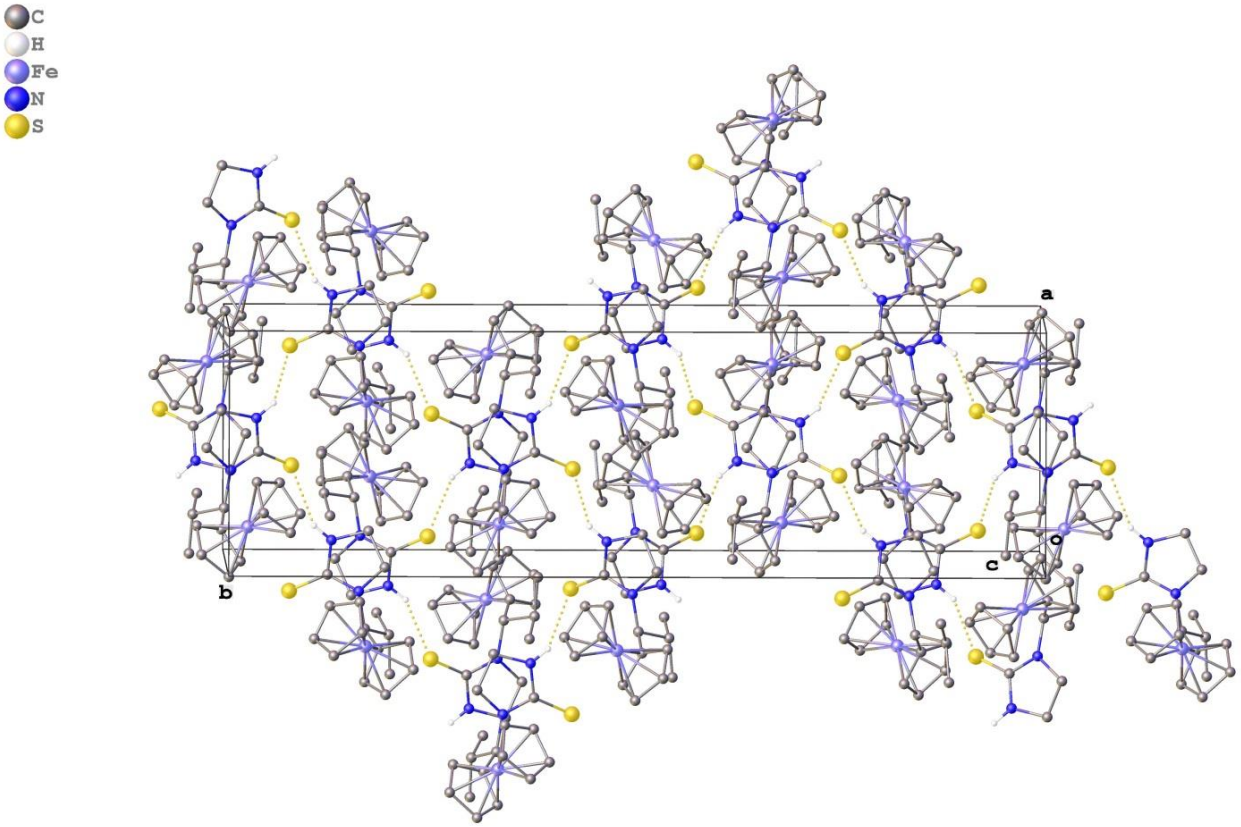

Table S1. Main crystallographic data and refinement parameters for compounds **5f**, **7a,e**

	5f	**7a**	**7e**
Molecular formula	$C_{21}H_{21}FeNS$	$C_{14}H_{16}FeN_2S$	$C_{17}H_{22}FeN_2S$
Molecular weight	375.30	300.20	342.27
T/K	120	120	120
Space group	Triclinic, P-1	Monoclinic C2/c	Orthorombic Pna21
Z	2	8	12
a/Å	10.2136(8)	34.485(5)	9.2562(11)
b/Å	11.4628(9)	5.7281(8)	30.749(4)
c/Å	15.7027(12)	13.0003(19)	16.798(2)
α/deg	86.230(2)	90	90
β/deg	86.922(2)	96.285(6)	90
γ/deg	72.937(2)	90	90
V/Å^3	1752.6(2)	2552.6(6)	4781.1(10)
d calc/g cm^{-3}	1.422	1.562	1.427
μ/cm–1	9.81	9.13	10.72
F(000)	784	1248	2148
2 θ max/deg	50.48	52	52
Number of measured reflections	15471	12940	45282
Number of independent reflections	6142	5838	9424
Number reflections with I> 2σ(I)	4784	5468	7285
Number of refined parameters	433	253	575
R1 [for refl with I>2σ(I)]	0.0351	0.0291	0.0539
wR2 [all data]	0.0892	0.0630	0.1113
GOF	1.021	0.986	1.010
Residual electron	0.771/-0.514	0.384/–0.205	0.765/-0.379

density (ρmax/ρmin)/eÅ–3			