

## Supplementary Material

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

Elena Yu. Rogatkina (Osipova)<sup>a</sup>, Anna S. Ivanova<sup>b</sup>, Alexey N. Rodionov<sup>a</sup>, Alexander S. Peregudov<sup>a</sup>, Alexander A. Korlyukov<sup>a</sup>, Alexander D. Volodin<sup>a</sup>, Yury A. Belousov,<sup>a</sup> and Alexander A. Simenel<sup>\*a,c</sup>

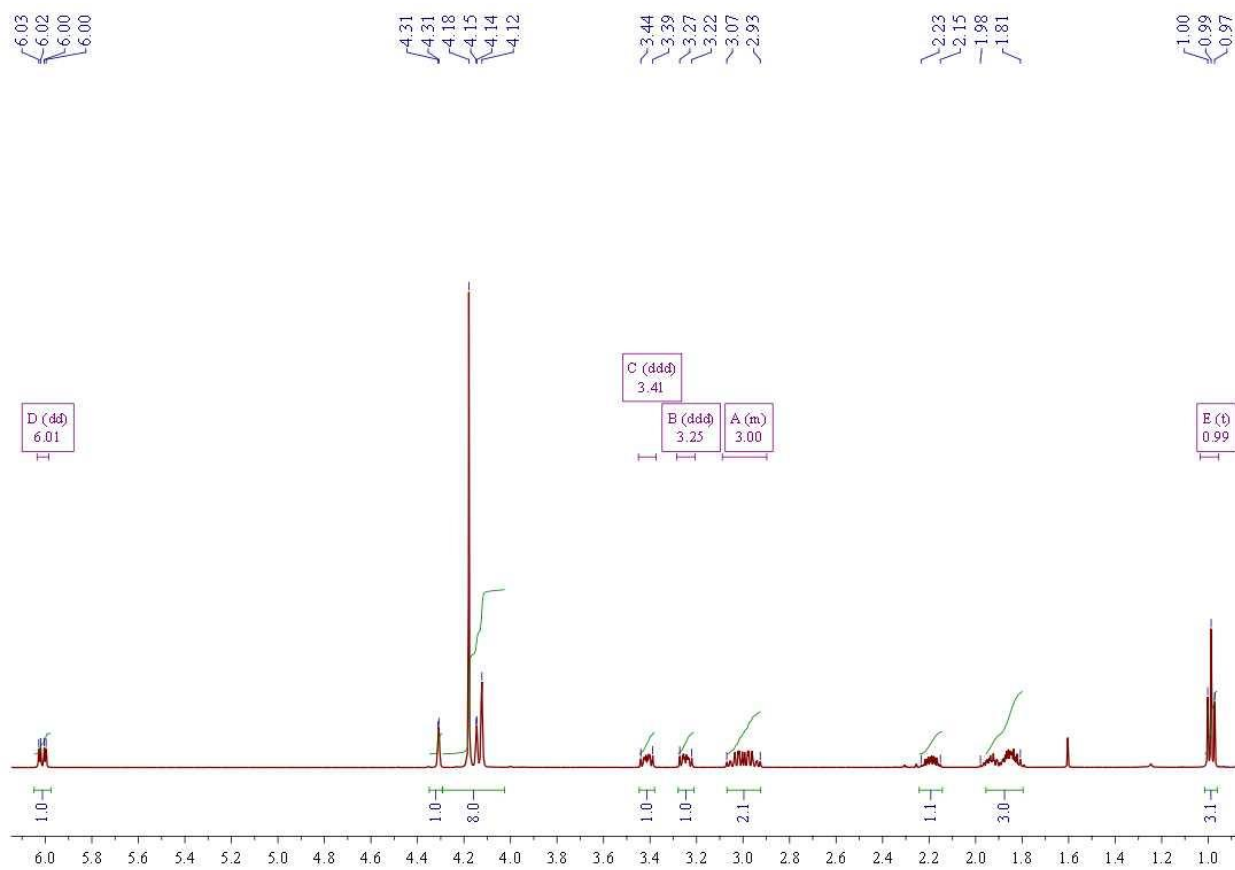
<sup>a</sup>A.N. Nesmeyanov Institute of OrganoElement Compounds, Russian Academy of Sciences, 28 Vavilov St., 119991 Moscow, Russian Federation

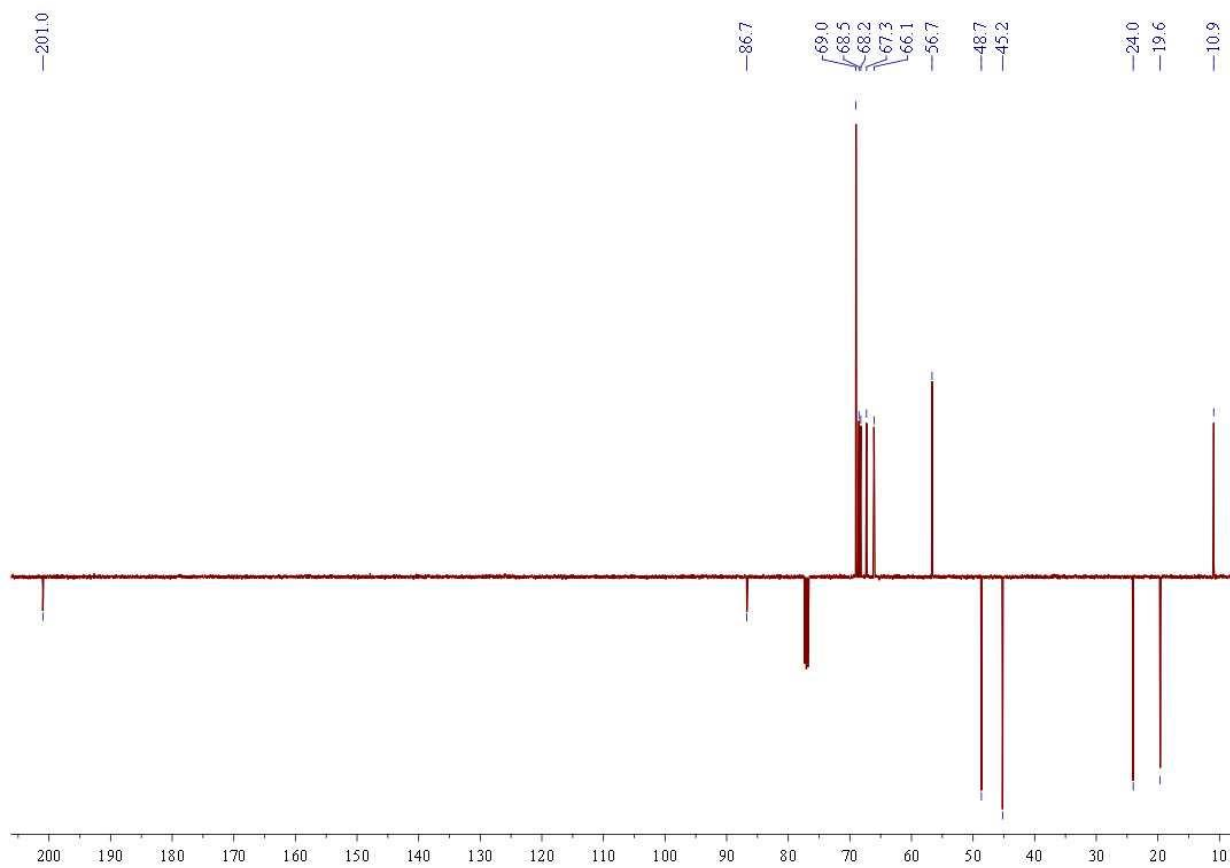
<sup>b</sup>Federal State Budget Educational Institution of Higher Education «Moscow Technological University», 78 Vernadsky prospect, 119454 Moscow, Russian Federation

<sup>c</sup>National University of Science and Technology "MISIS", Chemistry Department, 4 Leninskiy prospekt, 119049 Moscow, Russian Federation  
Email: [alexsim@ineos.ac.ru](mailto:alexsim@ineos.ac.ru)

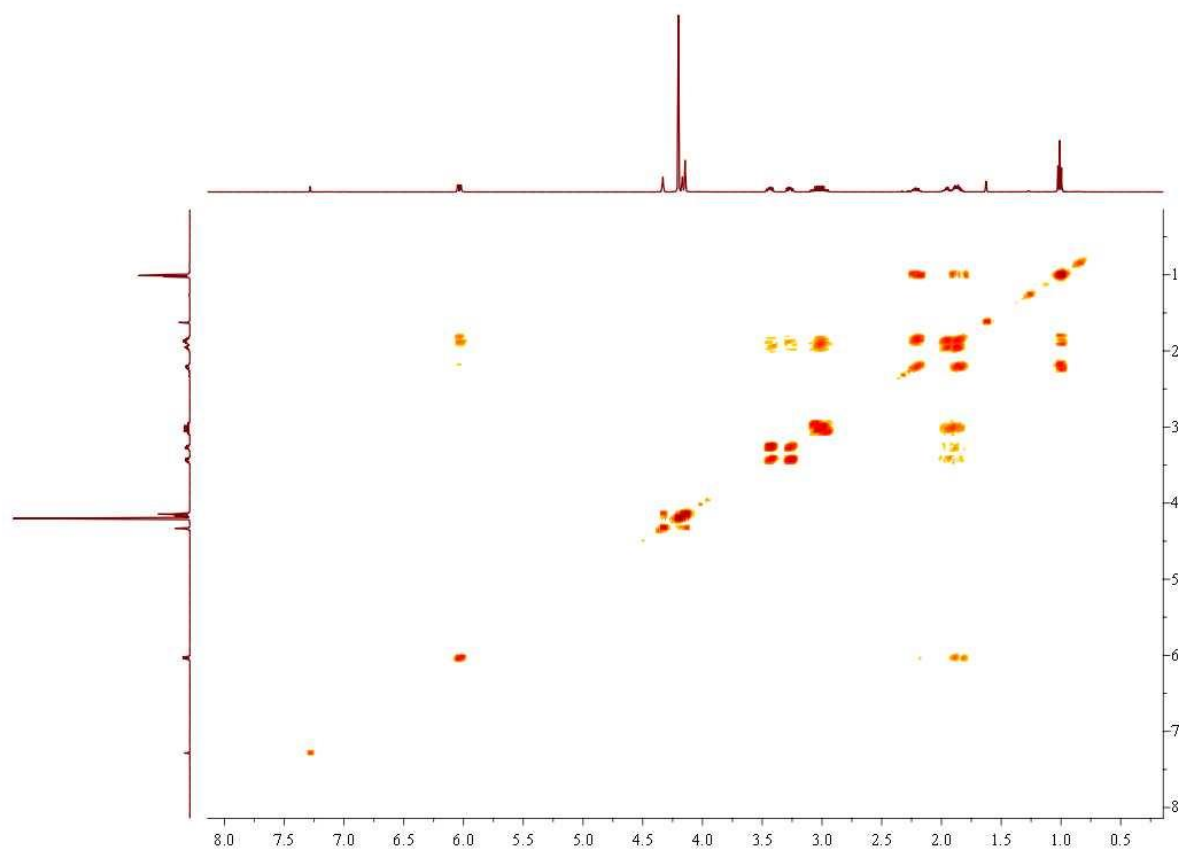
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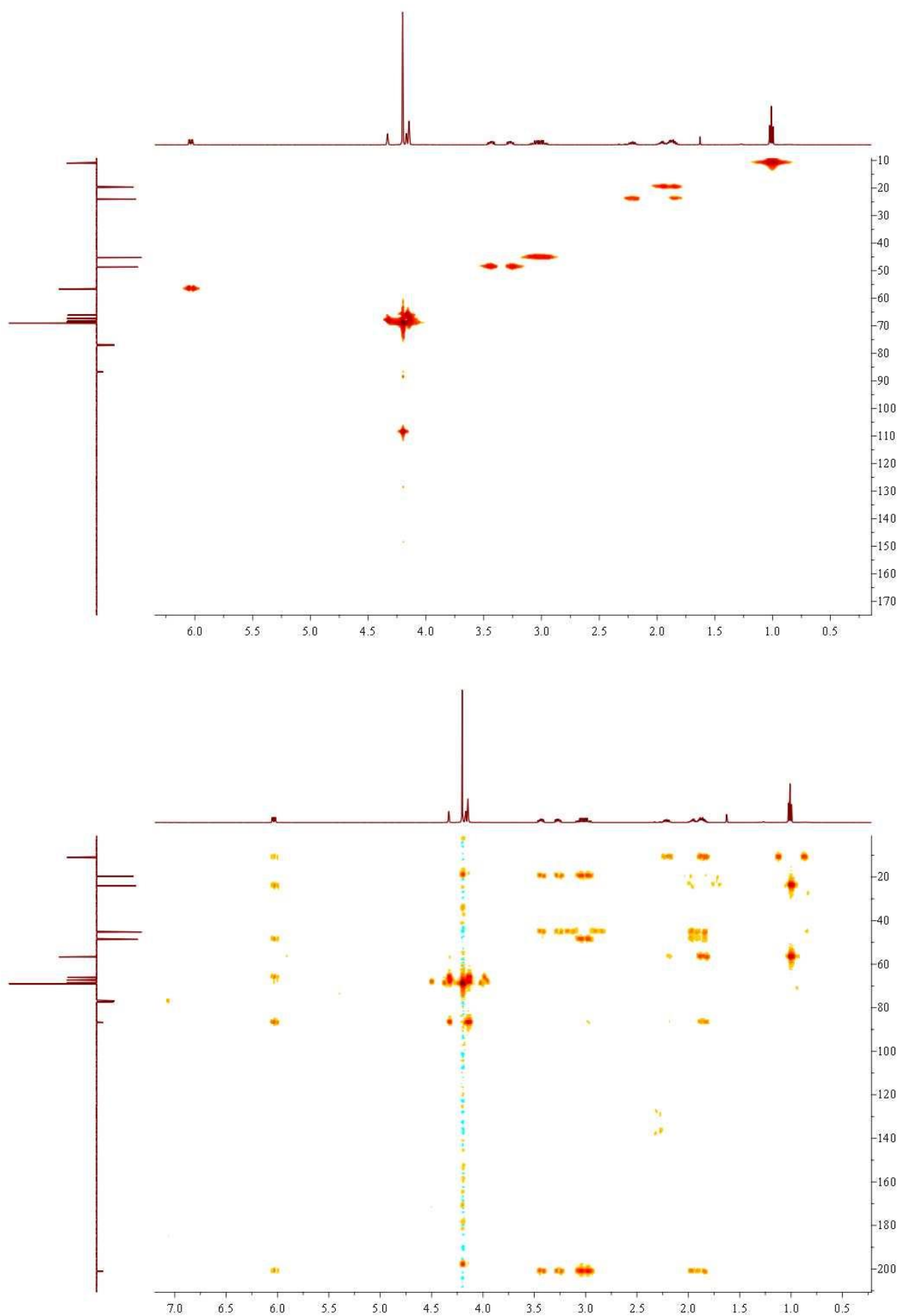
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**Figure S1.**  $^1\text{H}$  NMR spectrum of 1-(1-ferrocenylpropyl)pyrrolidine-2-thione **5c**

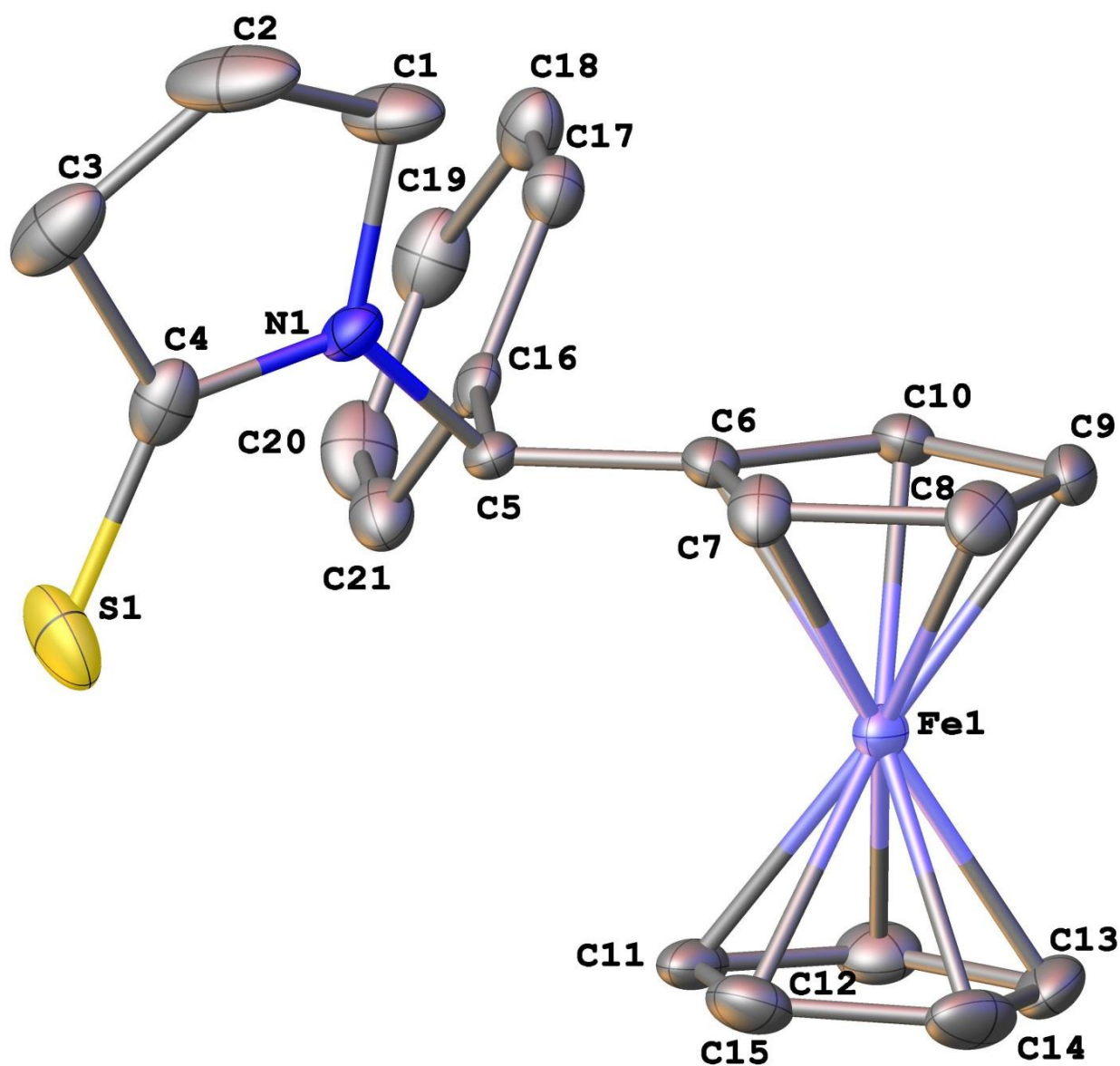
**Figure S2.**  $^{13}\text{C}$  NMR spectrum of 1-(1-ferrocenylpropyl)pyrrolidine-2-thione **5c**

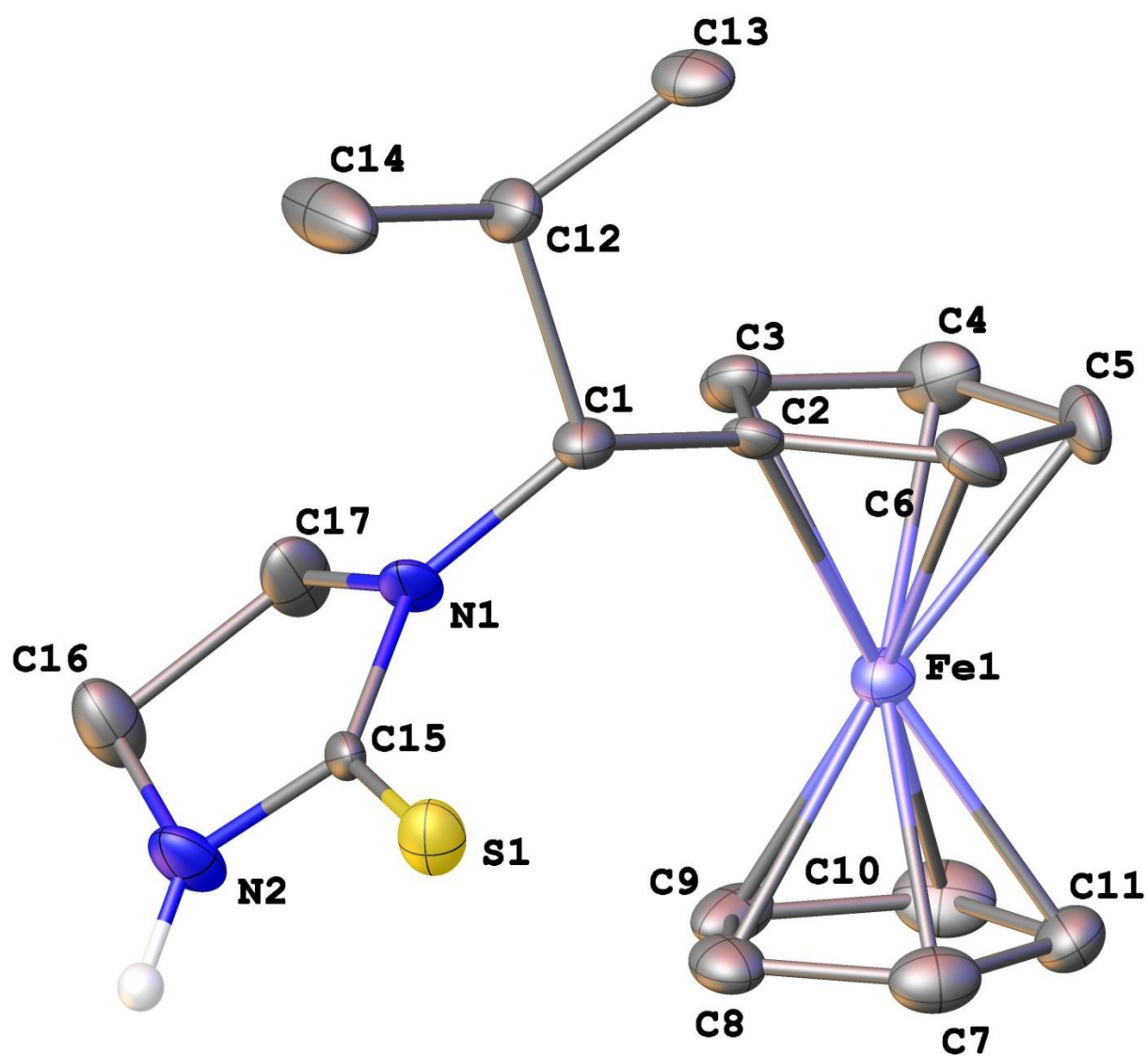
**Figure S3.** COSY NMR spectrum of 1-(1-ferrocenylpropyl)pyrrolidine-2-thione  
**5c**

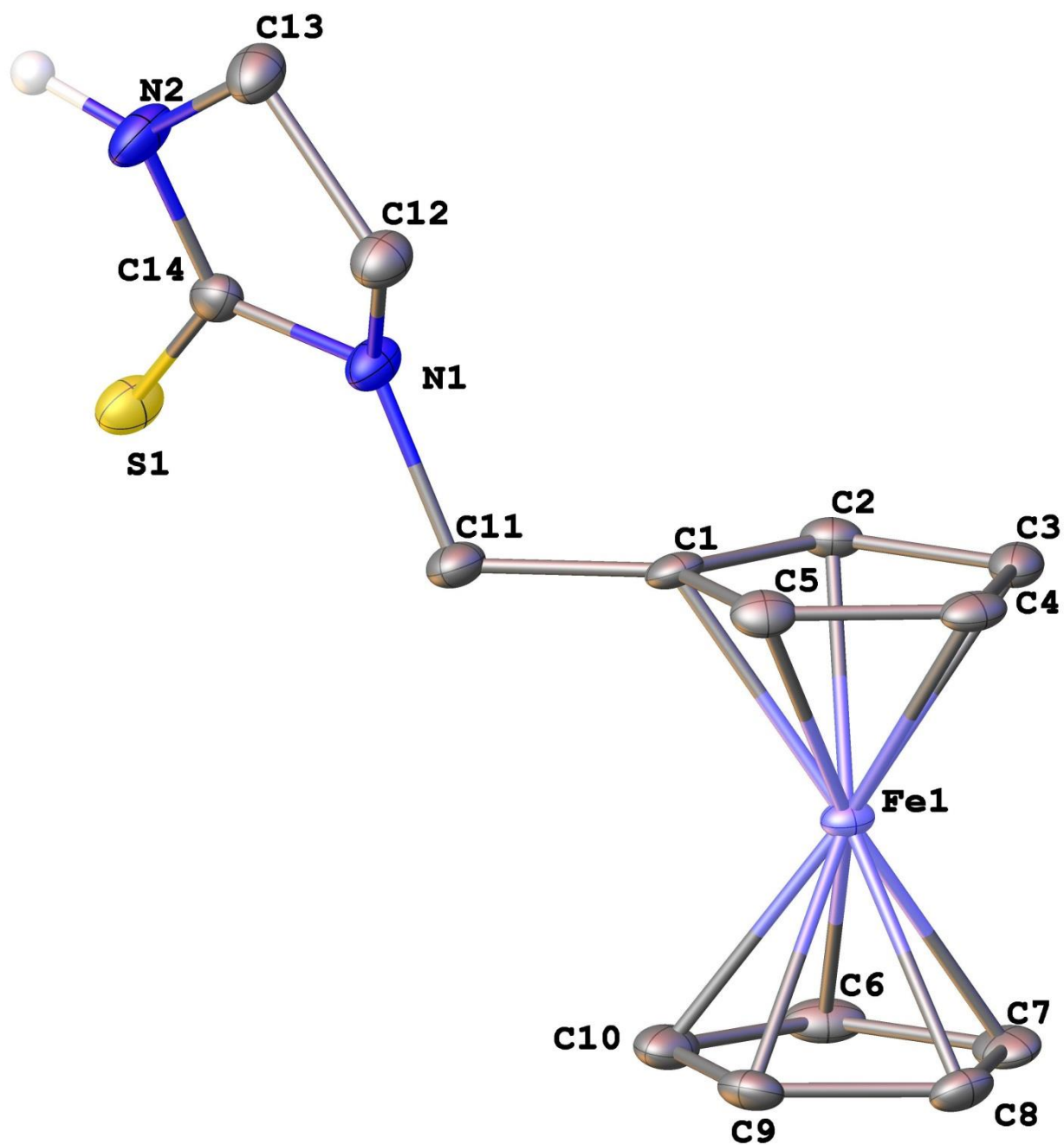


**Figure S4.** 2D NMR spectra of 1-(1-ferrocenylpropyl)pyrrolidine-2-thione **5c**

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

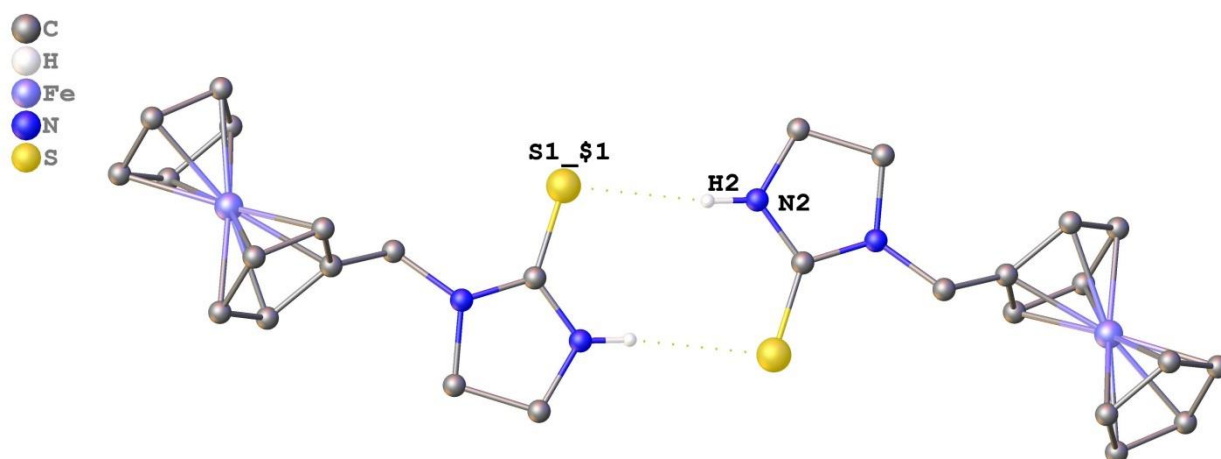


**Figure S6.** General view of 4,5-dihydro-1-(1-ferrocenyl(phenyl)methyl)-1H-imidazole-2-thiol **7e**

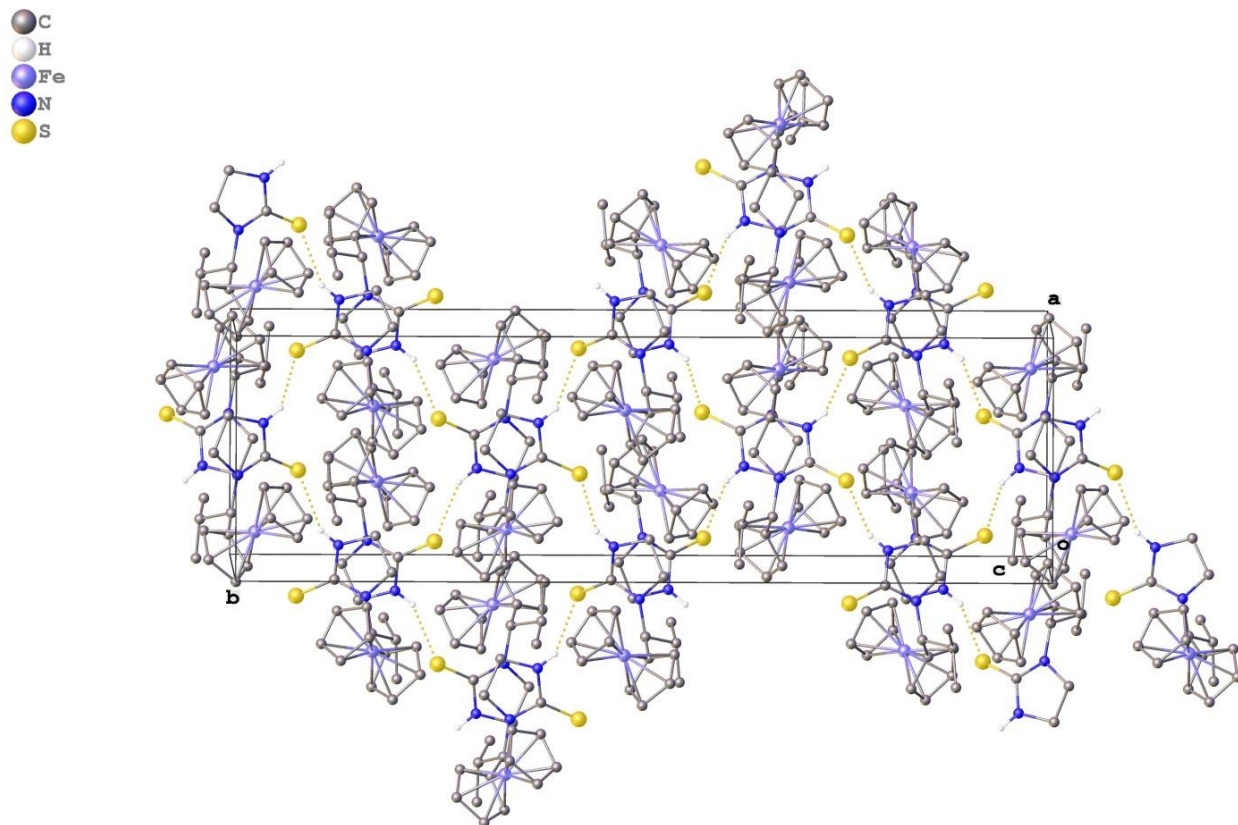
**Figure S7.** General view of 4,5-dihydro-1-(1-ferrocenylmethyl)-1H-imidazole-2-thiol **7a**



**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**

	<b>5f</b>	<b>7a</b>	<b>7e</b>
Molecular formula	C <sub>21</sub> H <sub>21</sub> FeNS	C <sub>14</sub> H <sub>16</sub> FeN <sub>2</sub> S	C <sub>17</sub> H <sub>22</sub> FeN <sub>2</sub> S
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 <sup>3</sup>	1752.6(2)	2552.6(6)	4781.1(10)
d calc/g cm <sup>-3</sup>	1.422	1.562	1.427
μ/cm <sup>-1</sup>	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 ( $\rho_{\max}/\rho_{\min}$ )/eÅ <sup>-3</sup>			
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