

Supplementary Materials

Synthesis of polysubstituted ferrocenesulfoxides

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² *UNESCO Chair of Belarusian State University, 220030 Minsk, Belarus*

³ *Research Institute for Physico-Chemical Problems of Belarusian State University, 220030 Minsk,
Belarus*

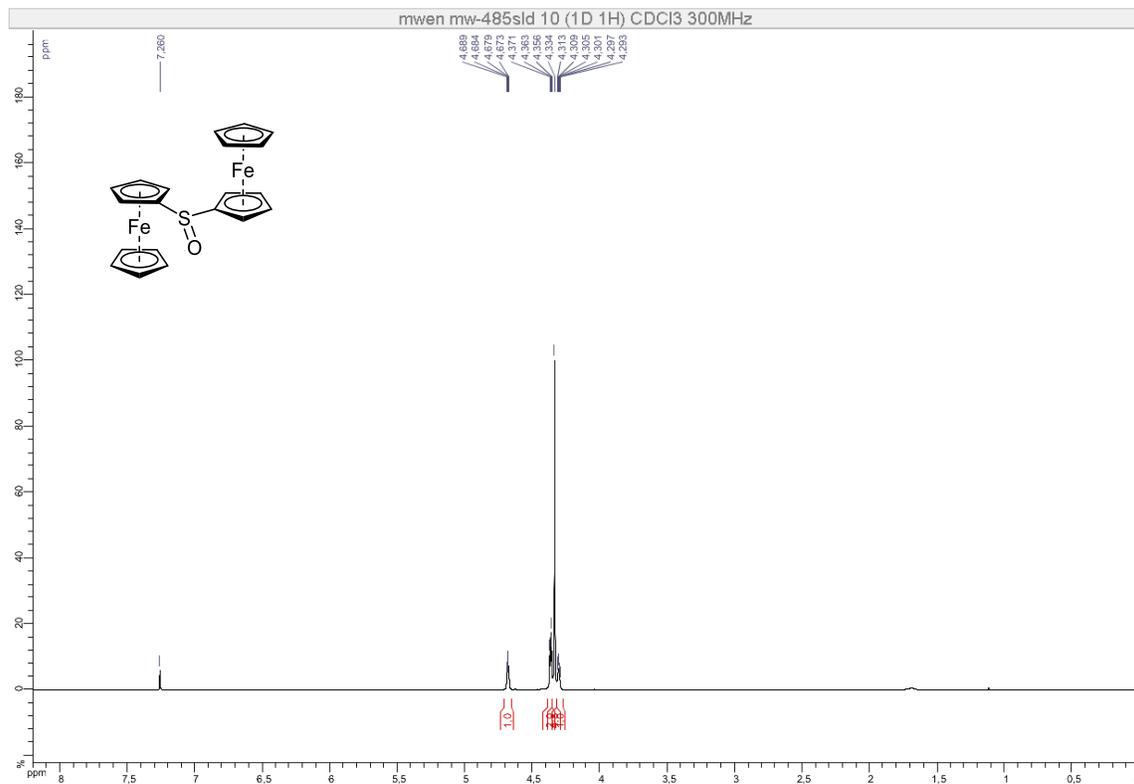
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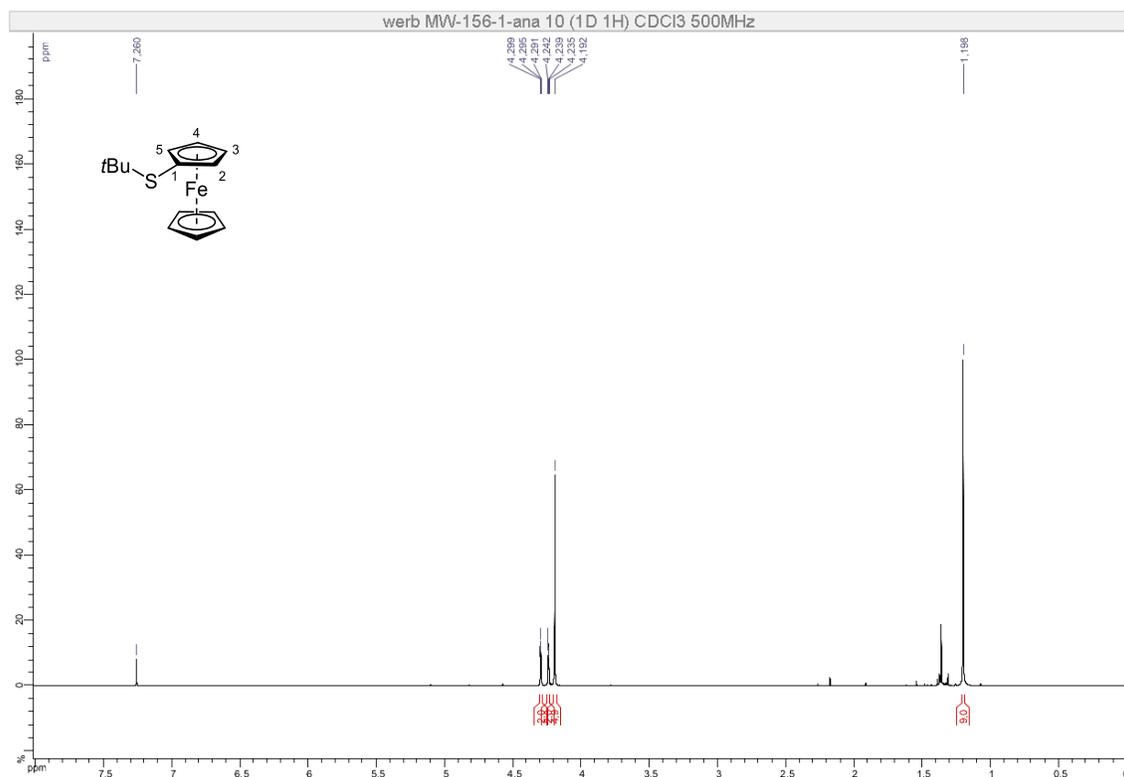
NMR Spectra

Diferrocenesulfoxide (FcSOFc)

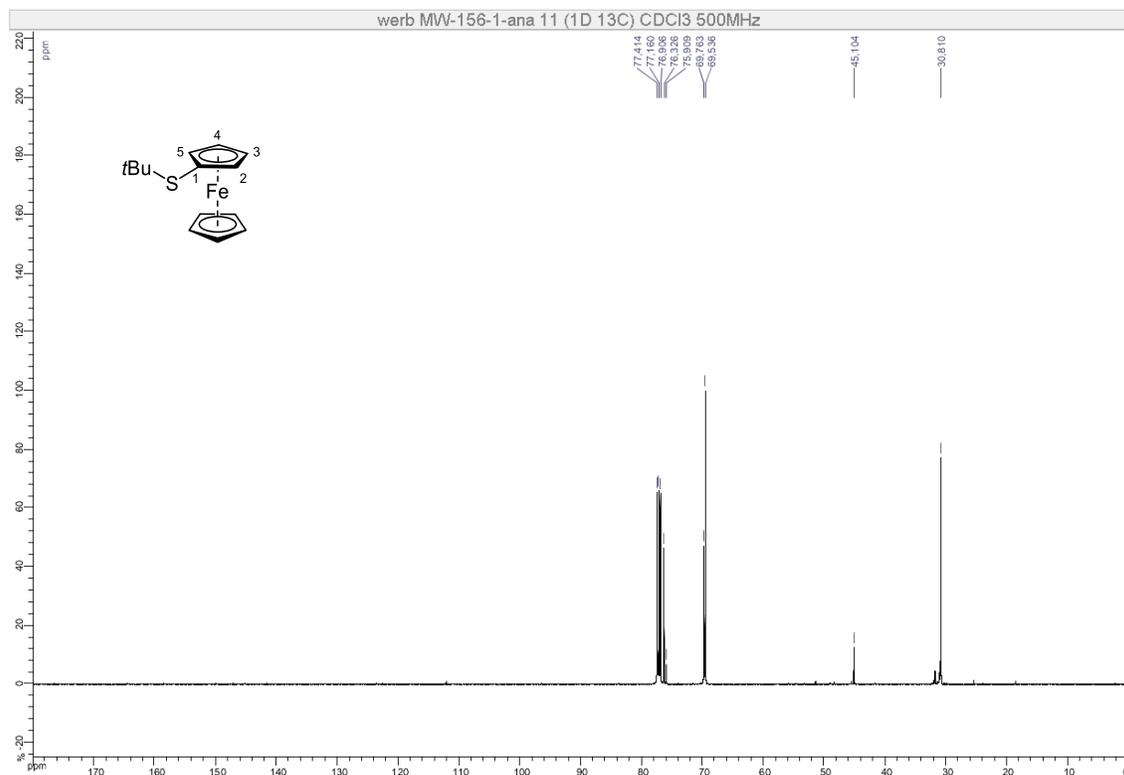


(*tert*-Butylthio)ferrocene

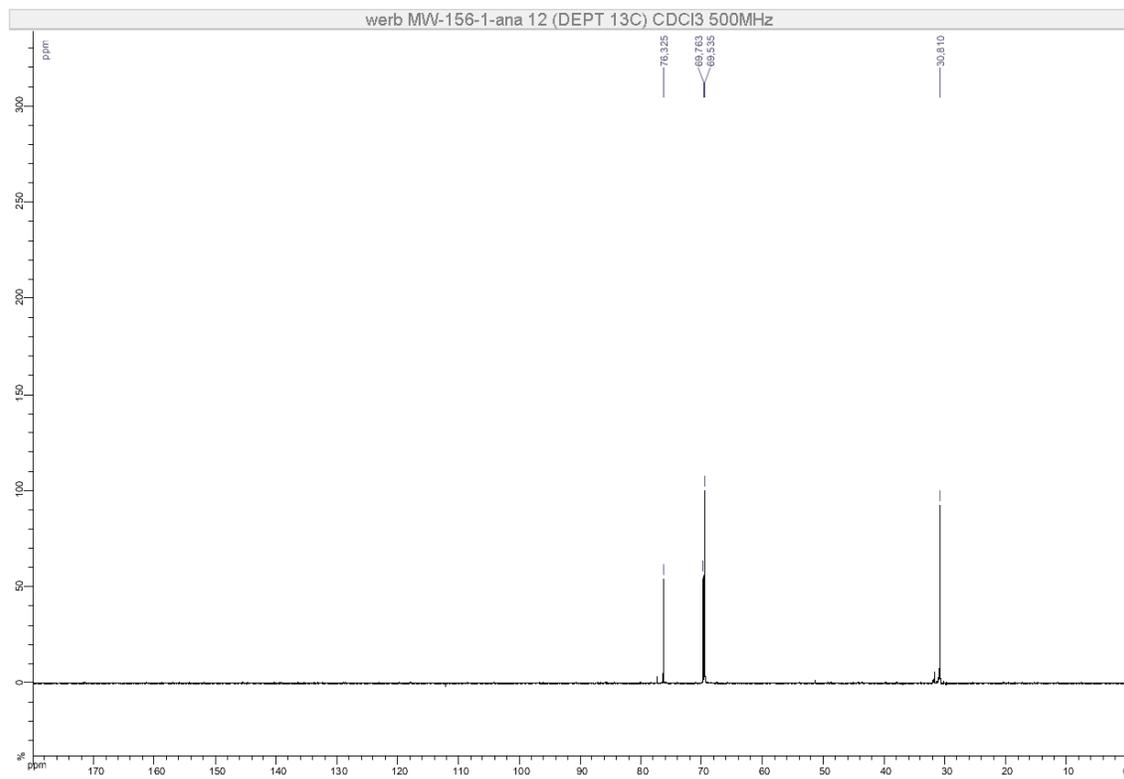
^1H NMR (500 MHz, CDCl_3)



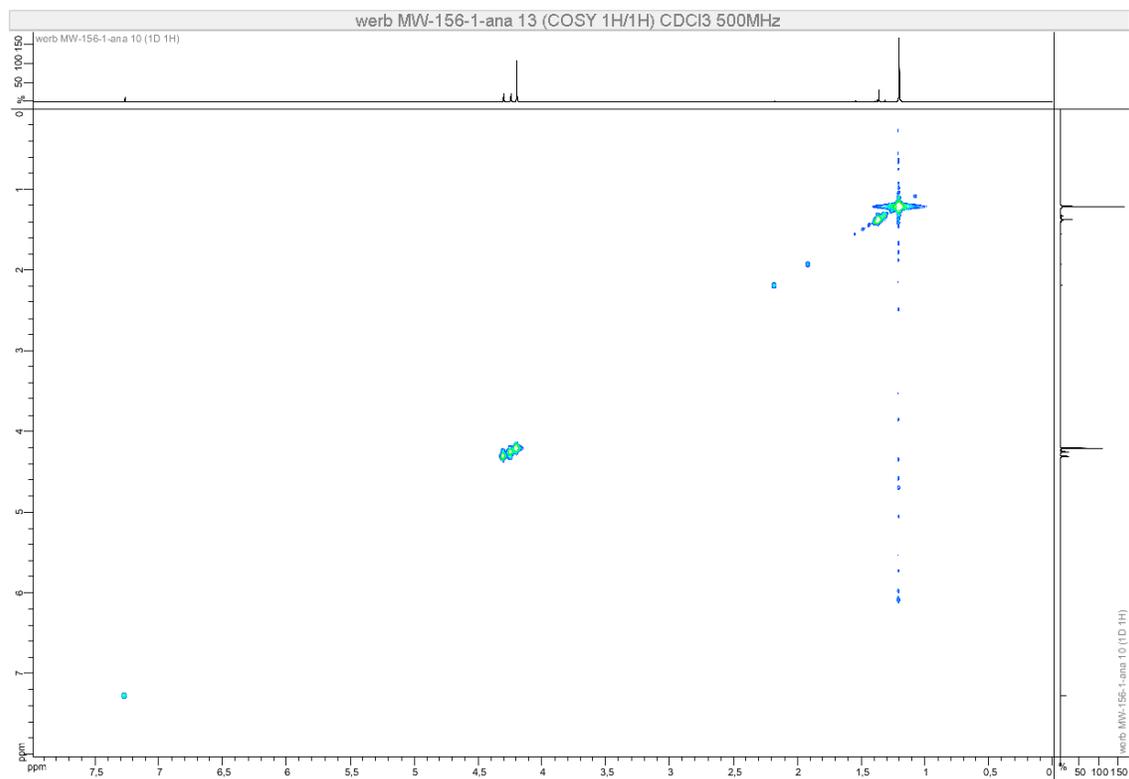
^{13}C NMR (126 MHz, CDCl_3)



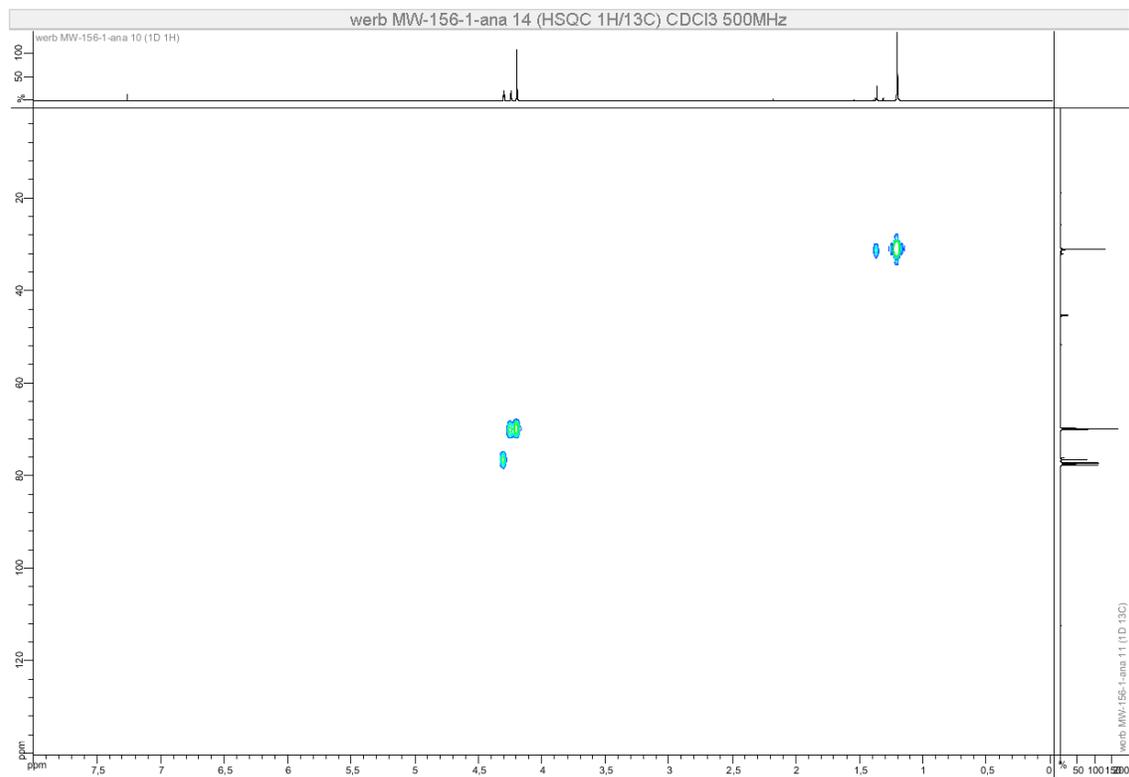
DEPT 135 (126 MHz, CDCl₃)



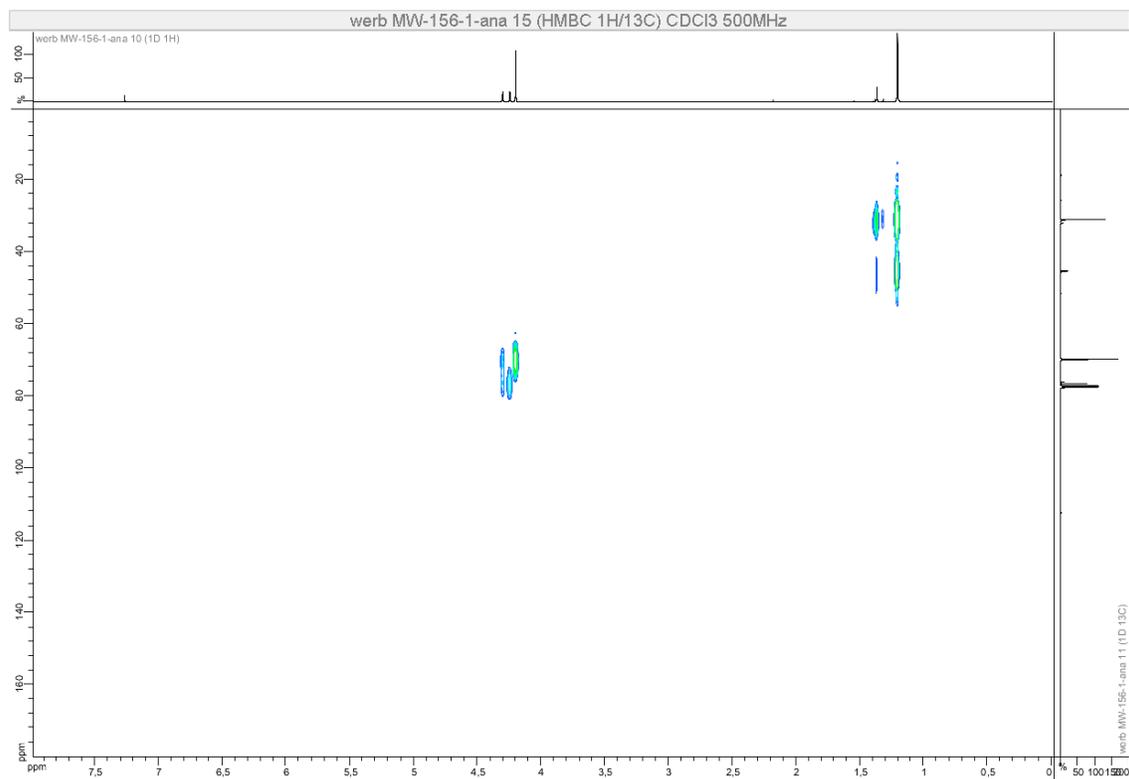
COSY (500 MHz, CDCl₃)



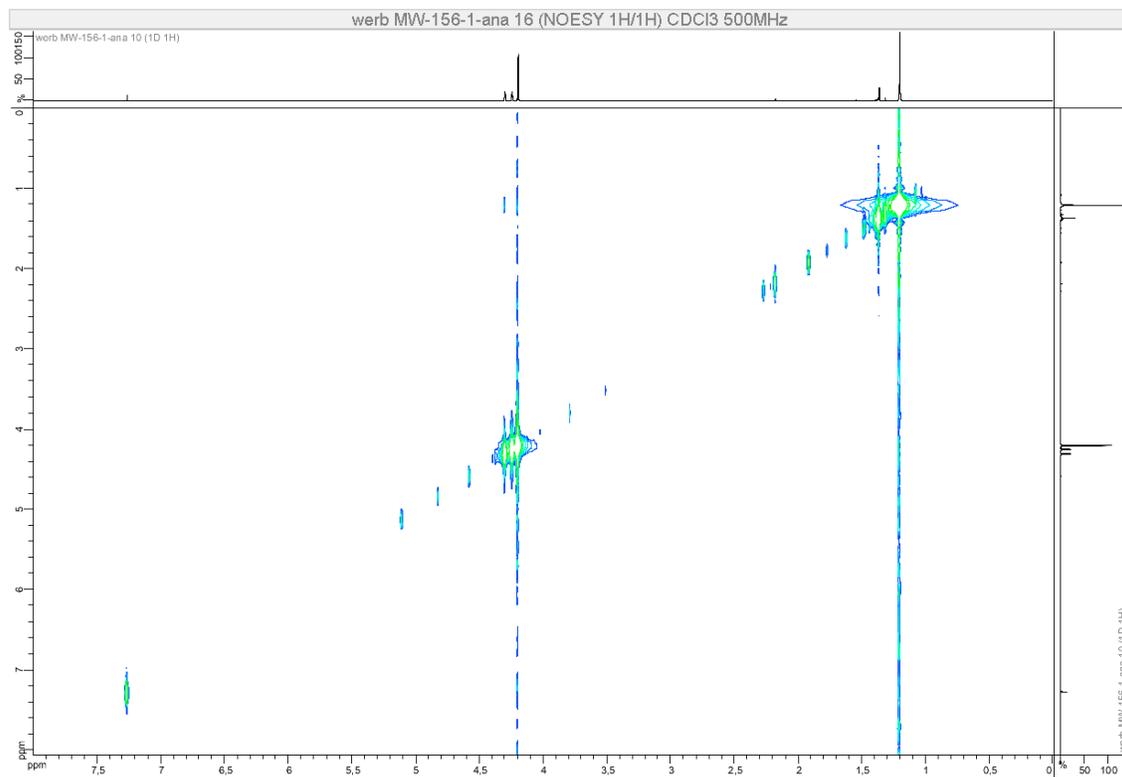
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

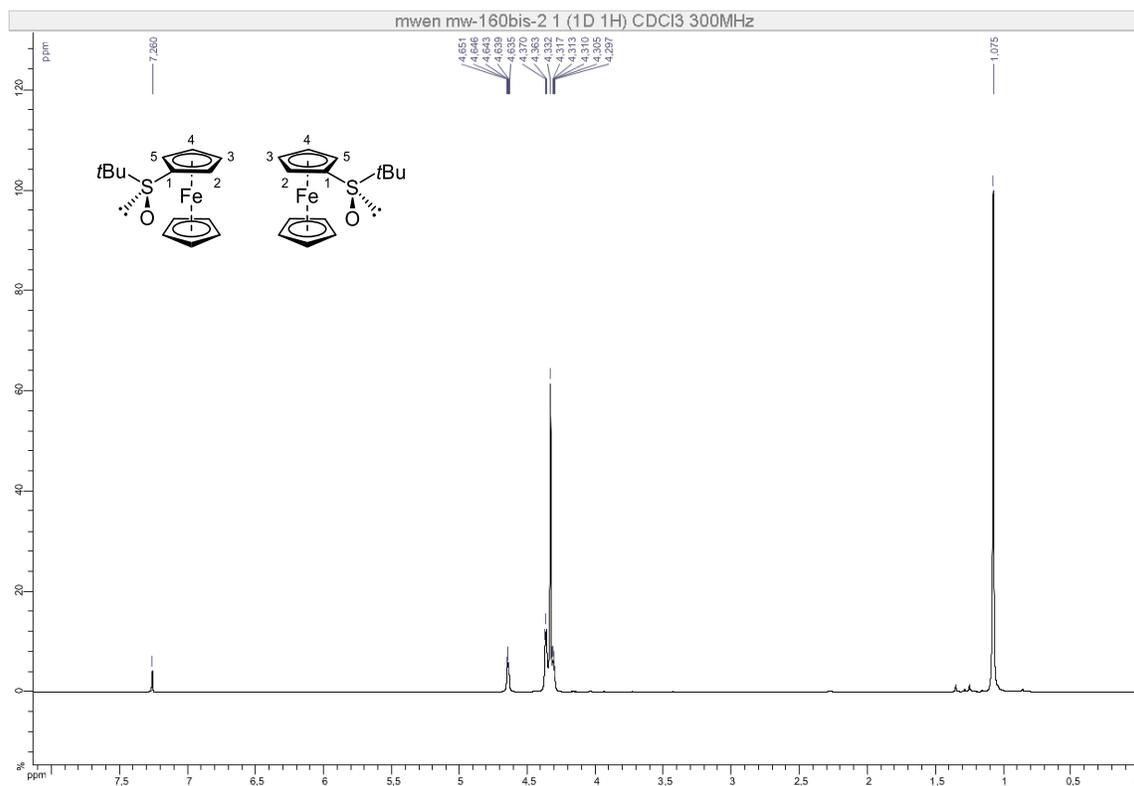


NOESY (500 MHz, CDCl₃)



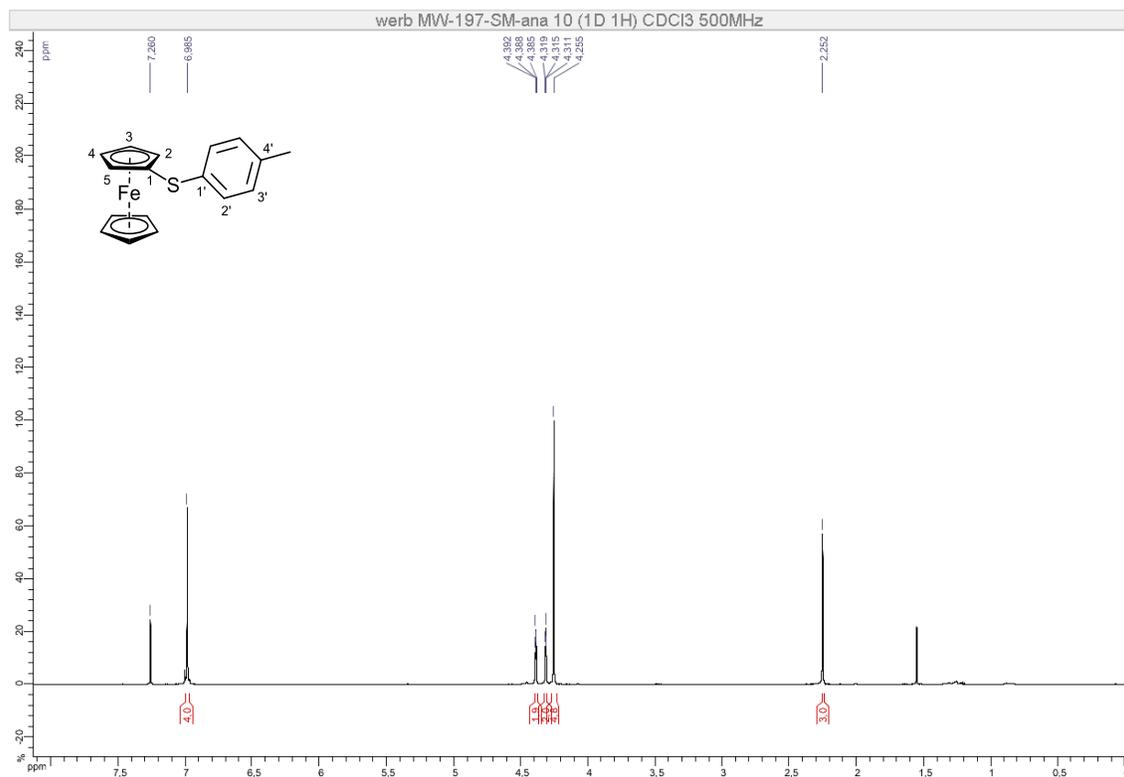
Racemic *S*-*tert*-Butylferrocenesulfoxide (*rac*-FcSO*t*Bu)

^1H NMR (300 MHz, CDCl_3)

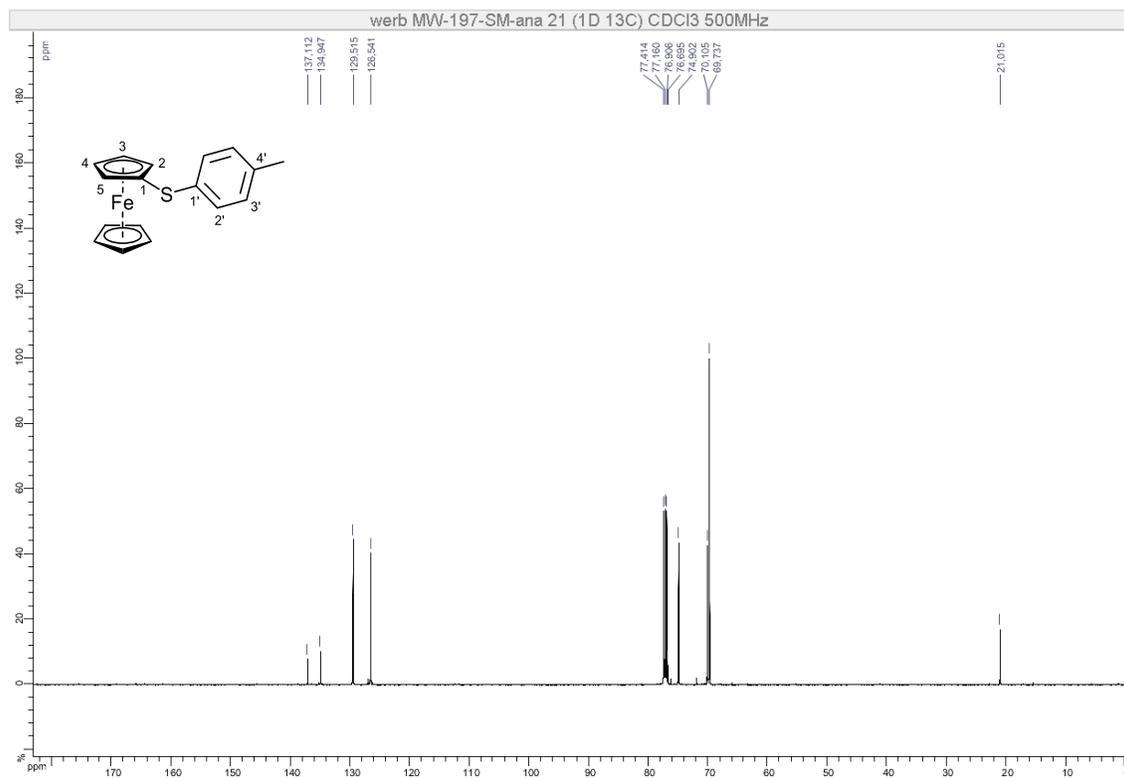


(4-Tolylthio)ferrocene

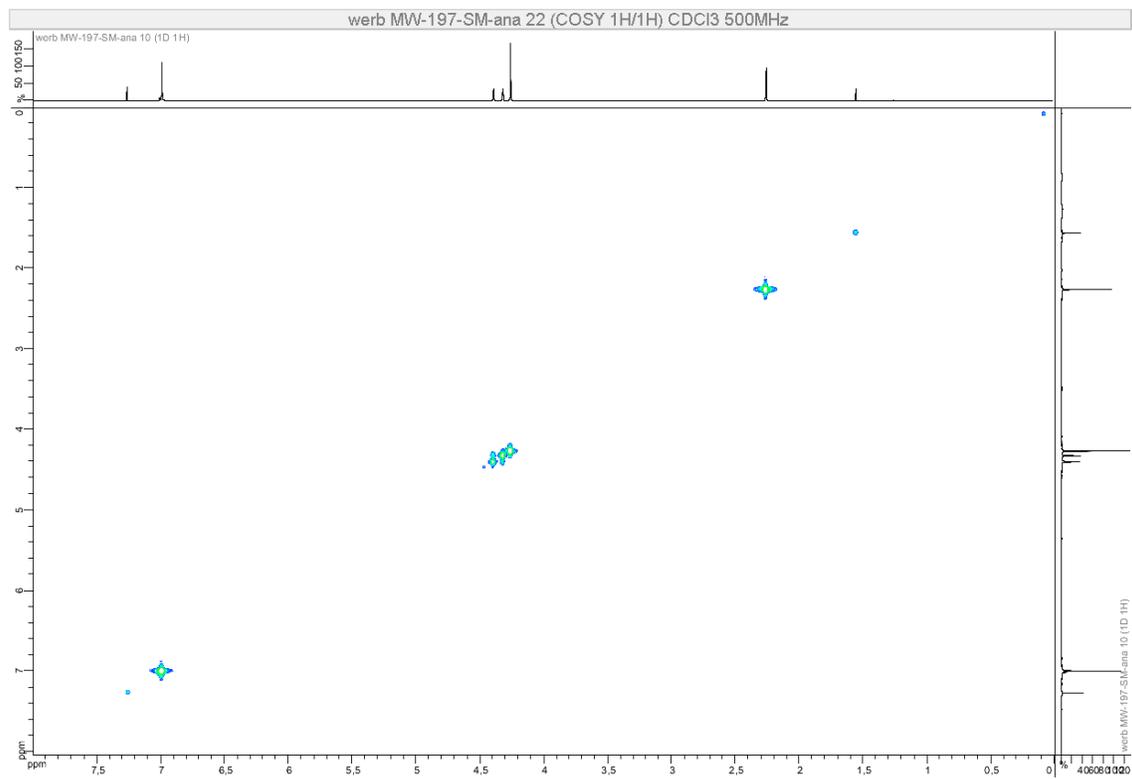
^1H NMR (500 MHz, CDCl_3)



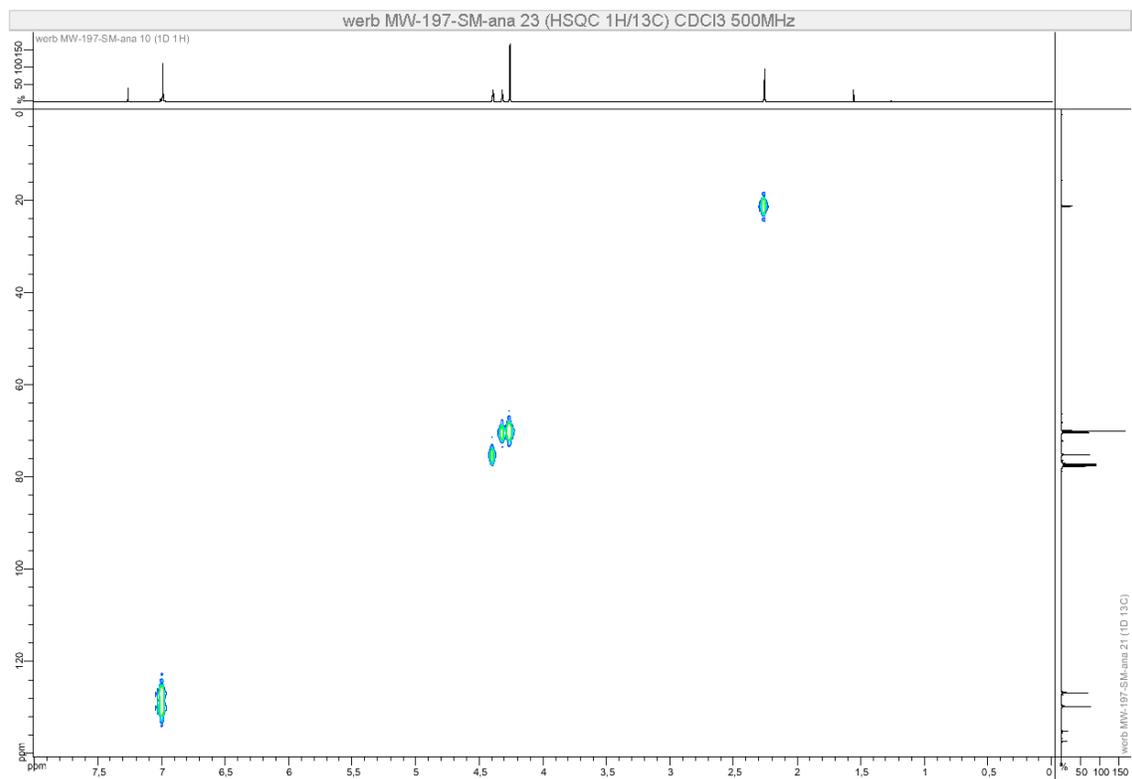
^{13}C NMR (126 MHz, CDCl_3)



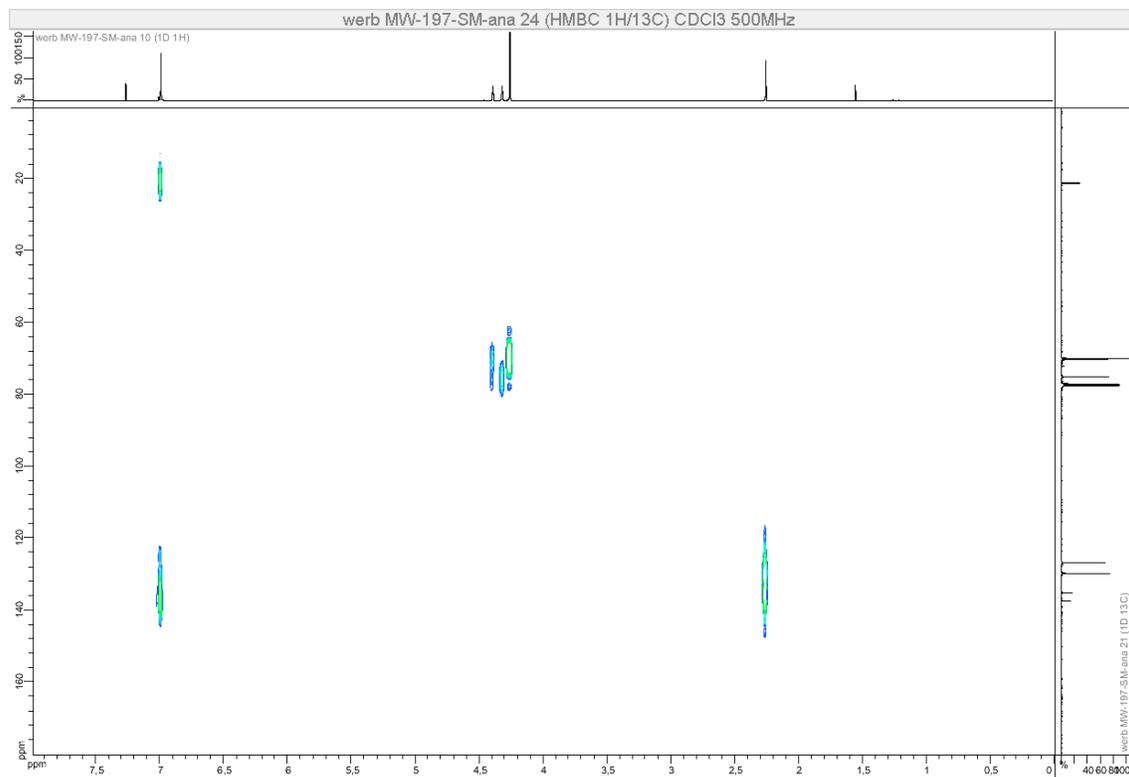
COSY (500 MHz, CDCl₃)



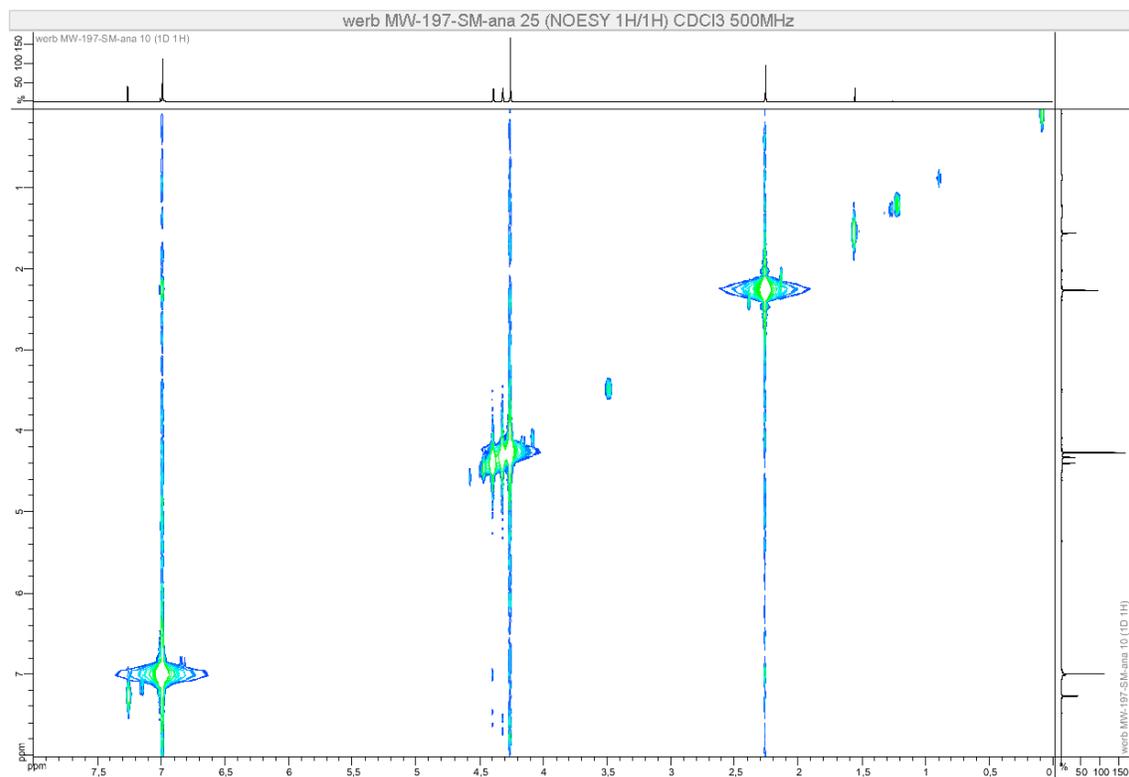
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

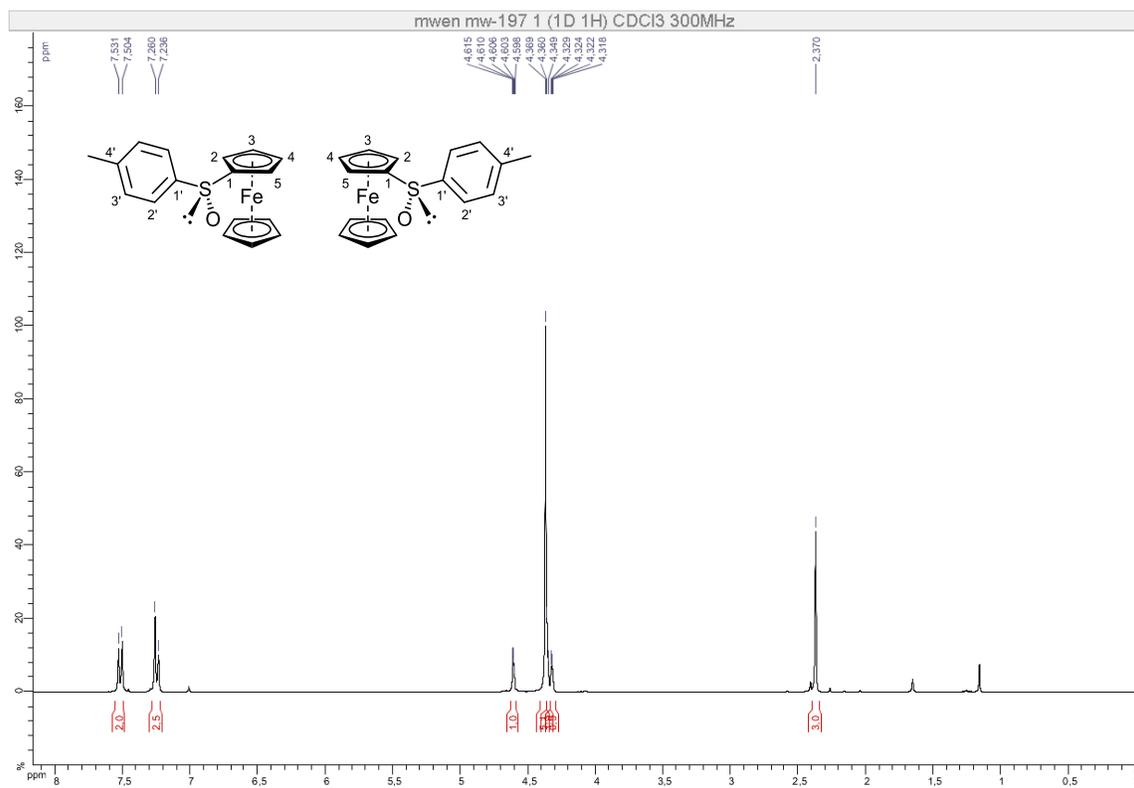


NOESY (500 MHz, CDCl₃)



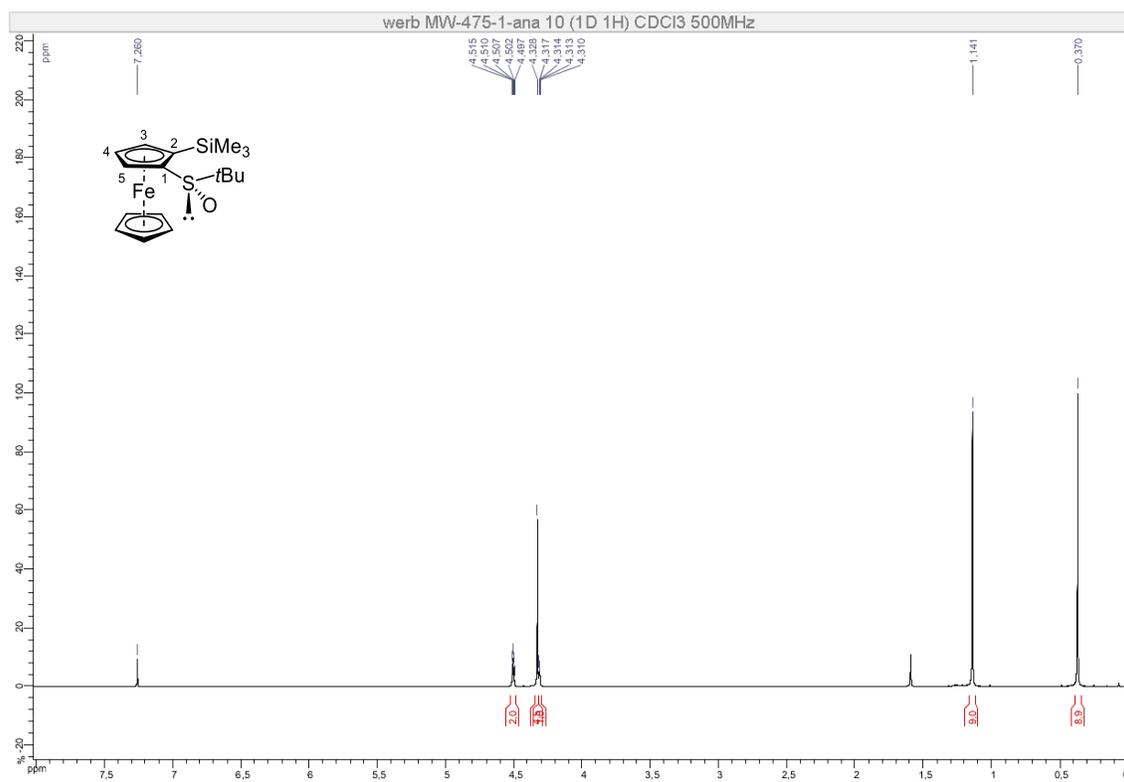
Racemic *S*-(4-Tolyl)ferrocenesulfoxide (*rac*-FcSO-*p*-Tol)

^1H NMR (300 MHz, CDCl_3)

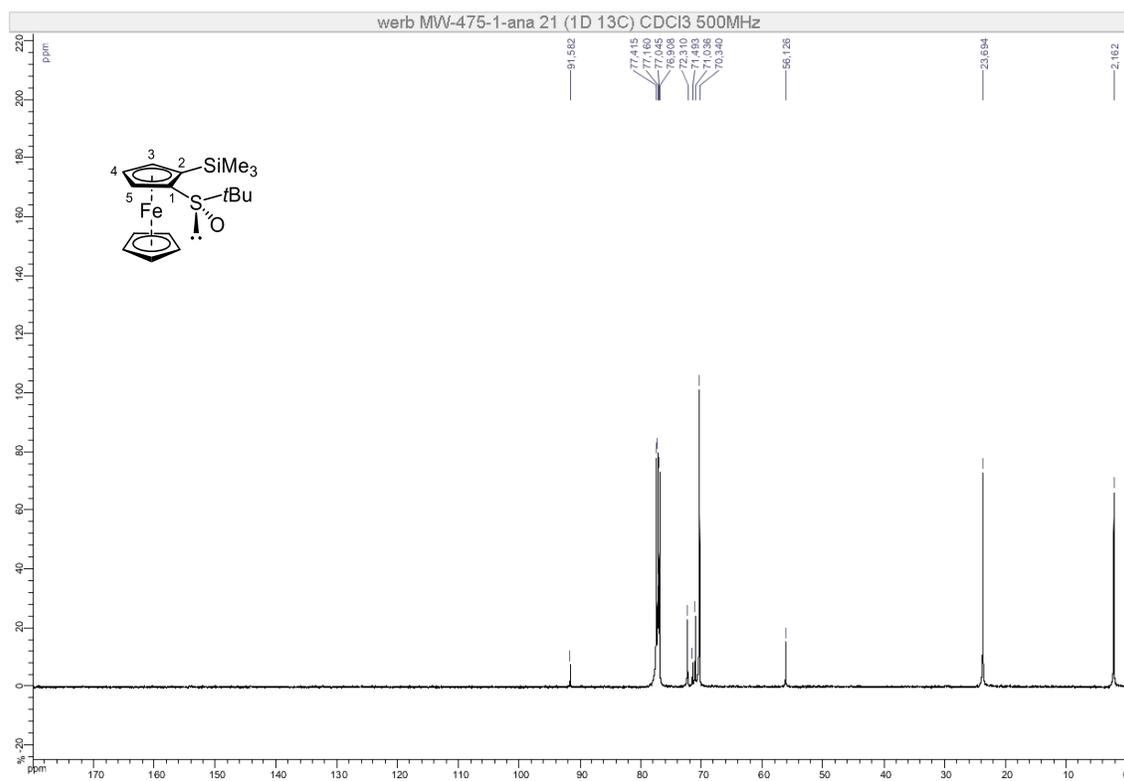


(*S,S*)-*S*-tert-Butyl-2-(trimethylsilyl)ferrocenesulfoxide (*S,S*-1a)

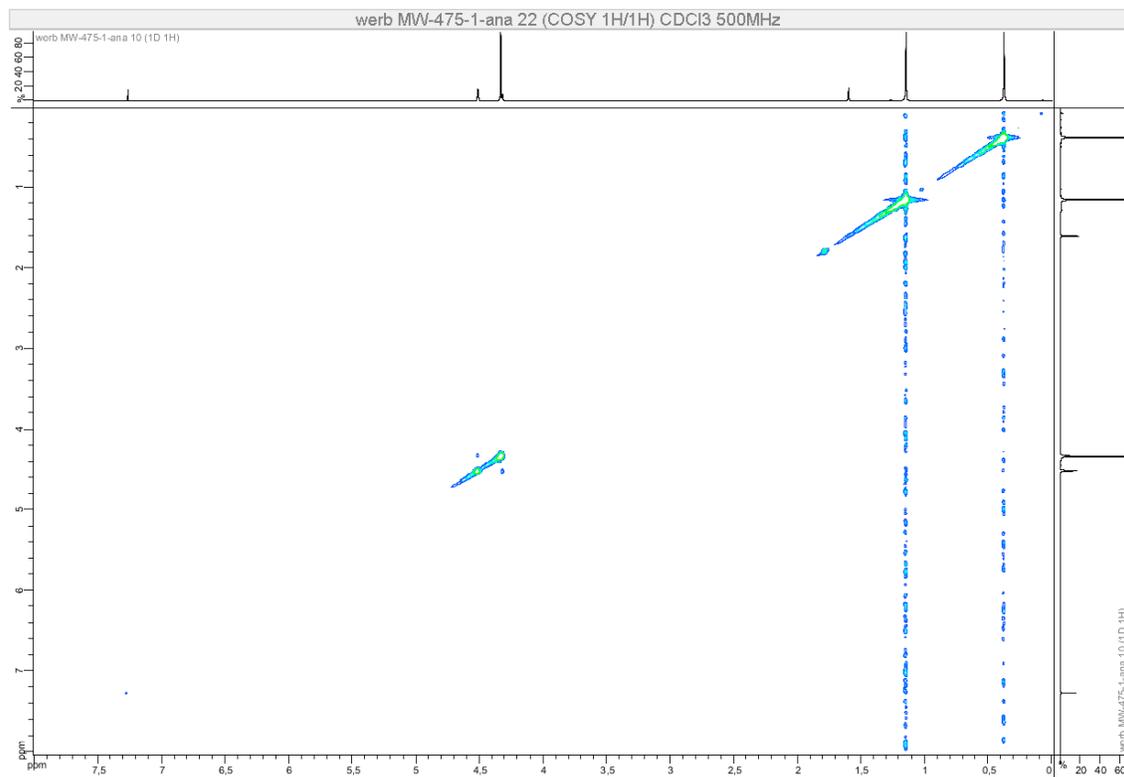
¹H NMR (500 MHz, CDCl₃)



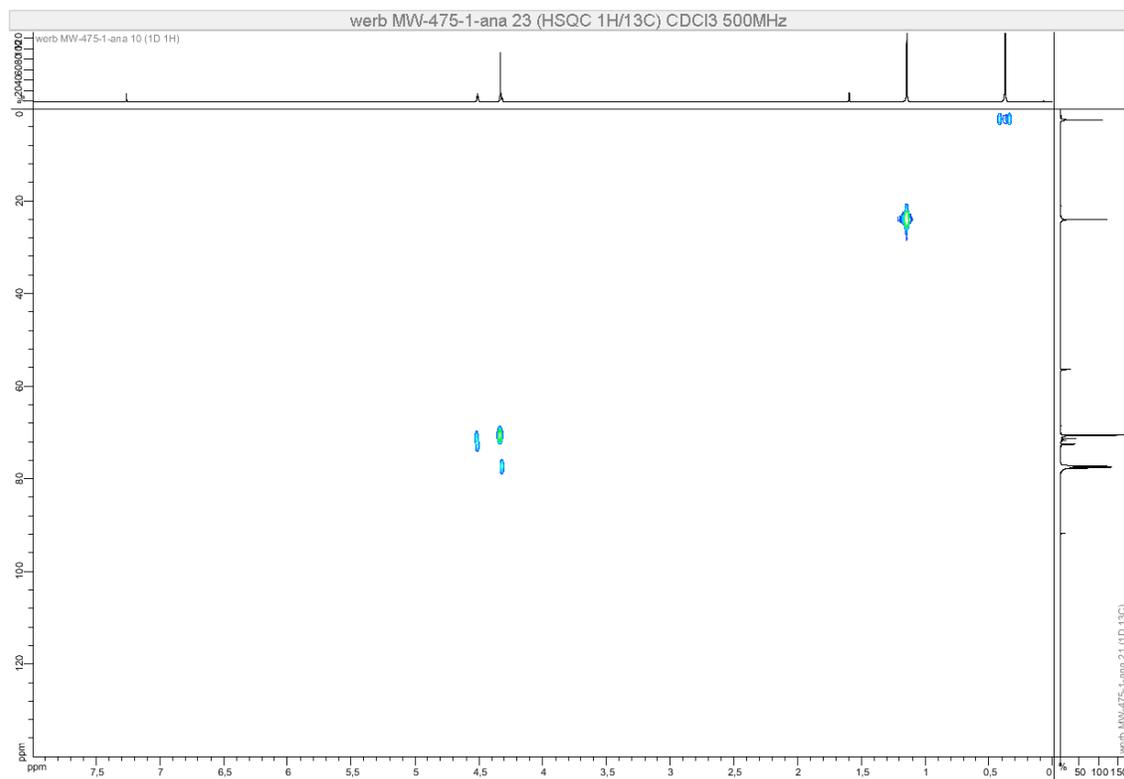
¹³C NMR (126 MHz, CDCl₃)



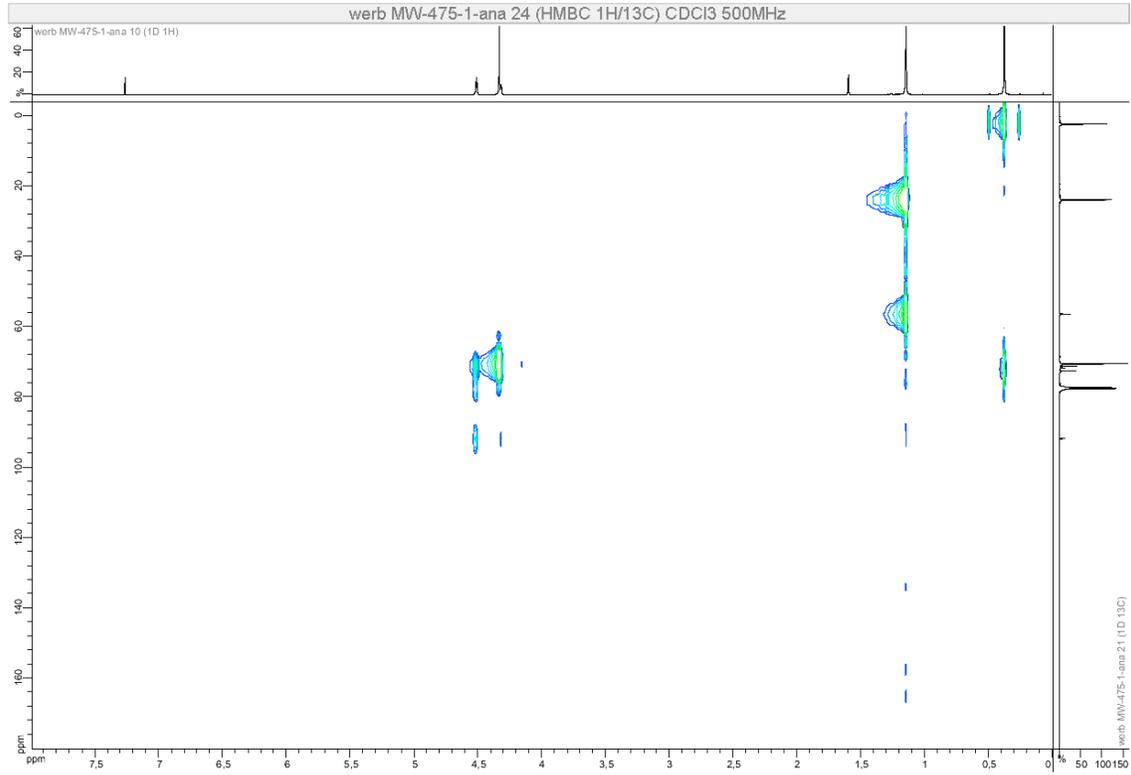
COSY (500 MHz, CDCl₃)



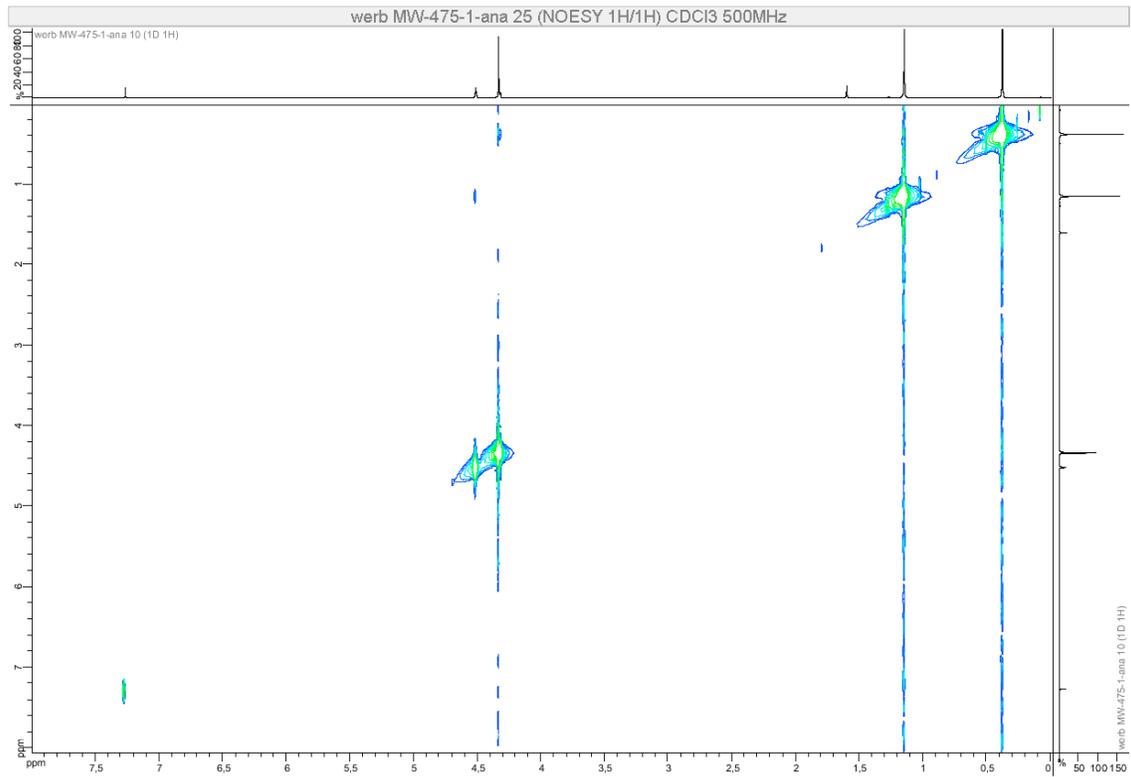
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

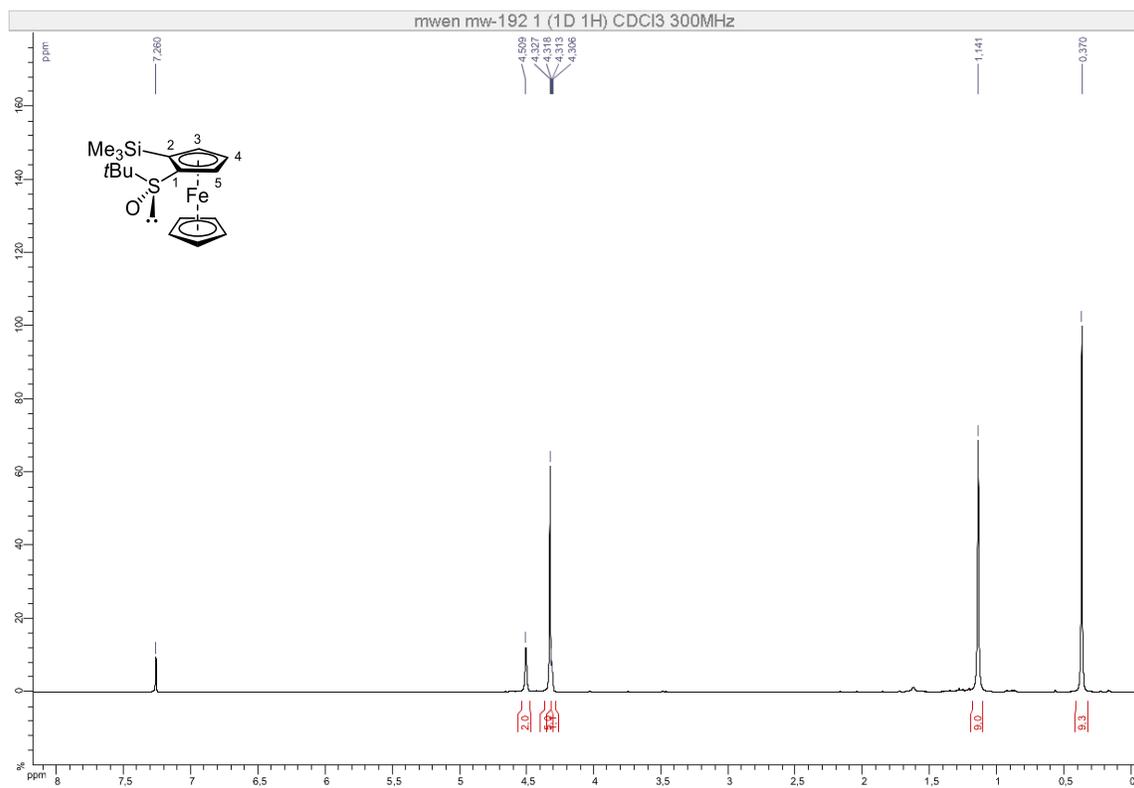


NOESY (500 MHz, CDCl₃)



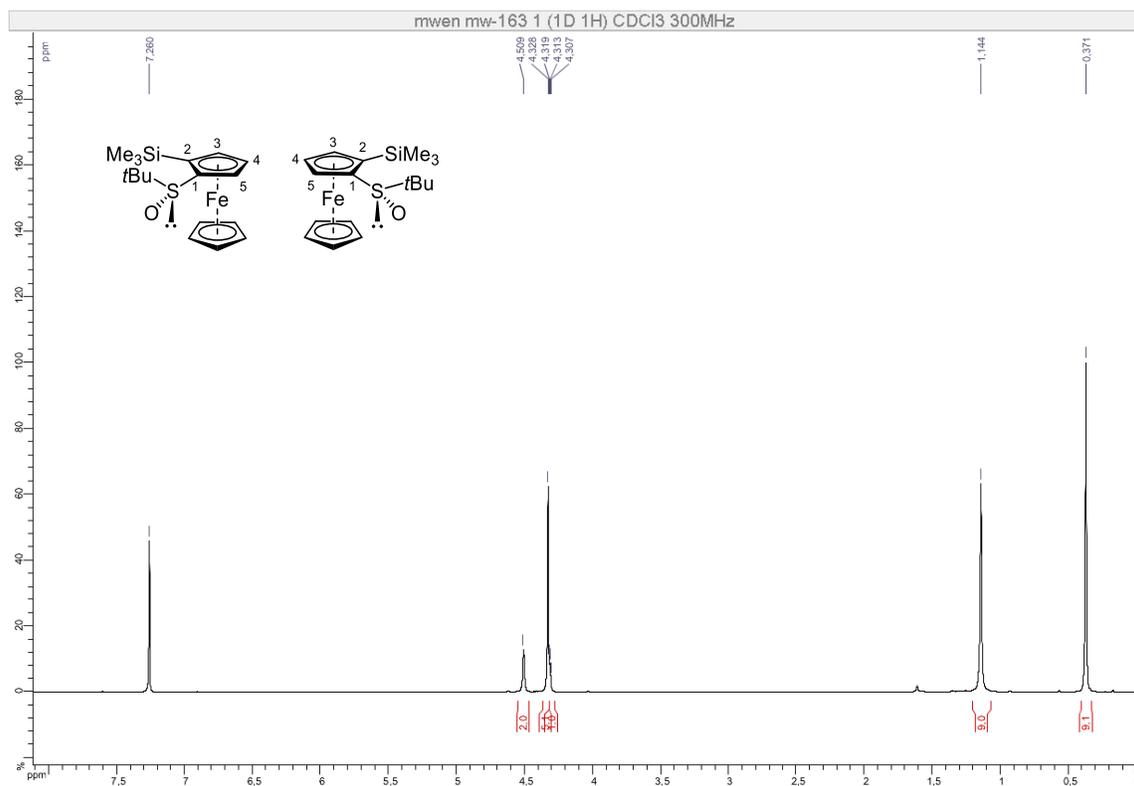
(*R,R*)-*S*-*tert*-Butyl-2-(trimethylsilyl)ferrocenesulfoxide (*R,R*-1a)

¹H NMR (300 MHz, CDCl₃)



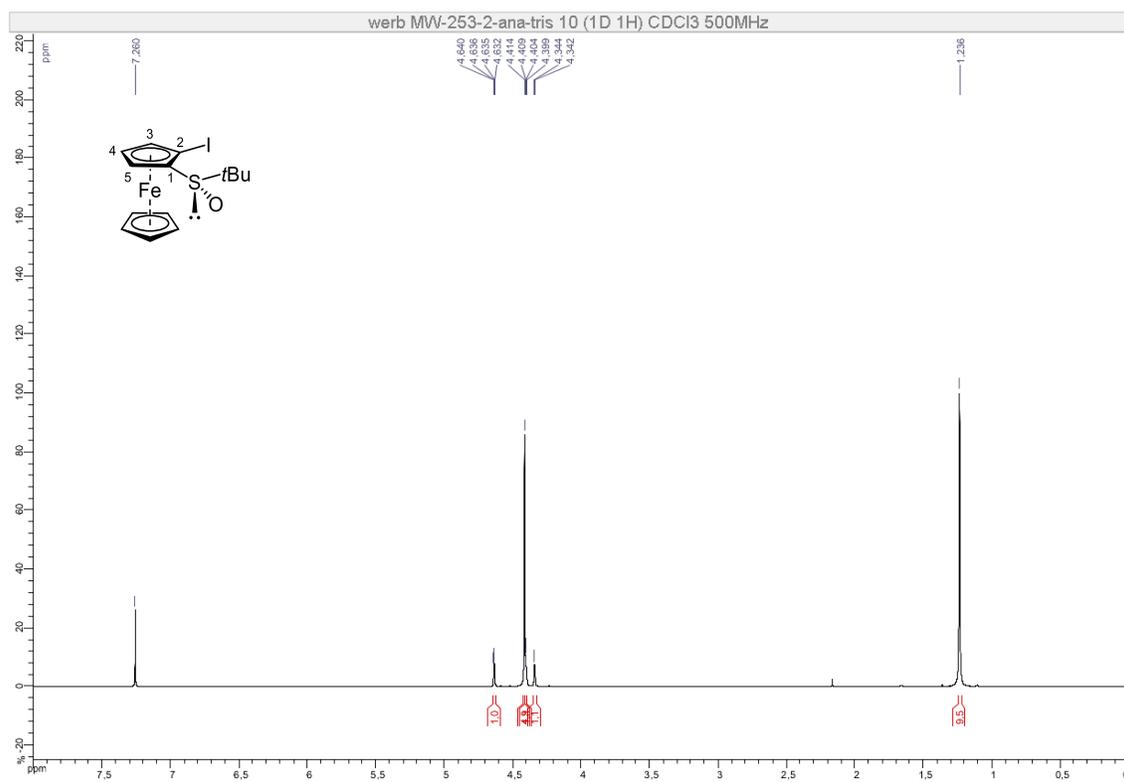
(*R,R*)- and (*S,S*)-*S*-*tert*-Butyl-2-(trimethylsilyl)ferrocenesulfoxide (*R,R*/*S,S*-1a)

^1H NMR (300 MHz, CDCl_3)

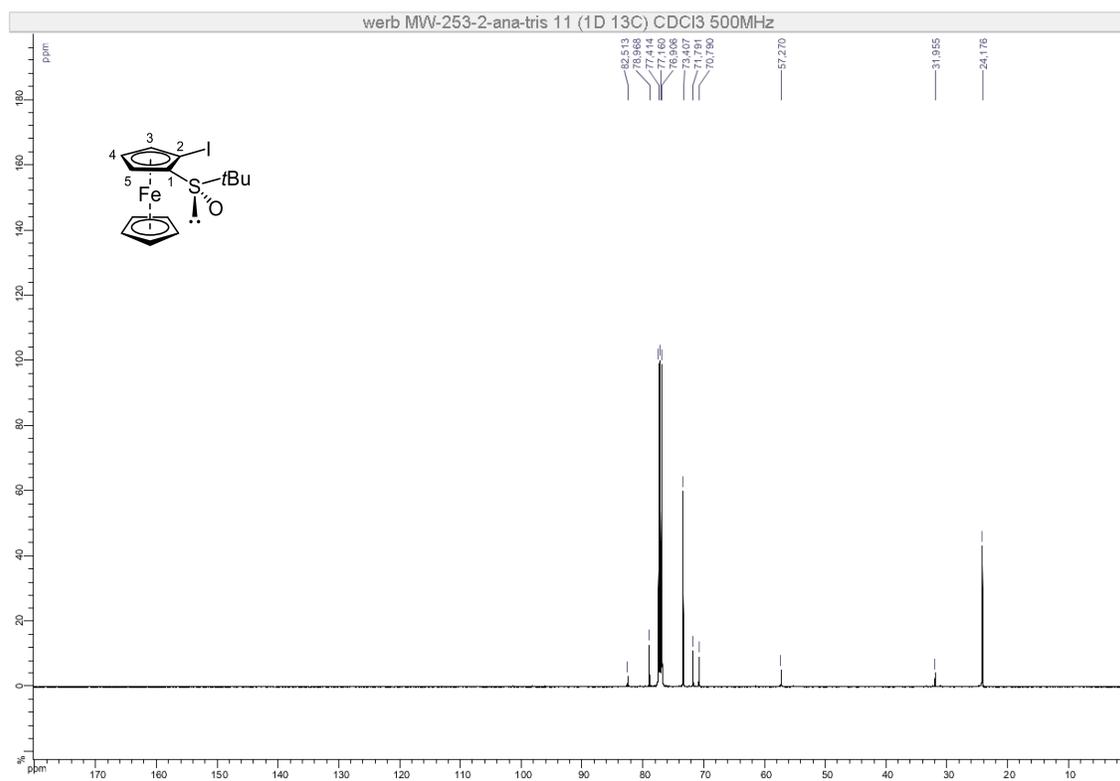


(*S,R_P*)-*S-tert*-Butyl-2-iodoferrocenesulfoxide (*S,R_P*-1b)

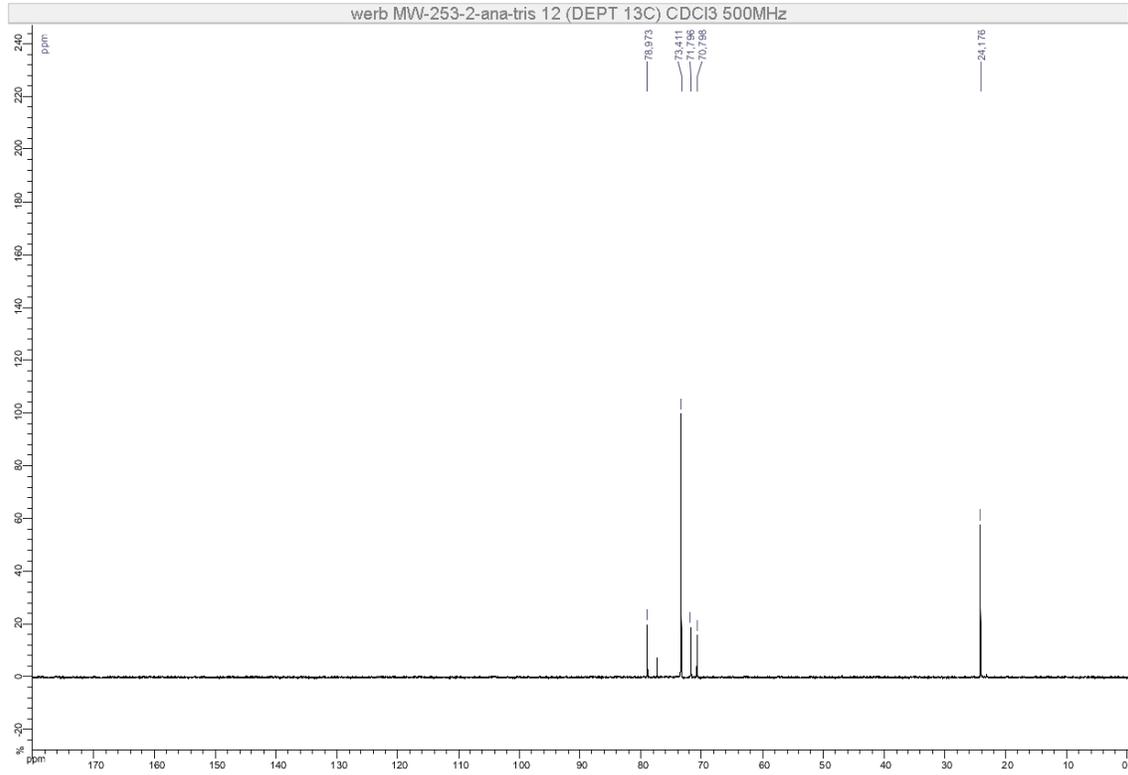
^1H NMR (500 MHz, CDCl_3)



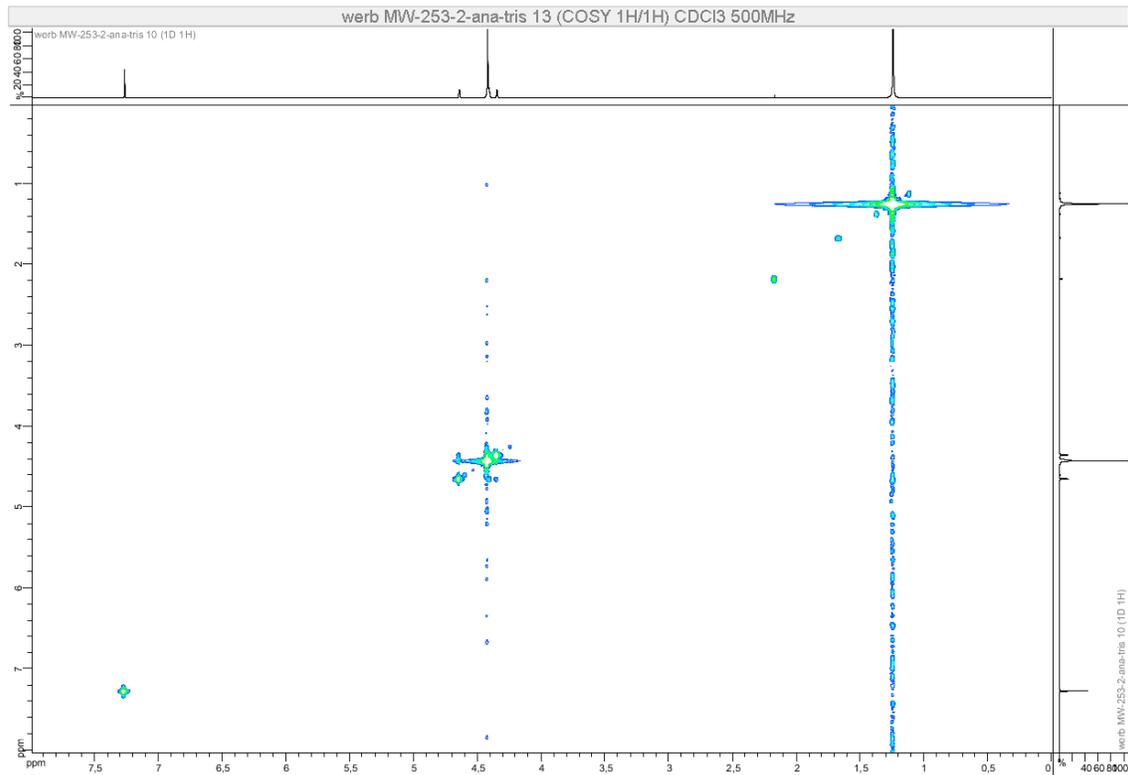
^{13}C NMR (126 MHz, CDCl_3)



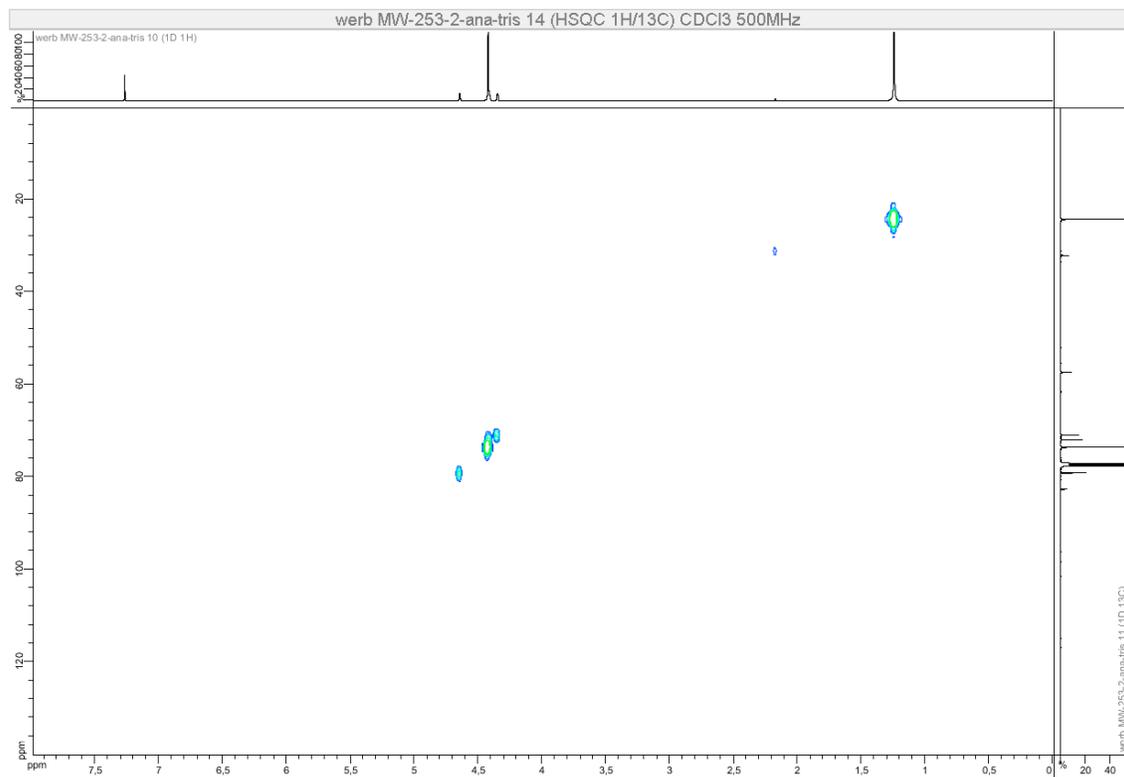
DEPT 135 (126 MHz, CDCl₃)



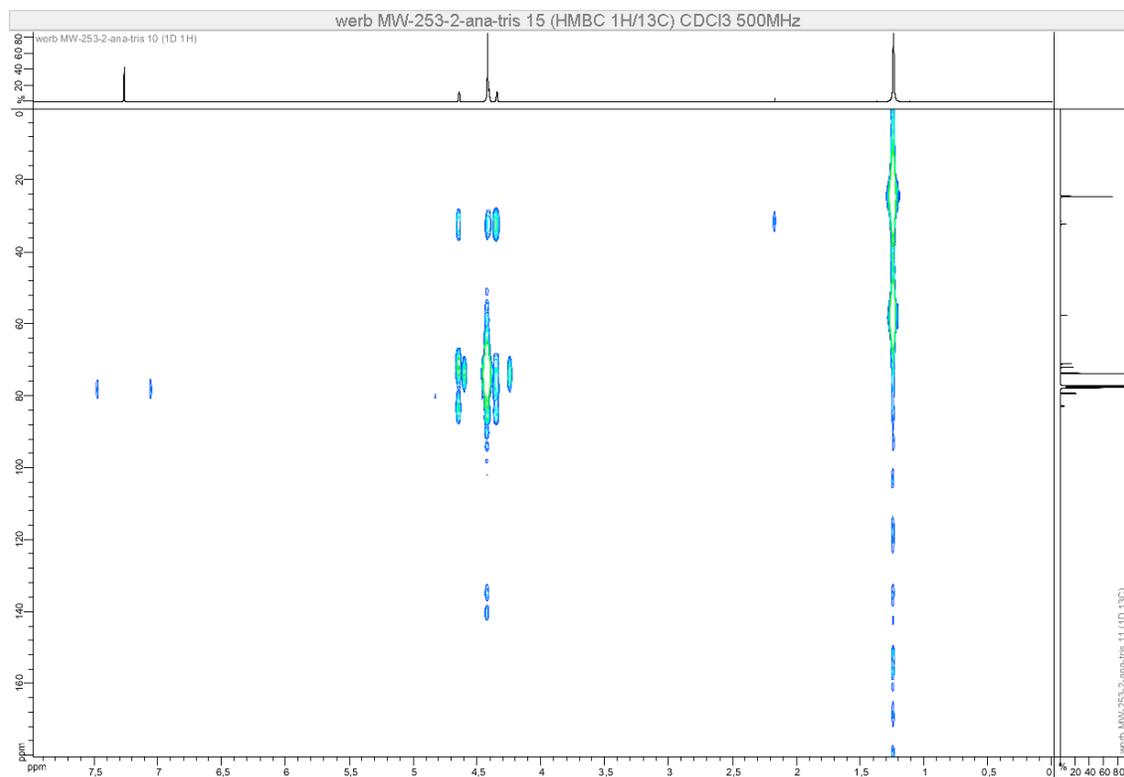
COSY (500 MHz, CDCl₃)



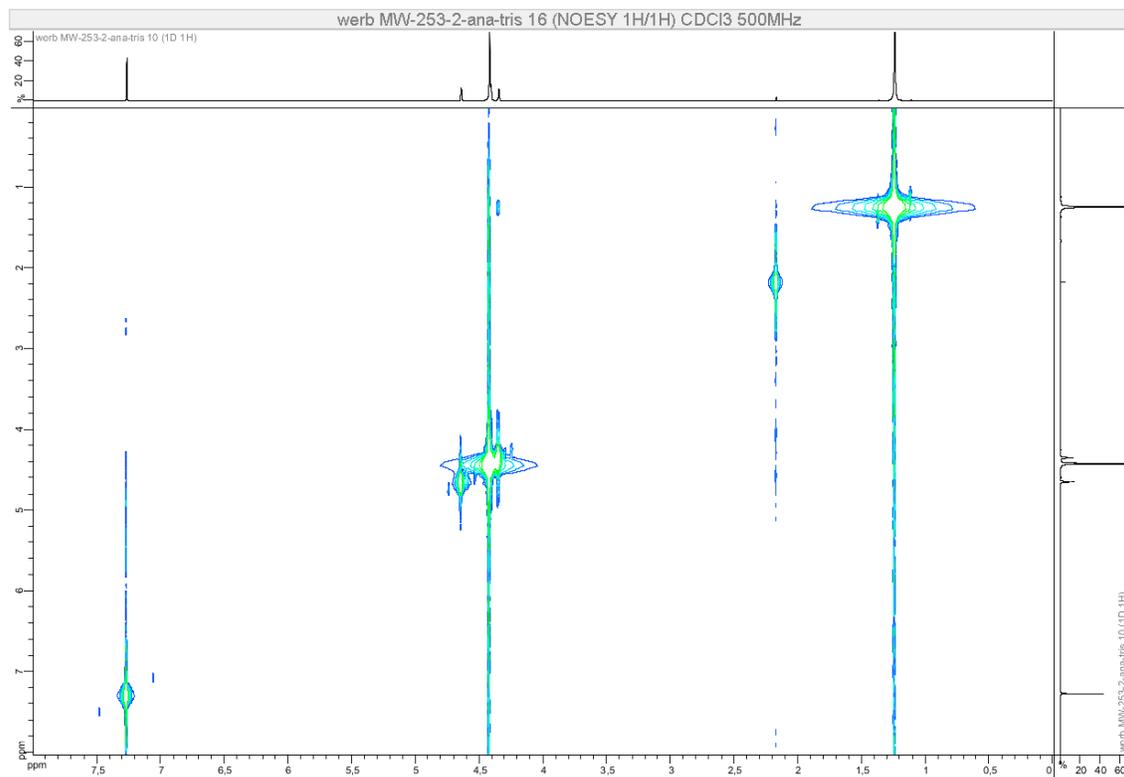
HSQC (500 MHz, CDCl₃)



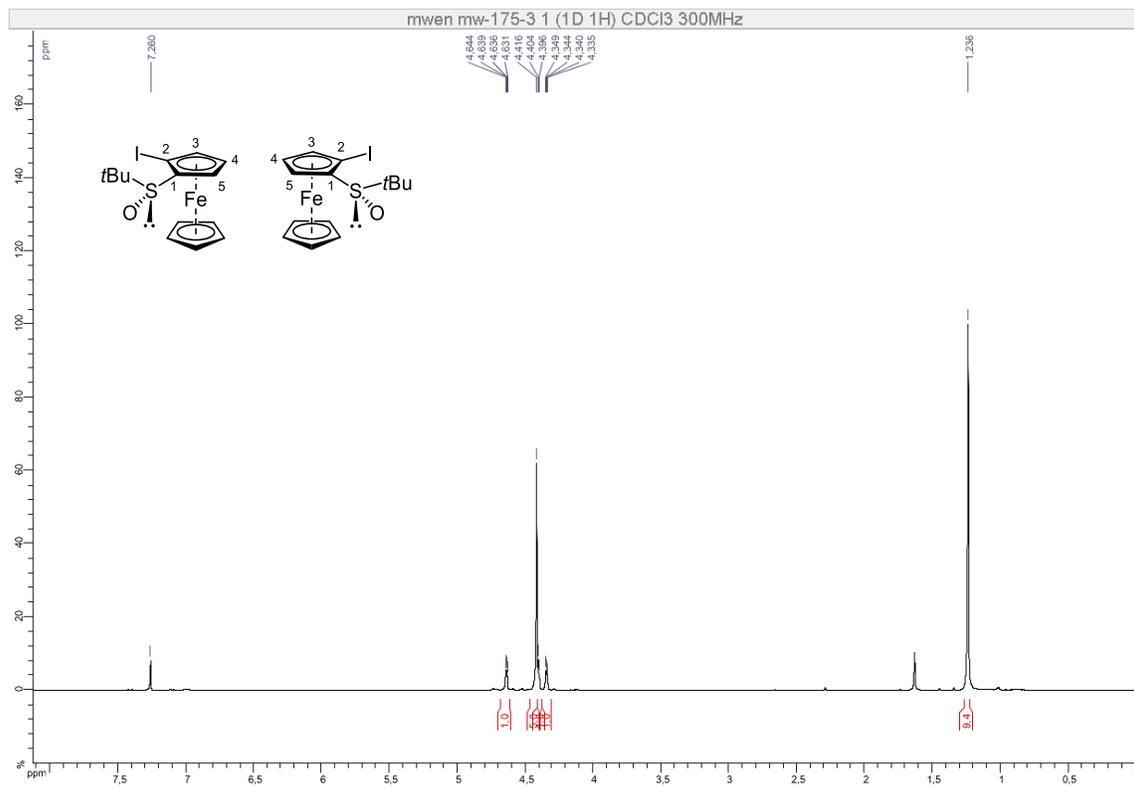
HMBC (500 MHz, CDCl₃)



NOESY (500 MHz, CDCl₃)

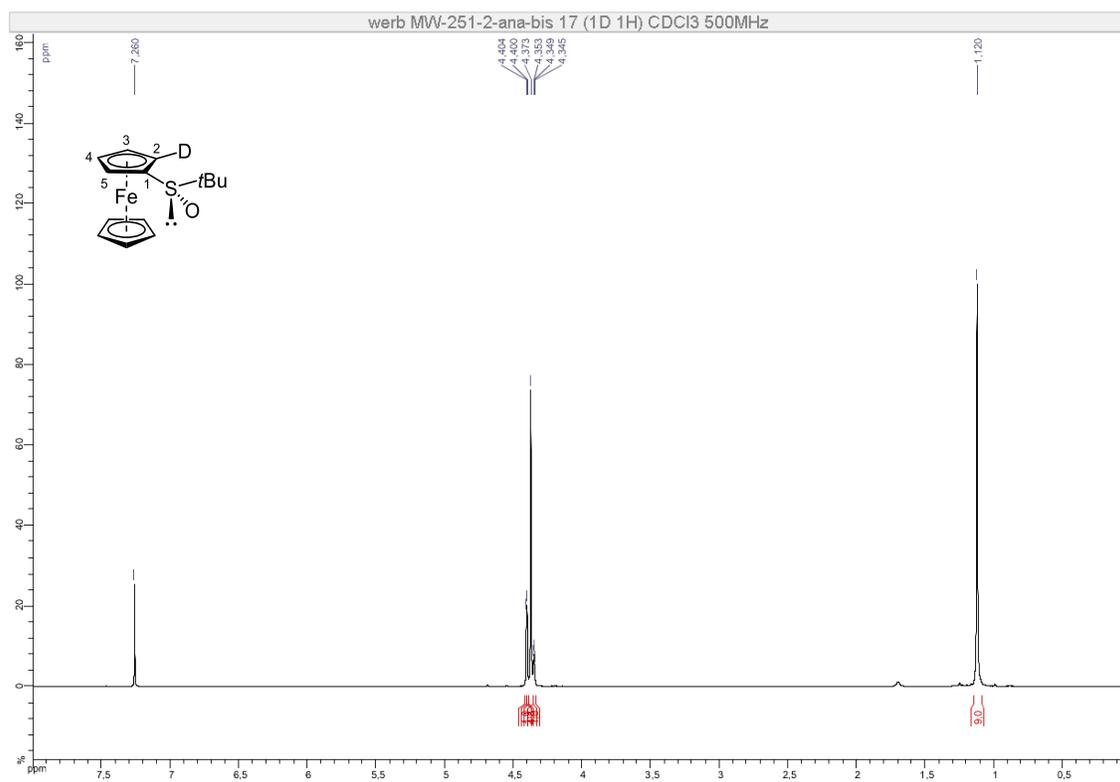


(*S,R_P*)- and (*R,S_P*)-*S-tert*-Butyl-2-iodoferrocenesulfoxide (*S,R_P*/*R,S_P*-1b)

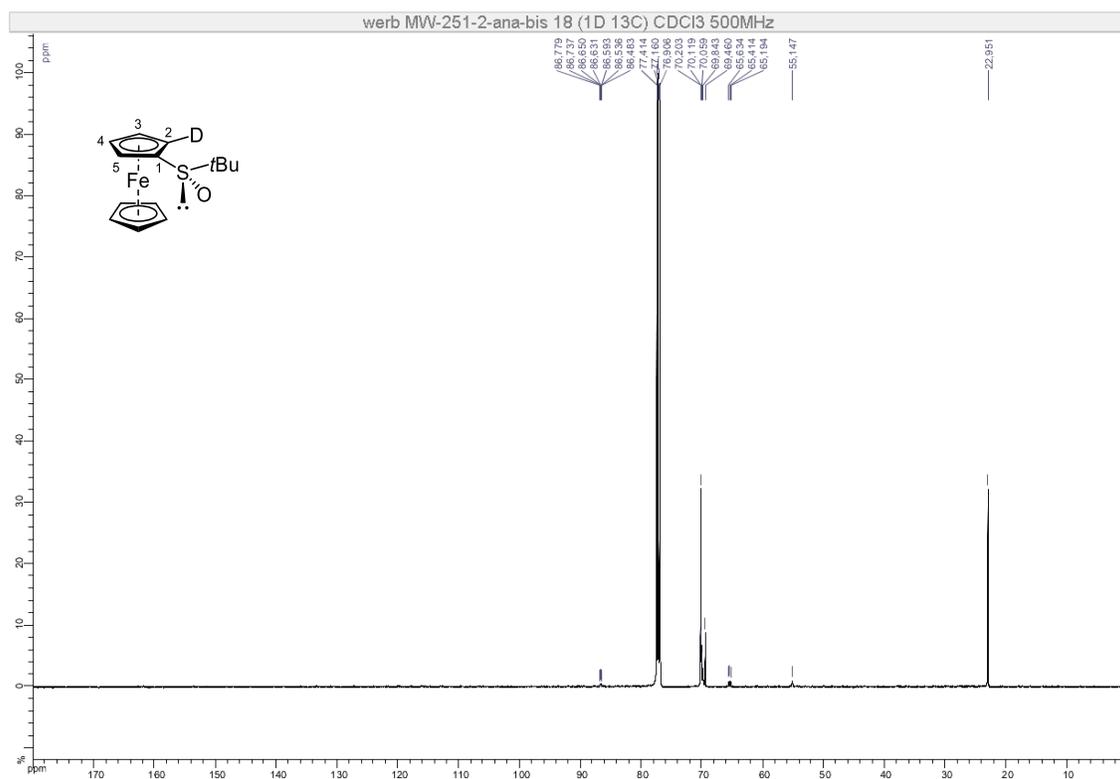


(*S,S*_P)-*S*-tert-Butyl-2-deuterioferrocenesulfoxide (*S,S*_P-1c)

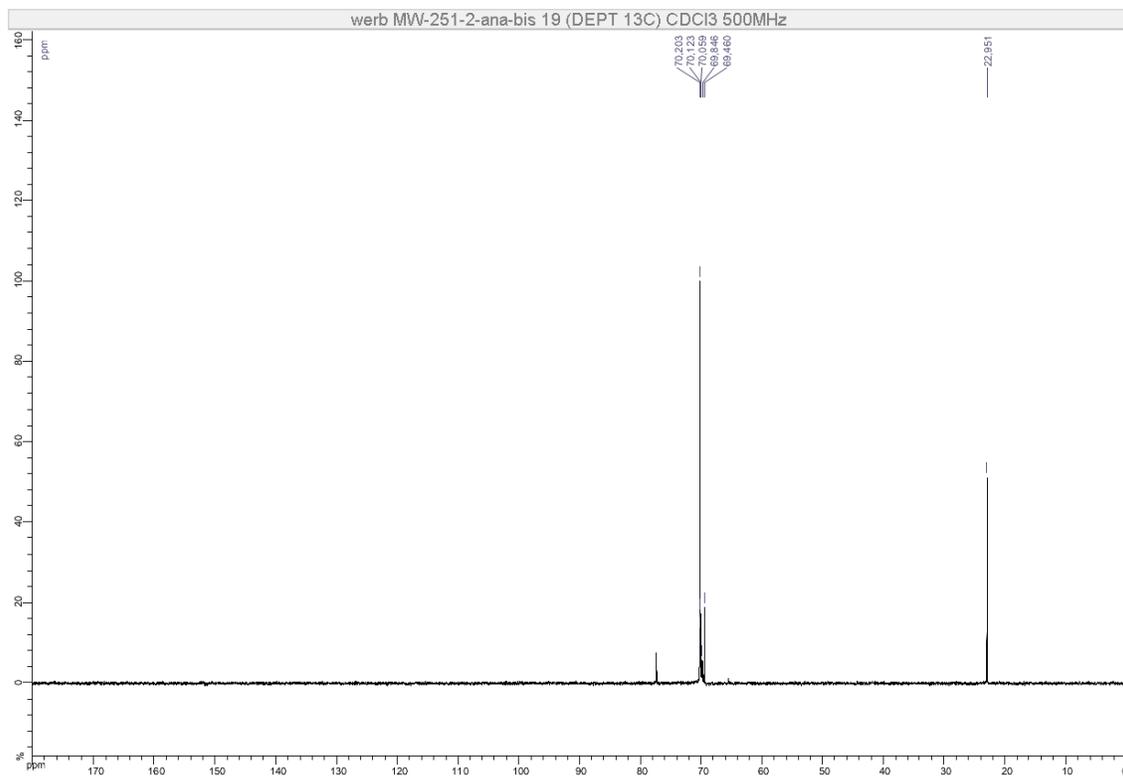
¹H NMR (500 MHz, CDCl₃)



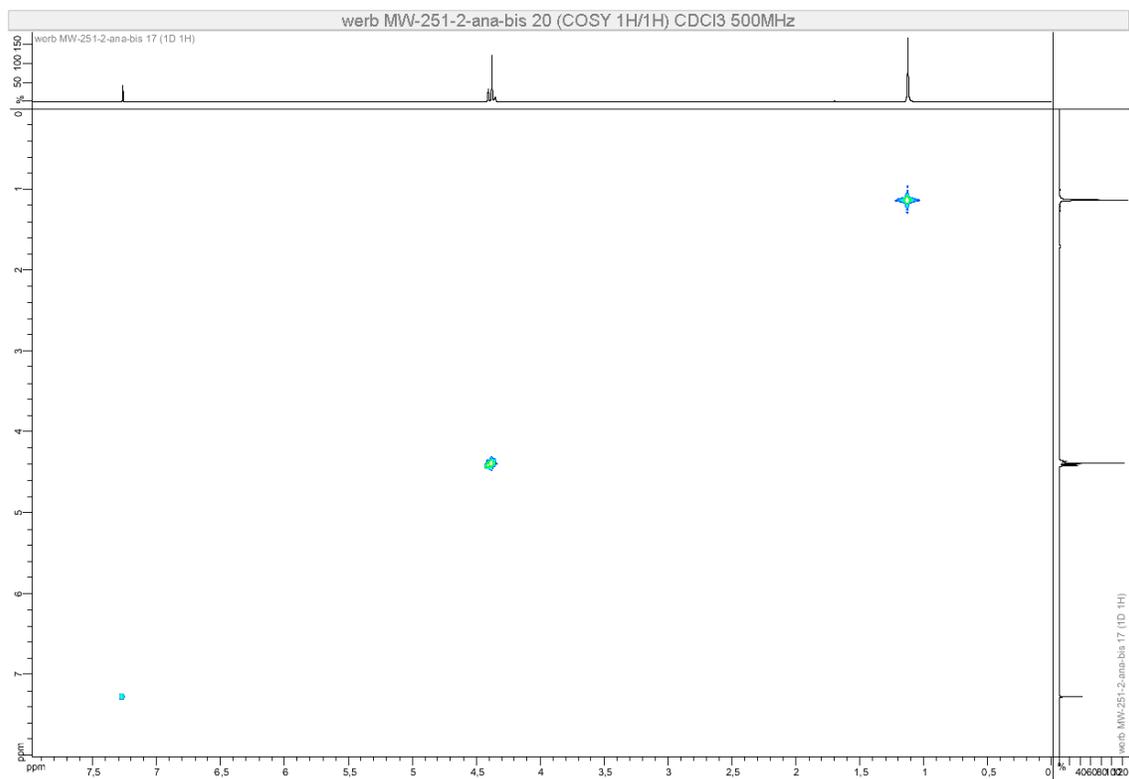
¹³C NMR (126 MHz, CDCl₃)



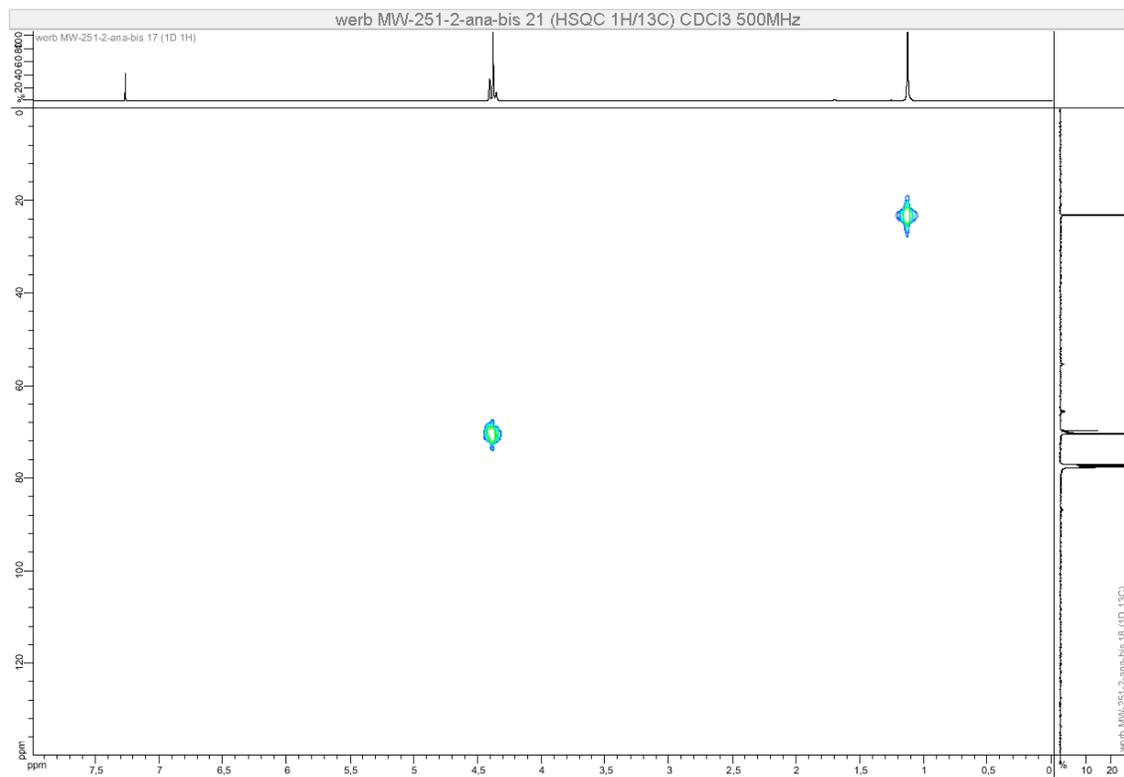
DEPT 135 (126 MHz, CDCl₃)



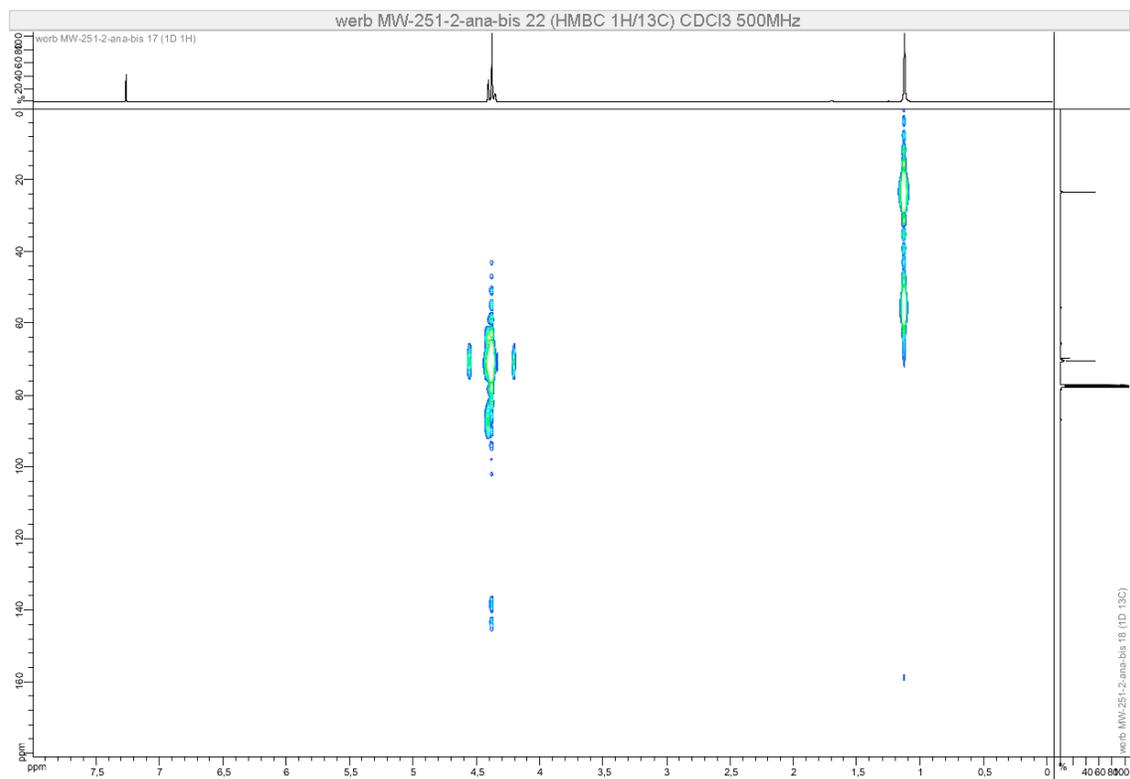
COSY (500 MHz, CDCl₃)



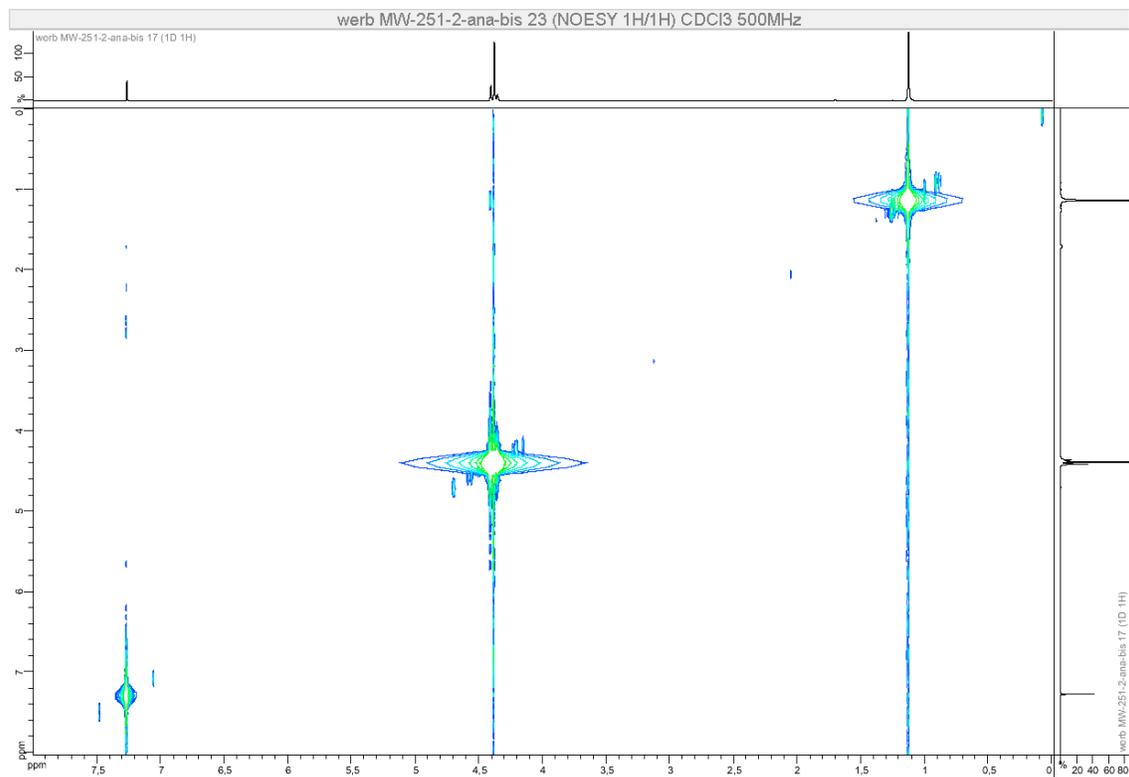
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

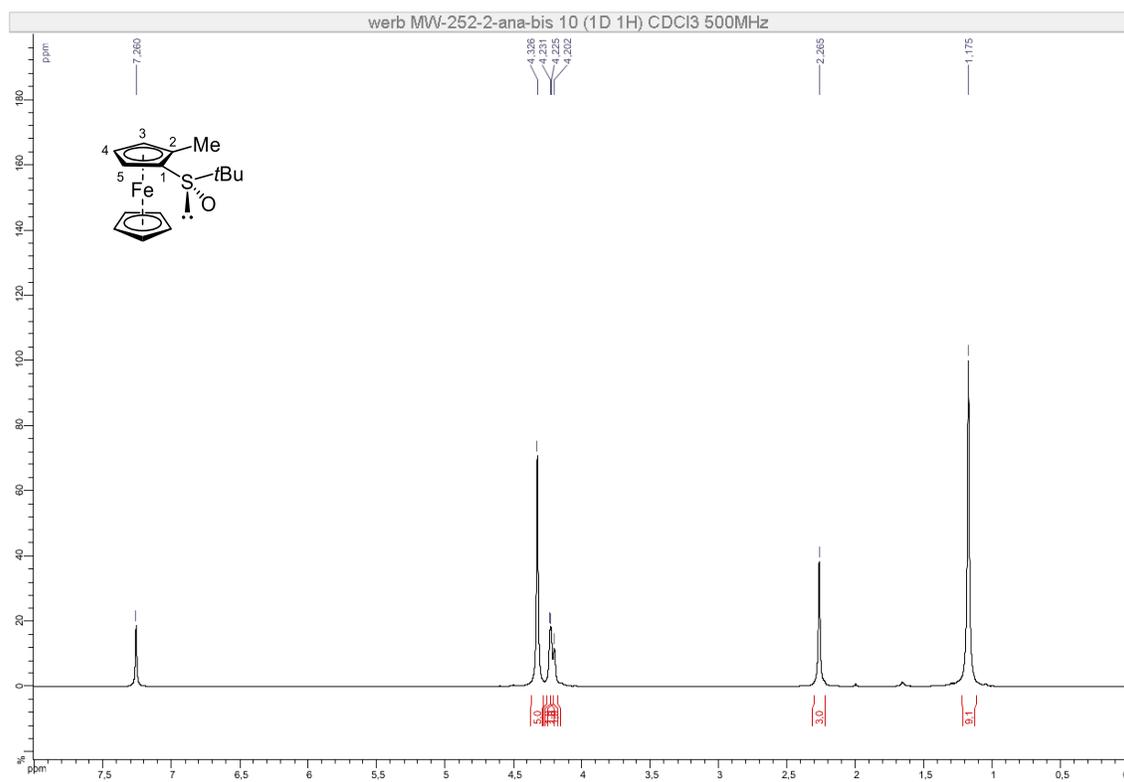


NOESY (500 MHz, CDCl₃)

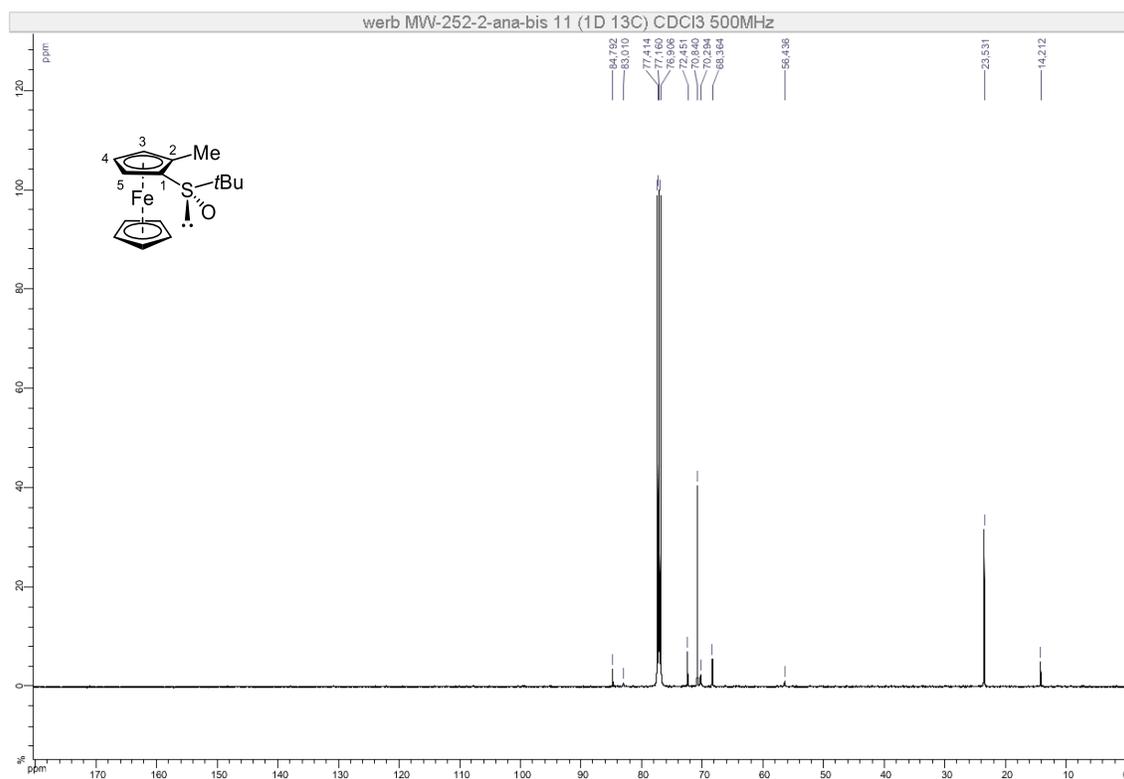


(*S,S*)-*S*-tert-Butyl-2-methylferrocenesulfoxide (*S,S*-1d)

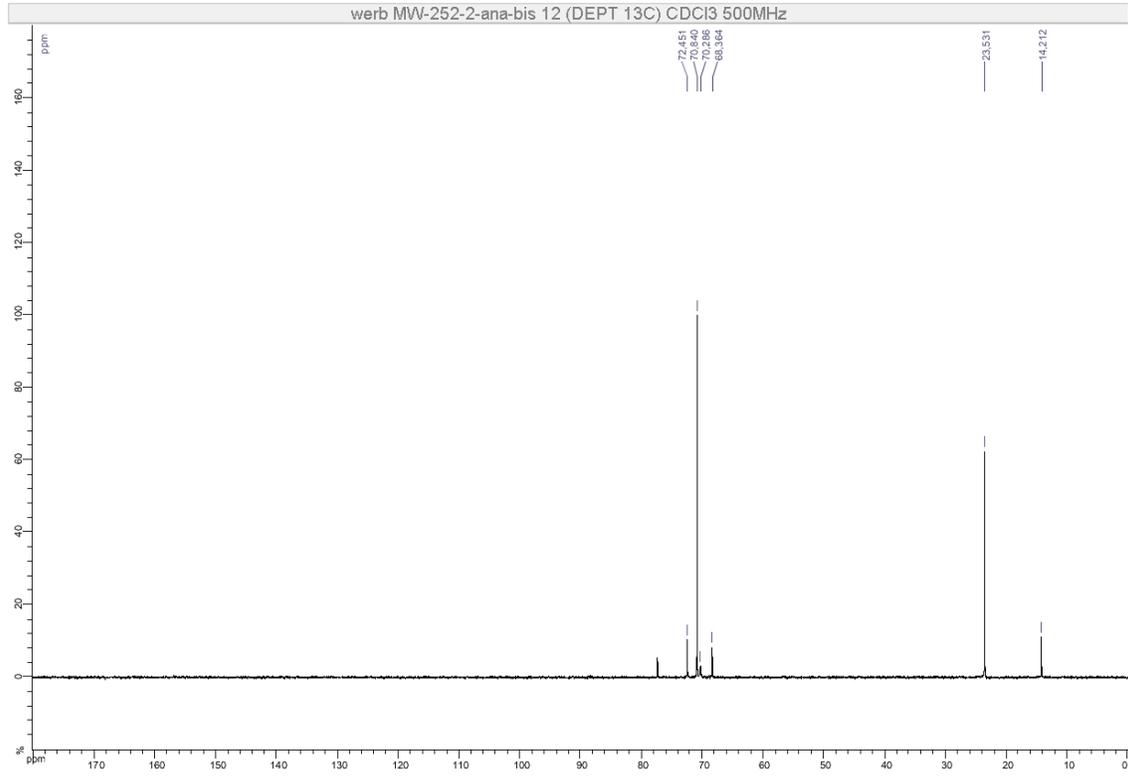
¹H NMR (500 MHz, CDCl₃)



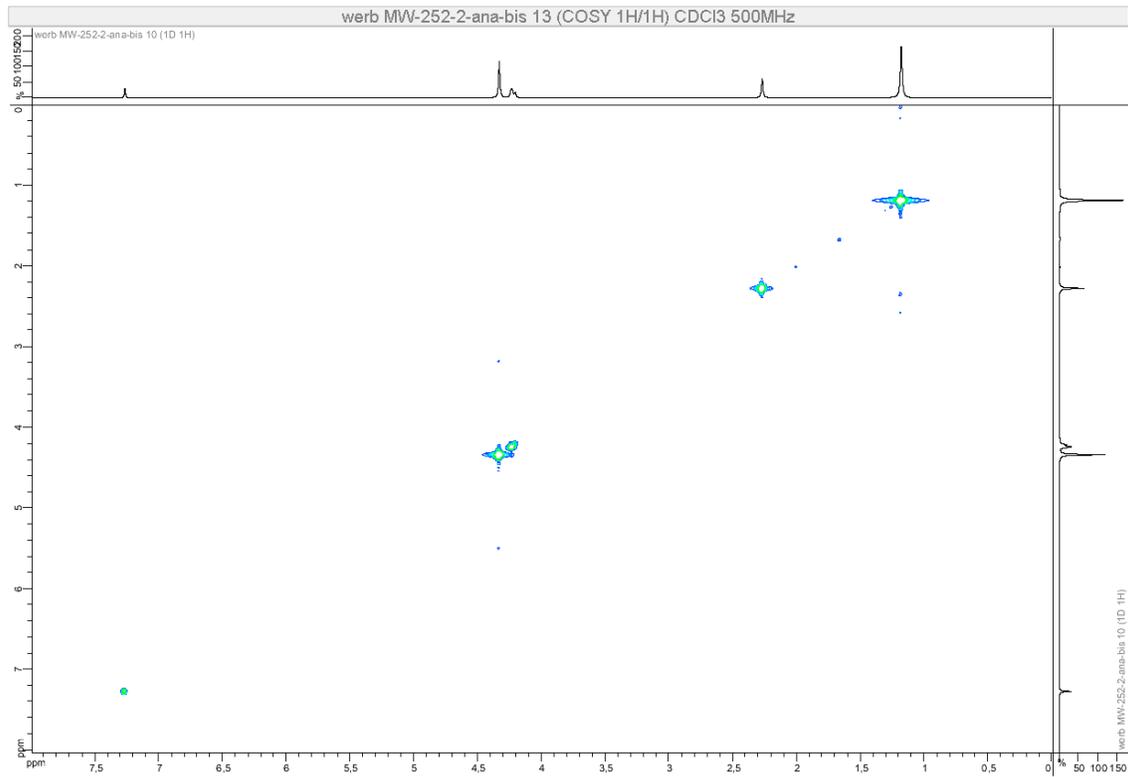
¹³C NMR (126 MHz, CDCl₃)



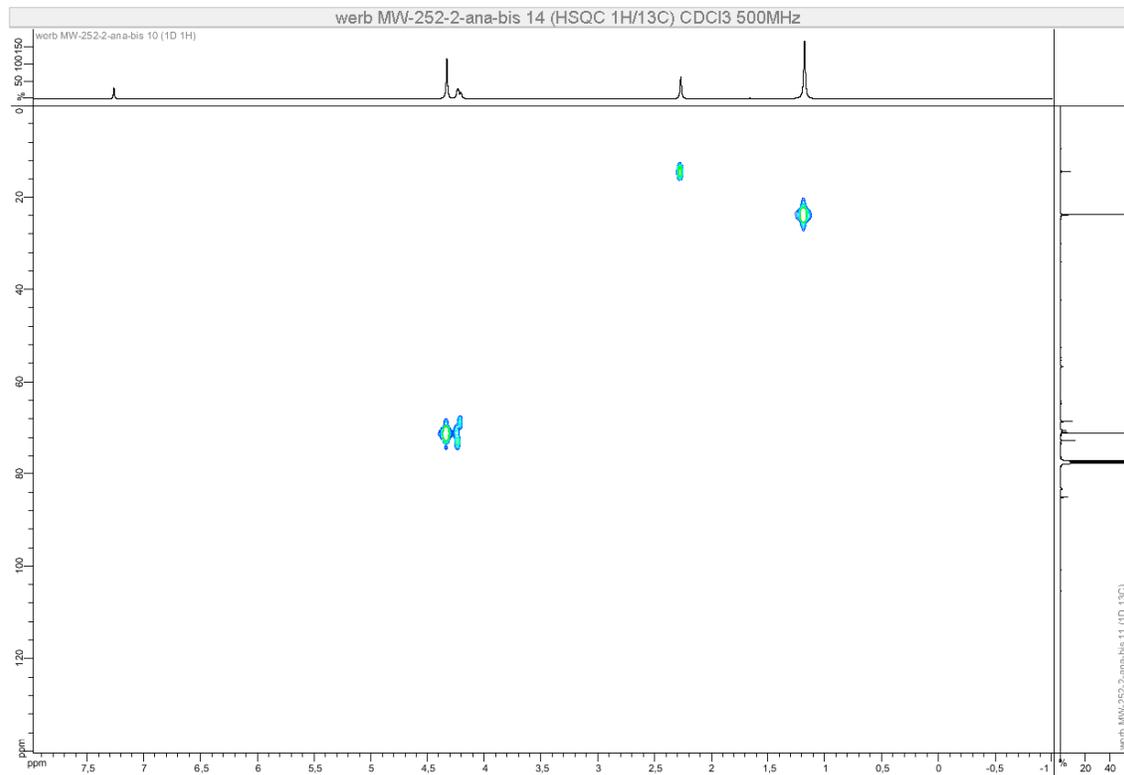
DEPT 135 (126 MHz, CDCl₃)



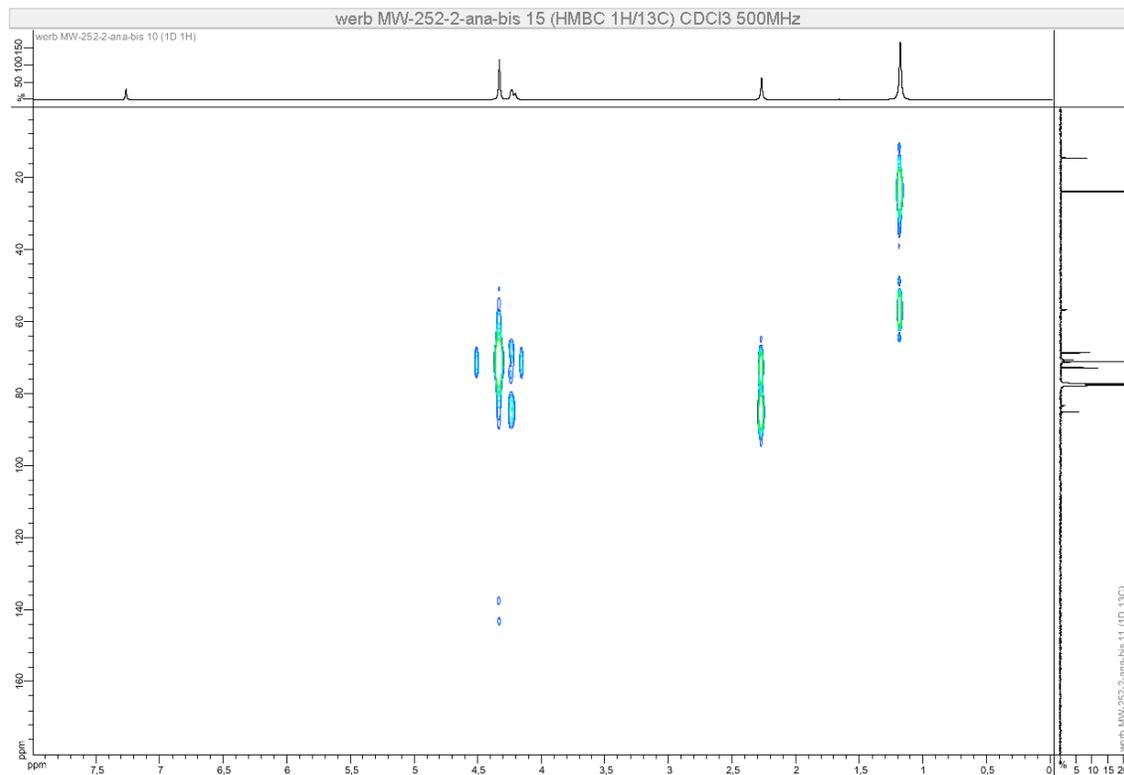
COSY (500 MHz, CDCl₃)



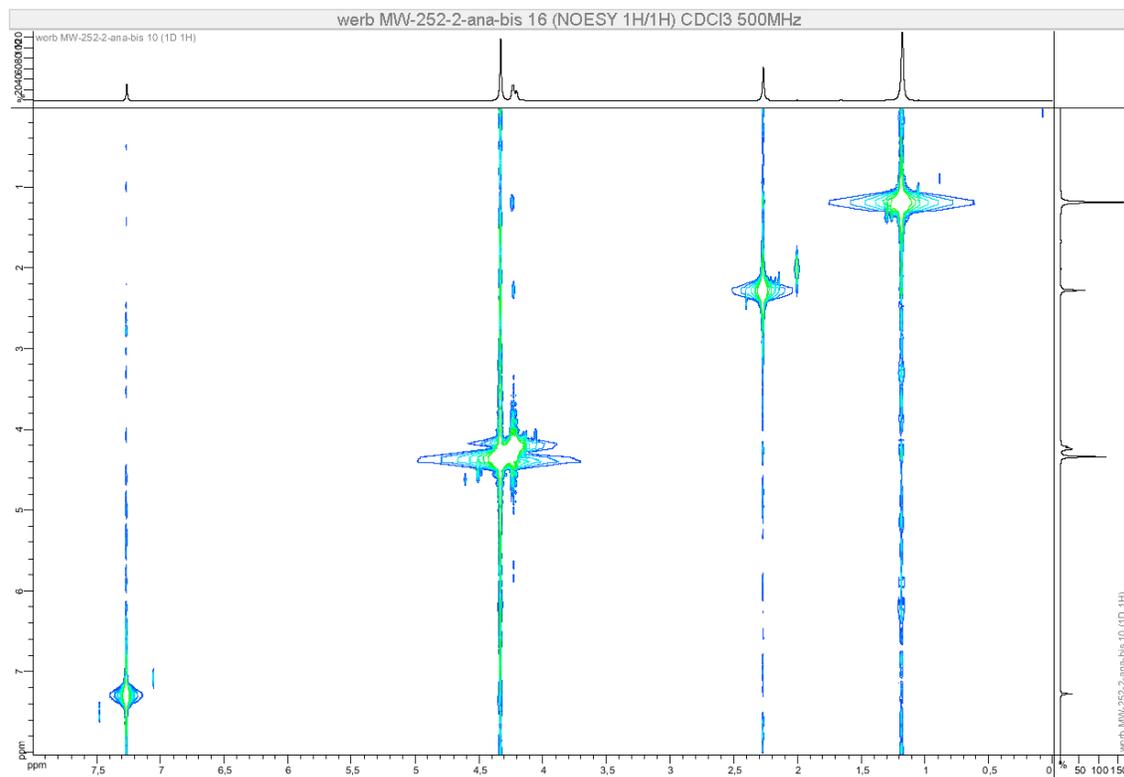
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

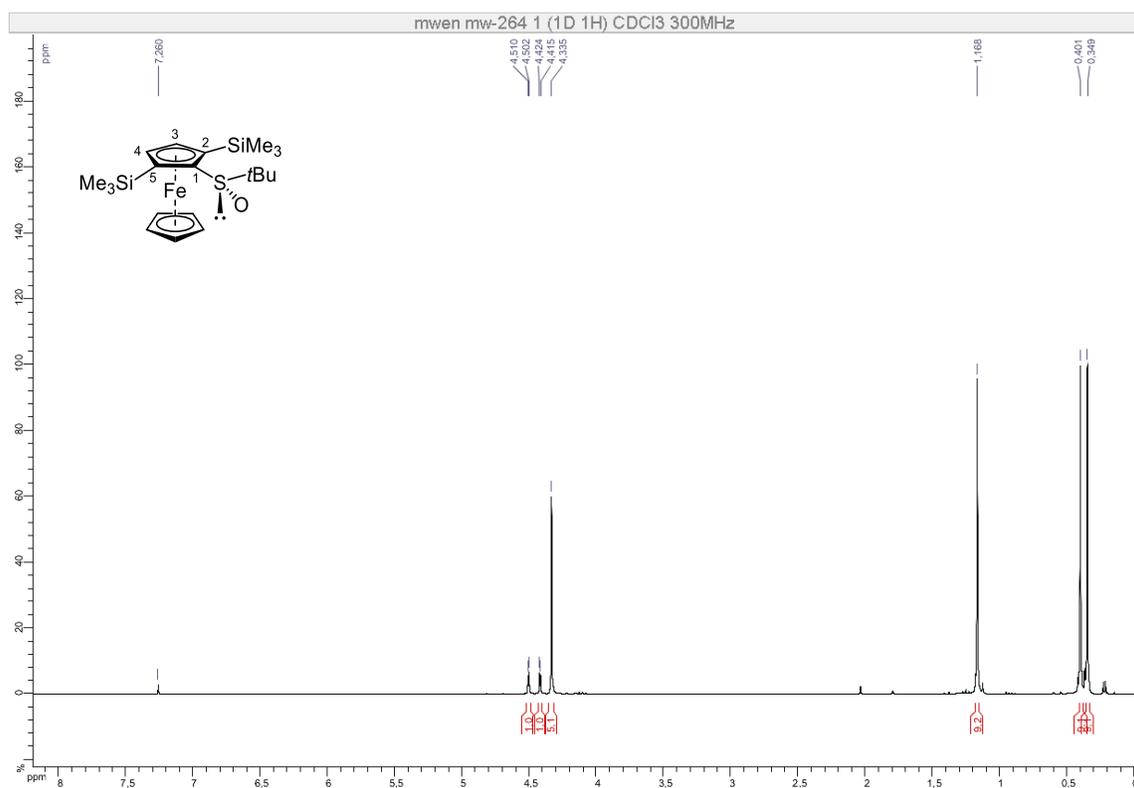


NOESY (500 MHz, CDCl₃)



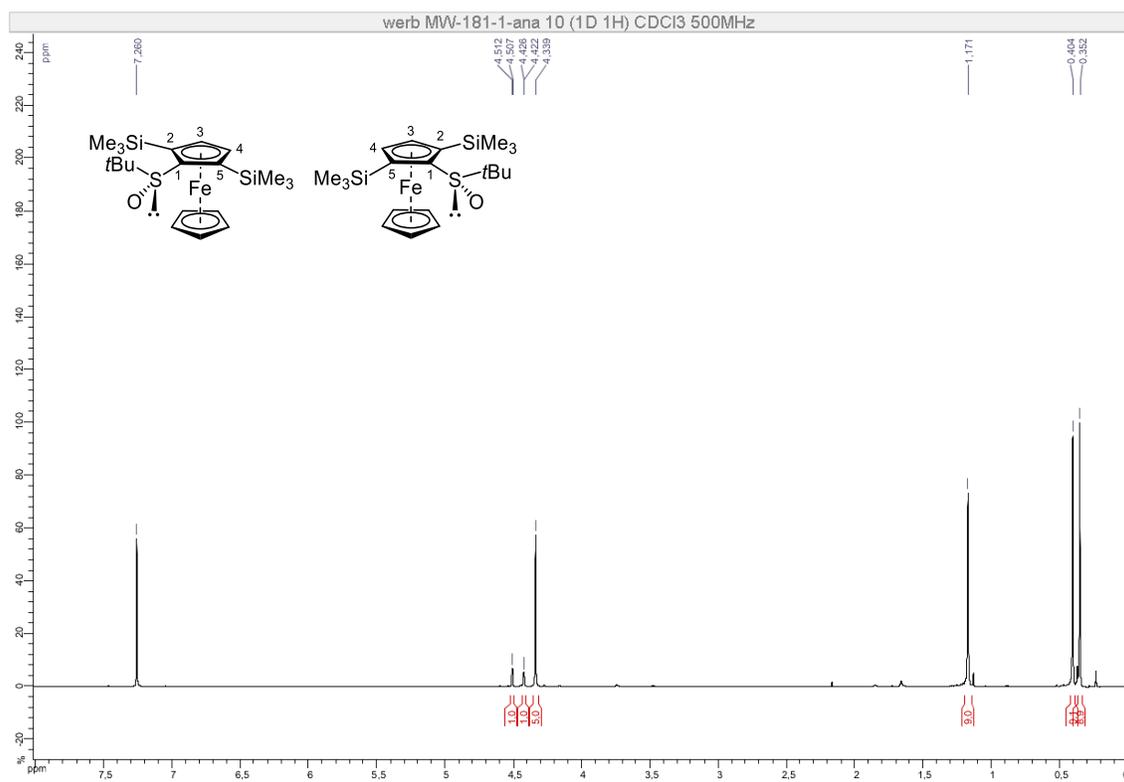
(S)-S-tert-Butyl-2,5-bis(trimethylsilyl)ferrocenesulfoxide (S-2aa)

¹H NMR (300 MHz, CDCl₃)

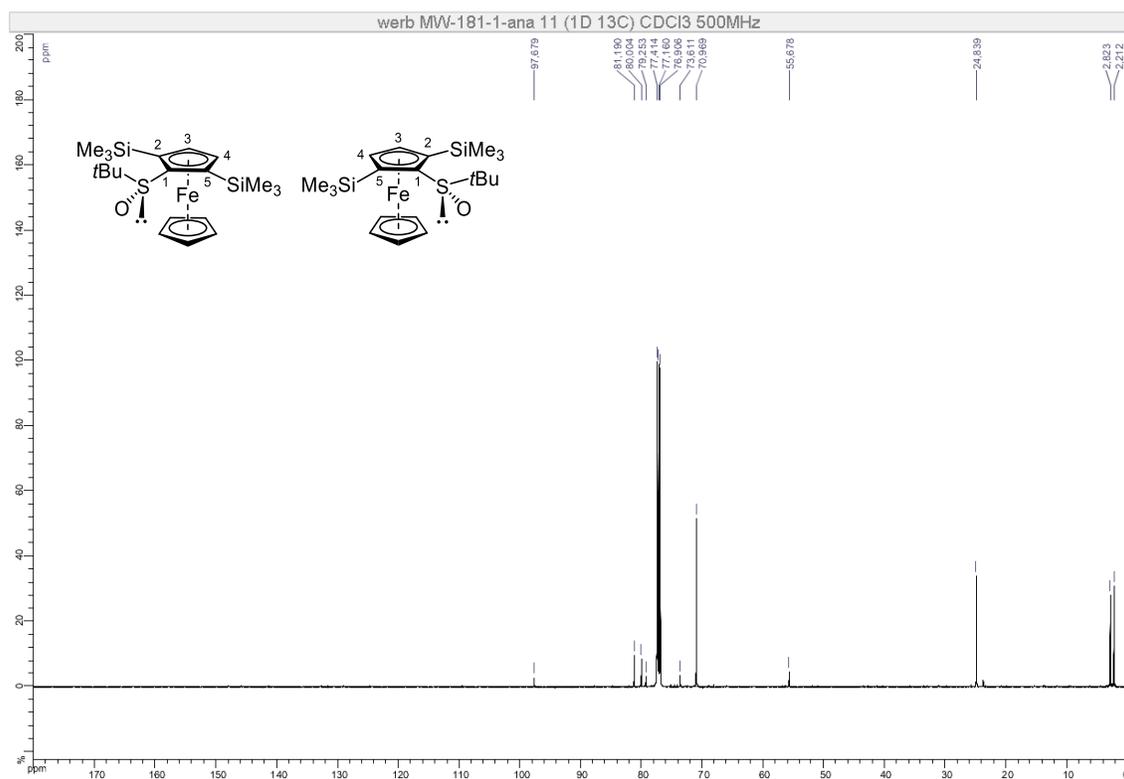


(R)- and (S)-*tert*-Butyl-2,5-bis(trimethylsilyl)ferrocenesulfoxide (*rac*-2aa)

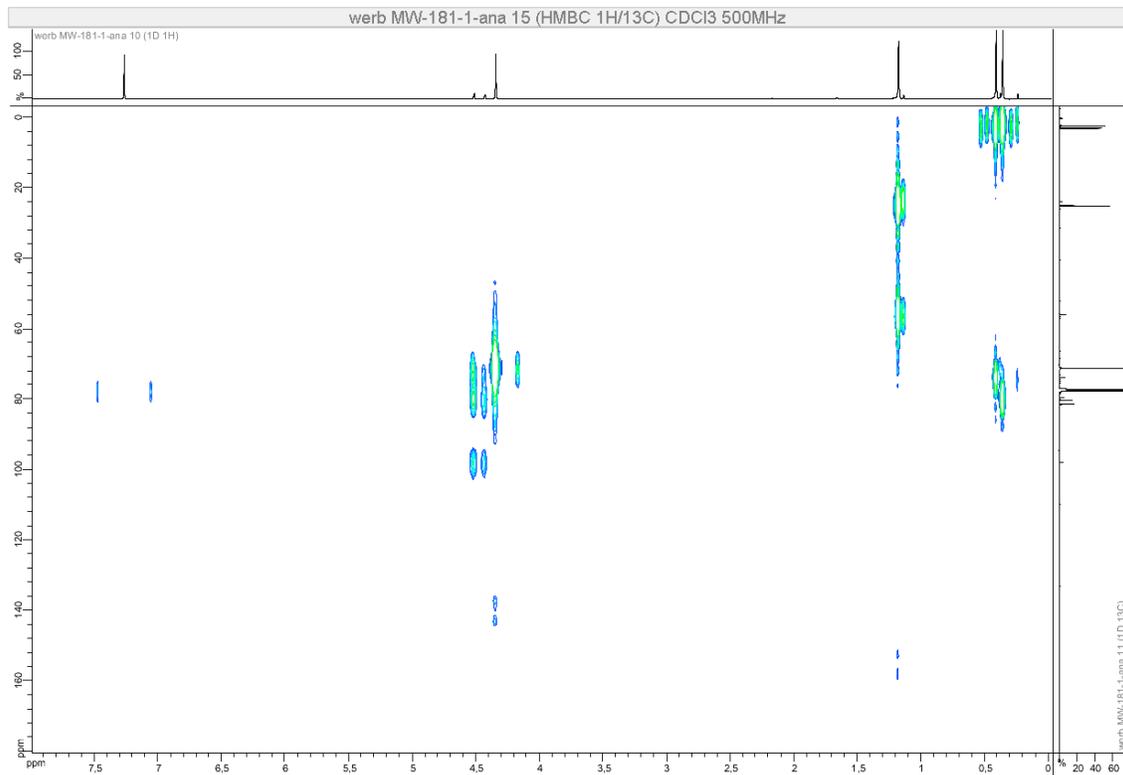
¹H NMR (500 MHz, CDCl₃)



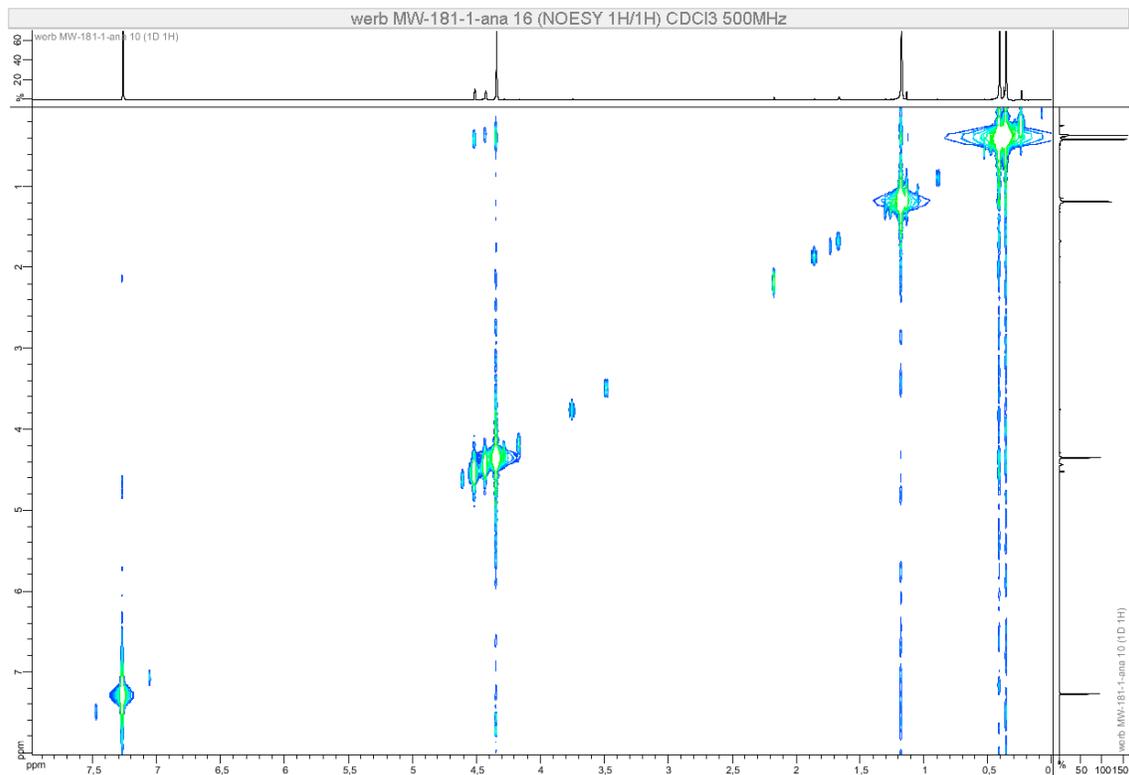
¹³C NMR (126 MHz, CDCl₃)



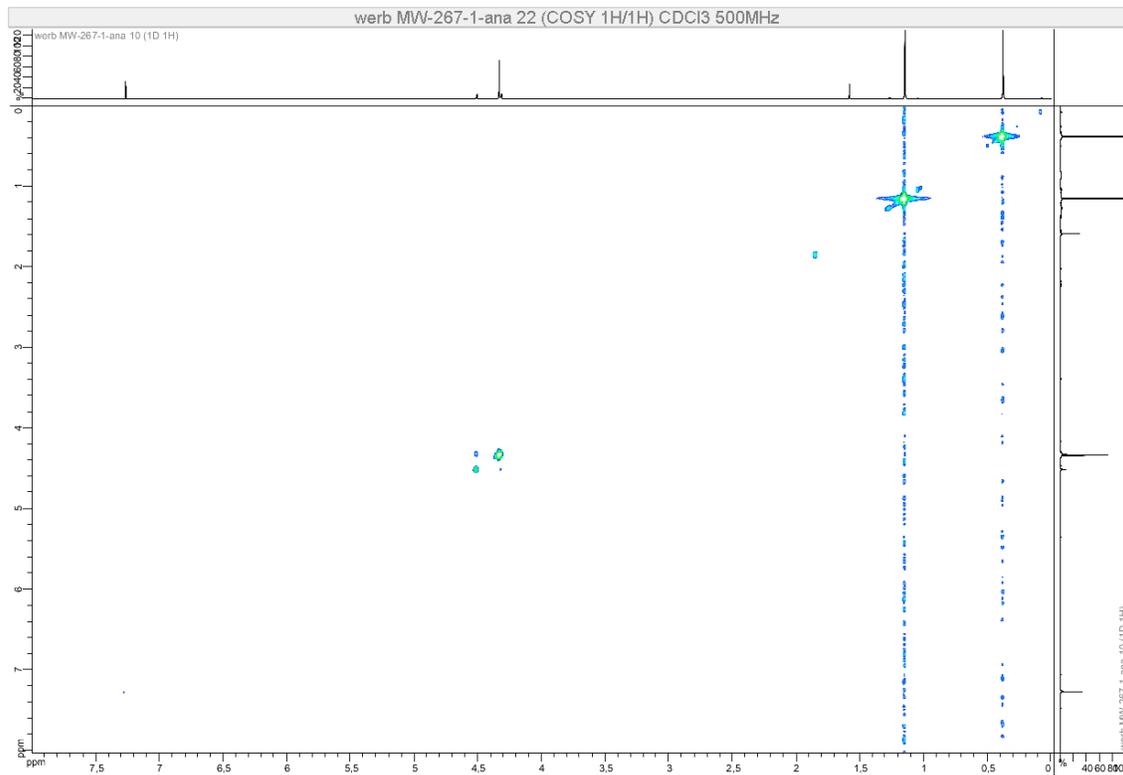
HMBC (500 MHz, CDCl₃)



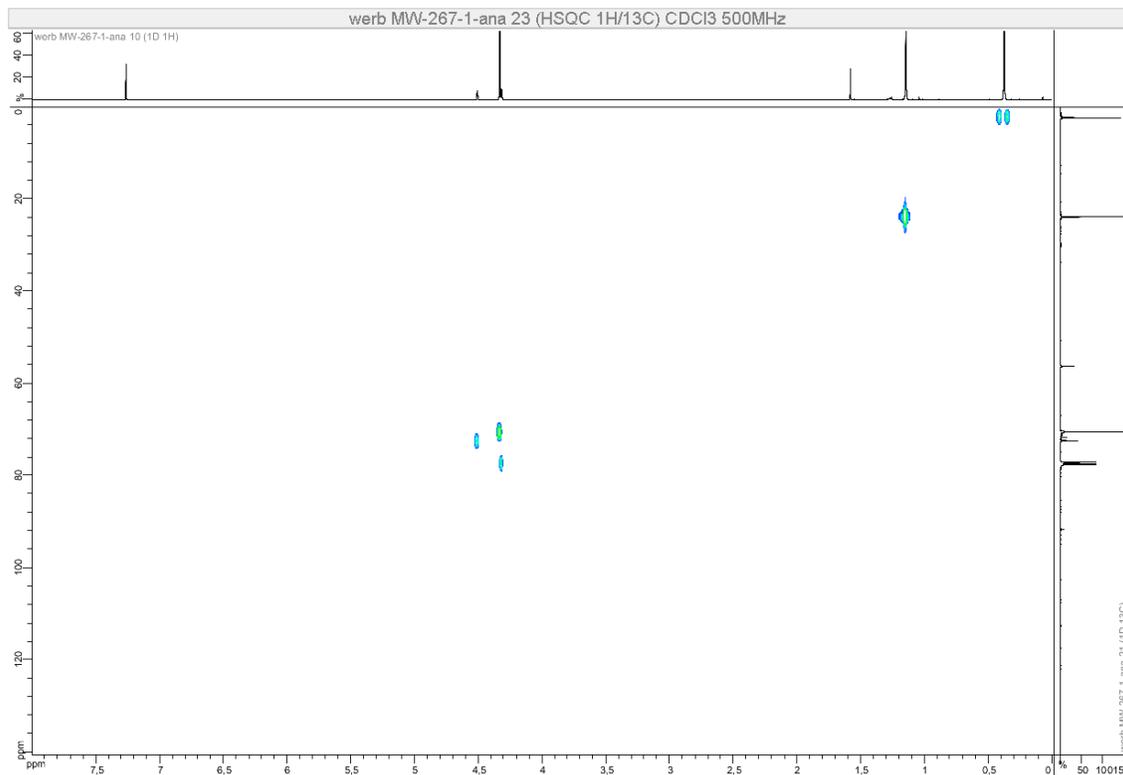
NOESY (500 MHz, CDCl₃)



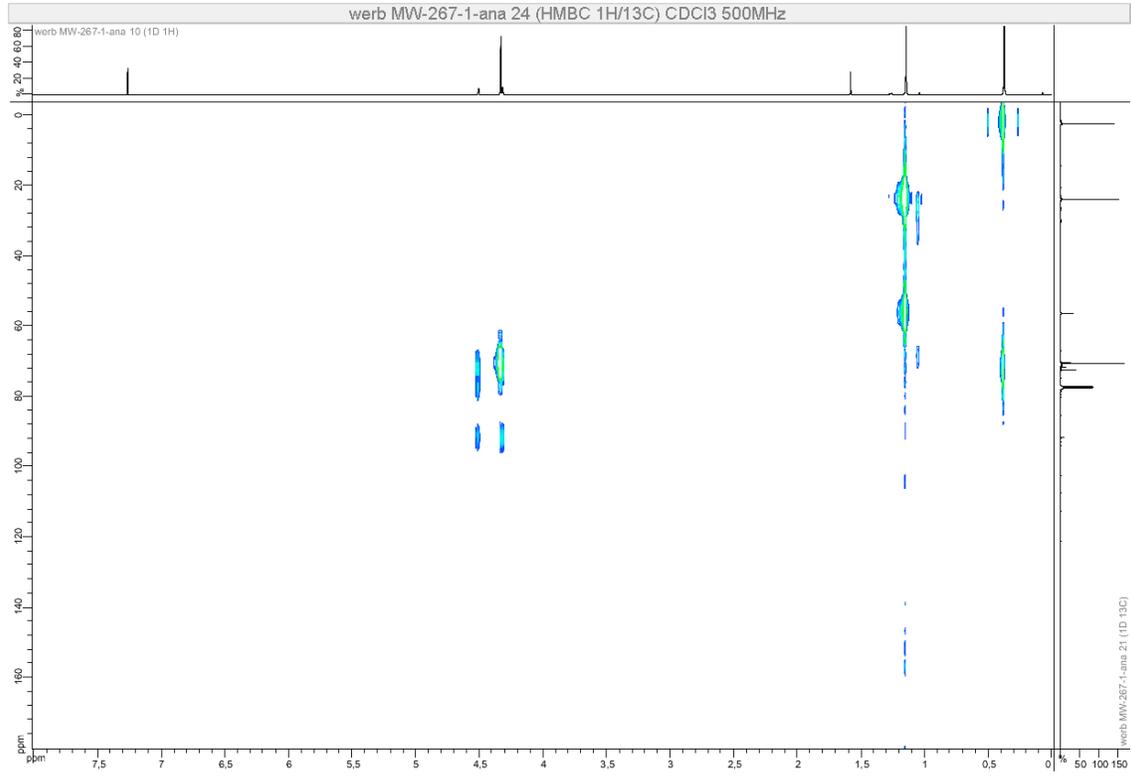
COSY (500 MHz, CDCl₃)



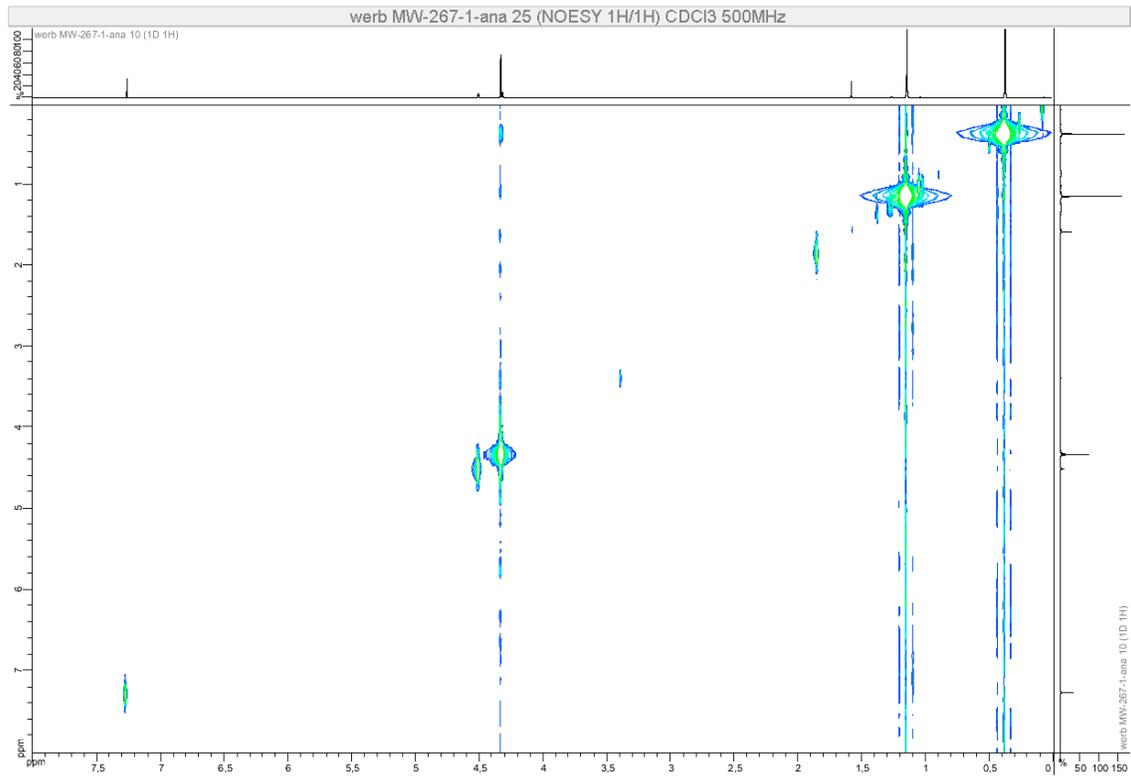
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

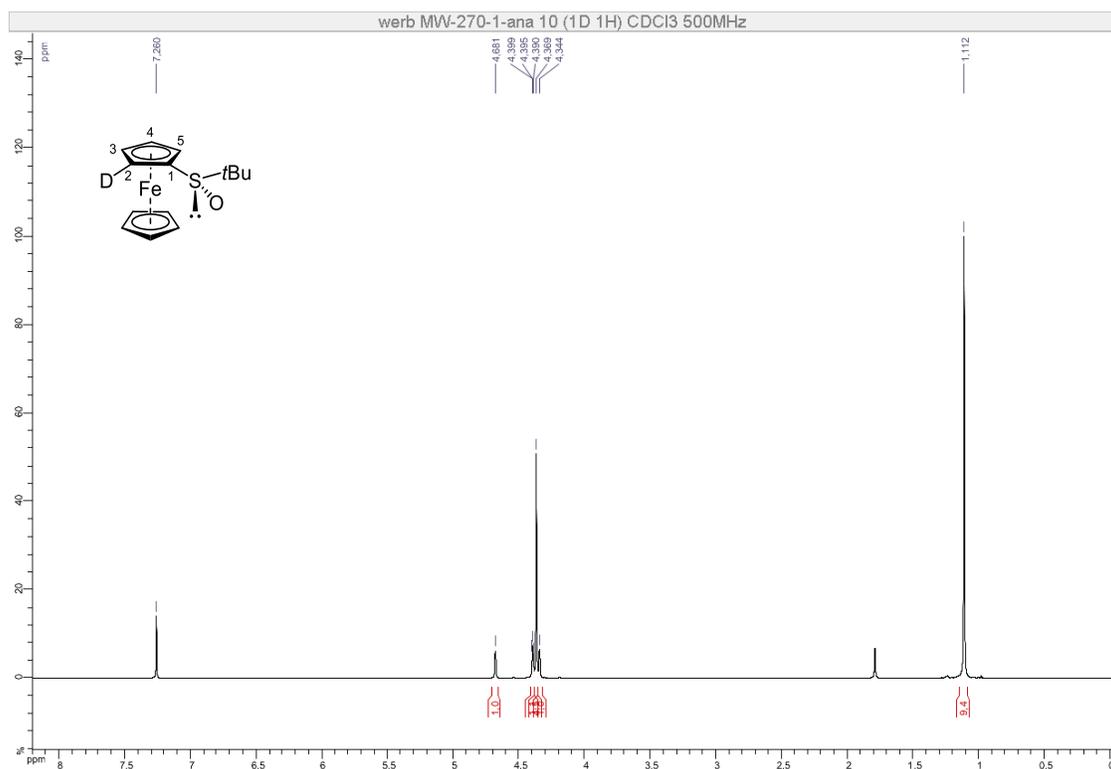


NOESY (500 MHz, CDCl₃)

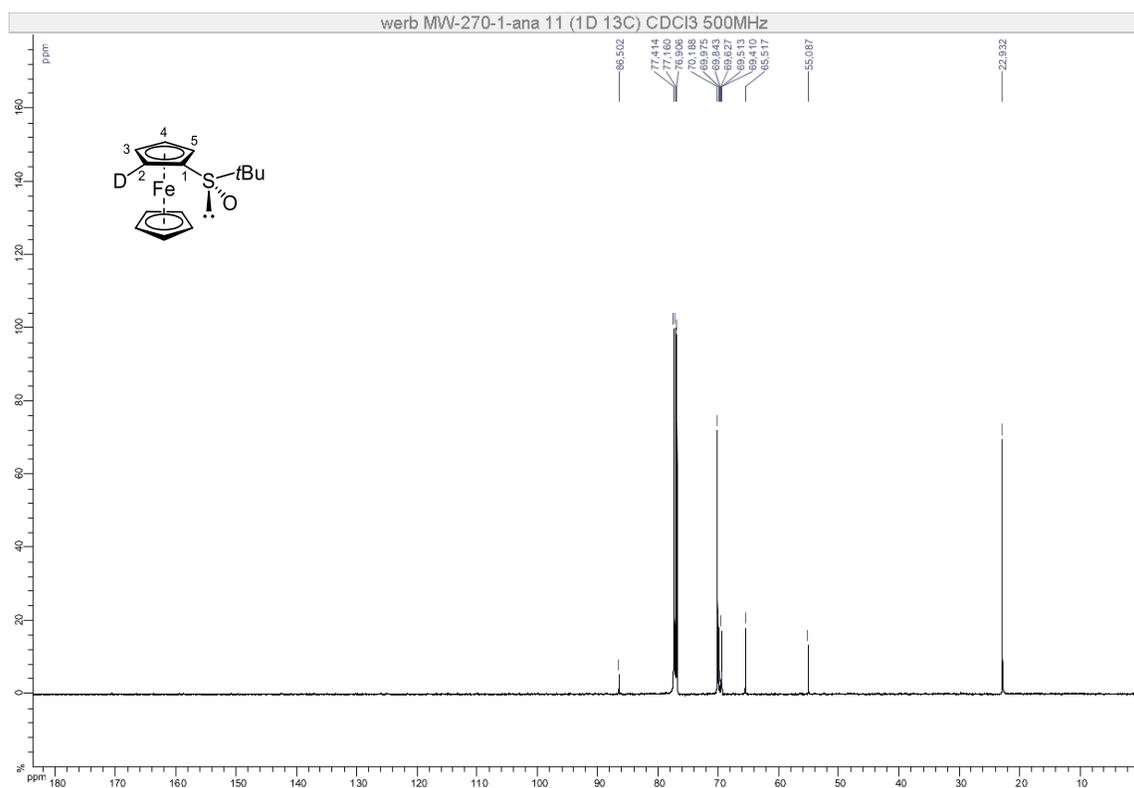


(*S,R*_P)-*S*-tert-Butyl-2-deuterioferrocenesulfoxide (*S,R*_P-1c)

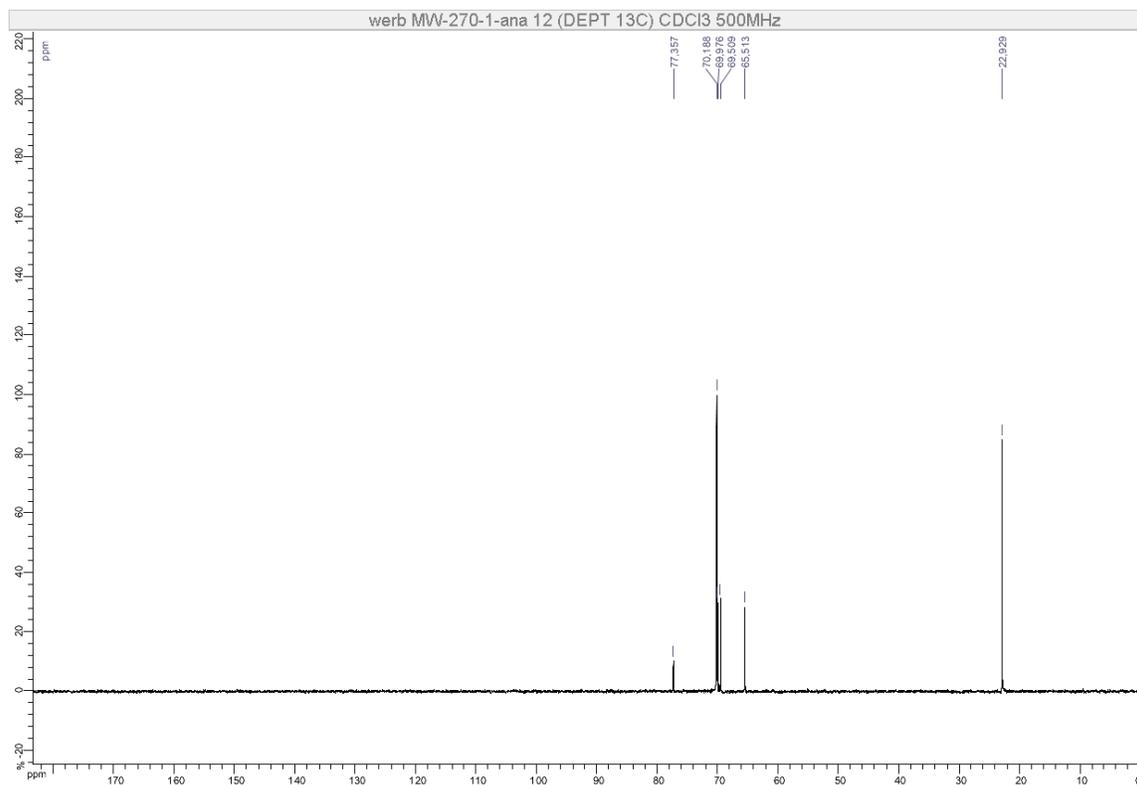
¹H NMR (500 MHz, CDCl₃)



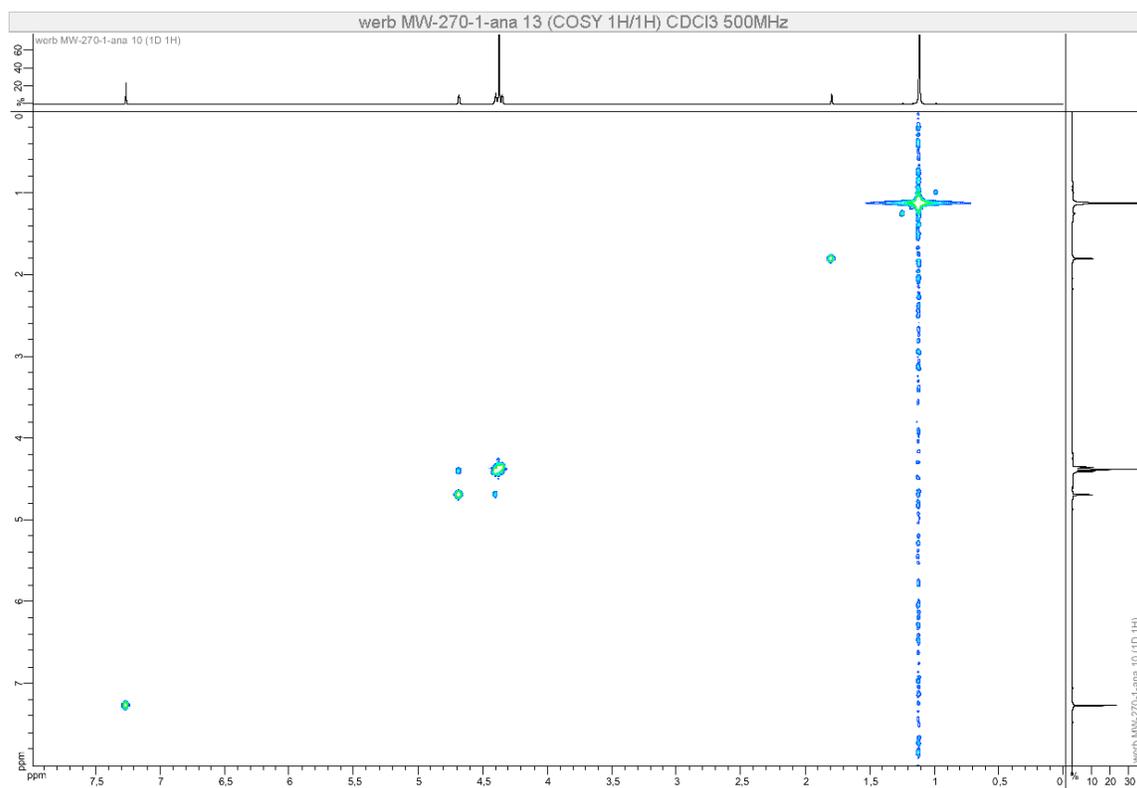
¹³C NMR (126 MHz, CDCl₃)



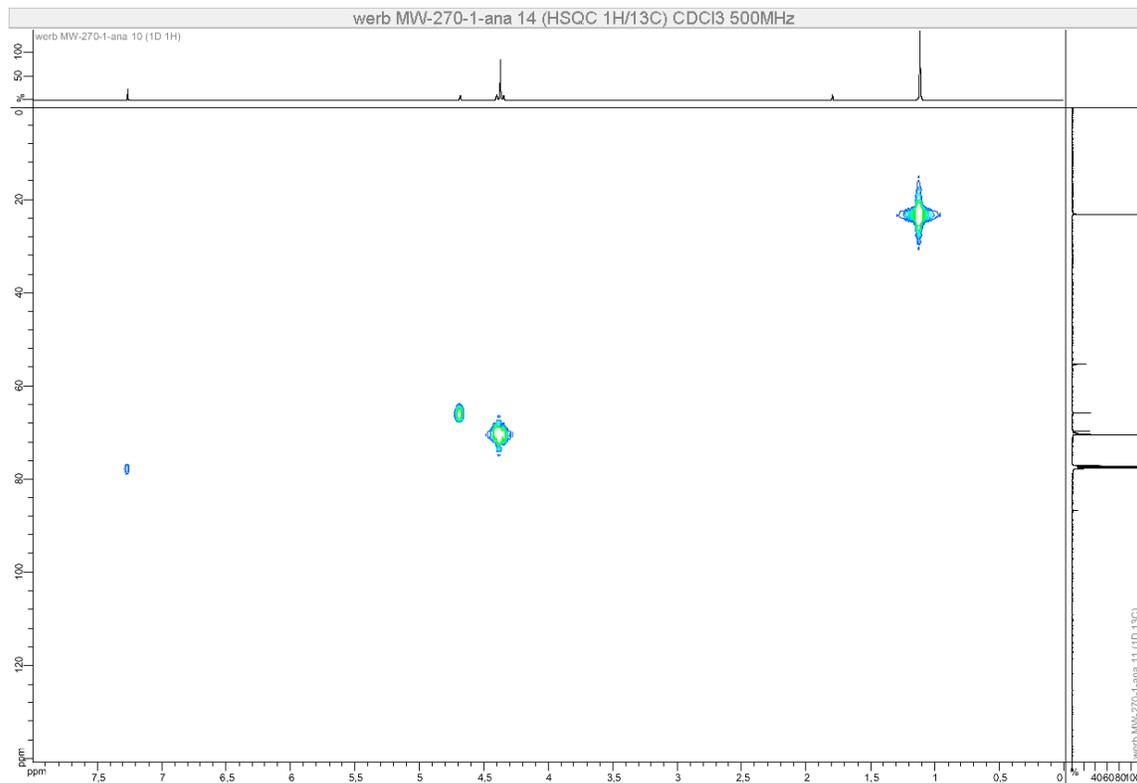
DEPT 135 (126 MHz, CDCl₃)



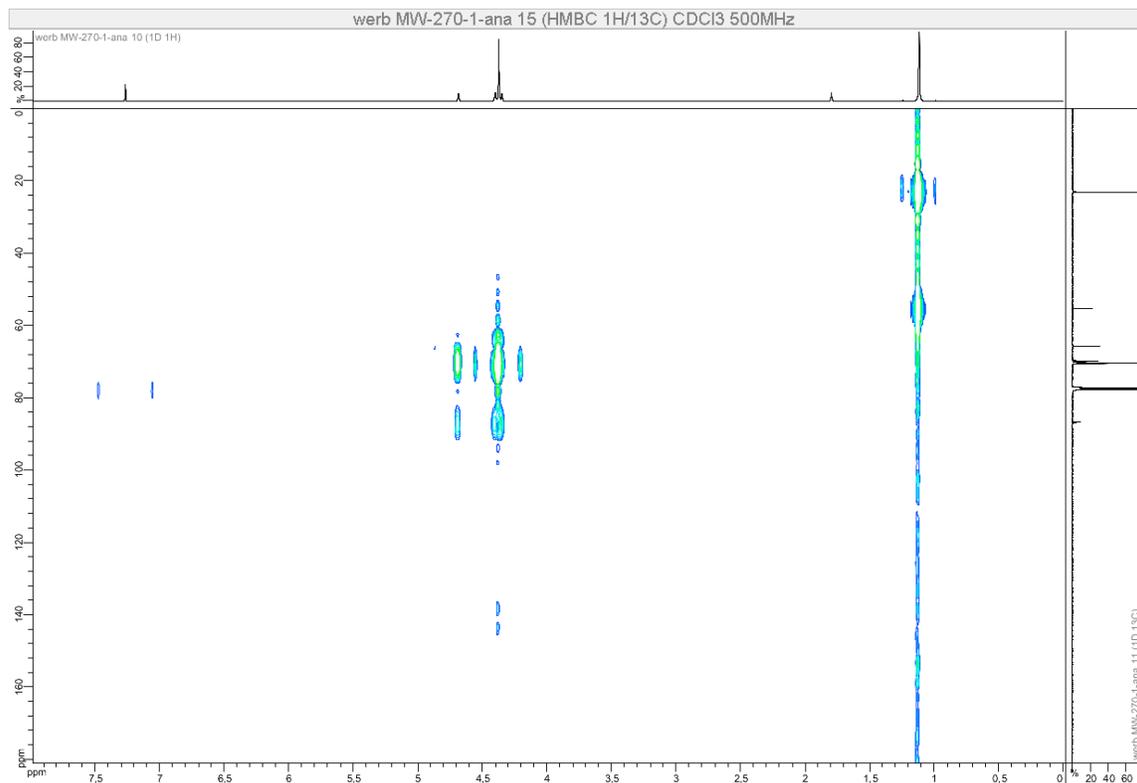
COSY (500 MHz, CDCl₃)



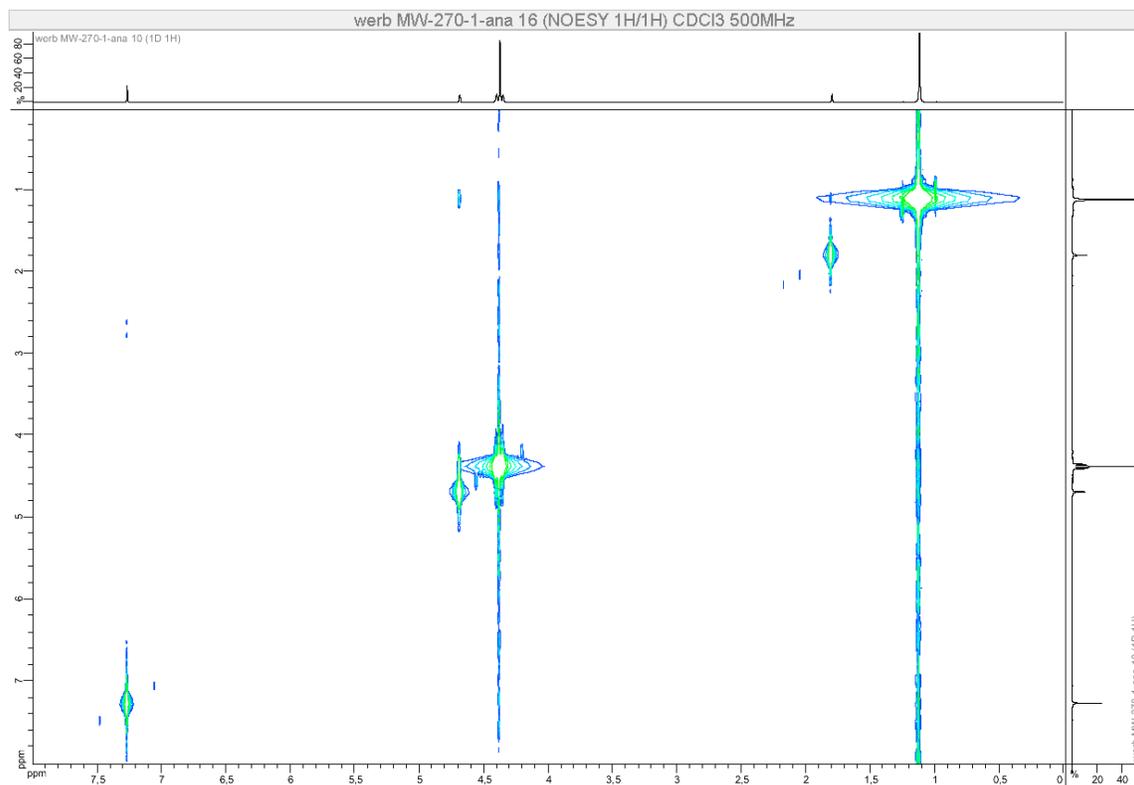
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

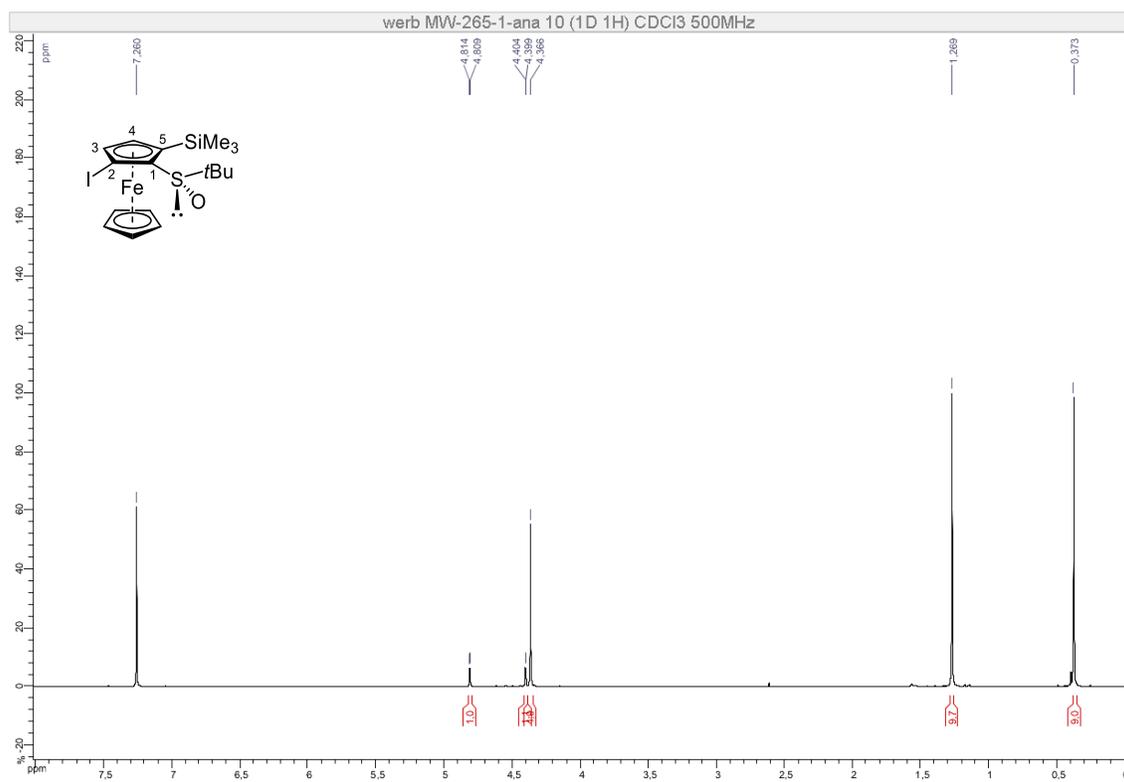


NOESY (500 MHz, CDCl₃)

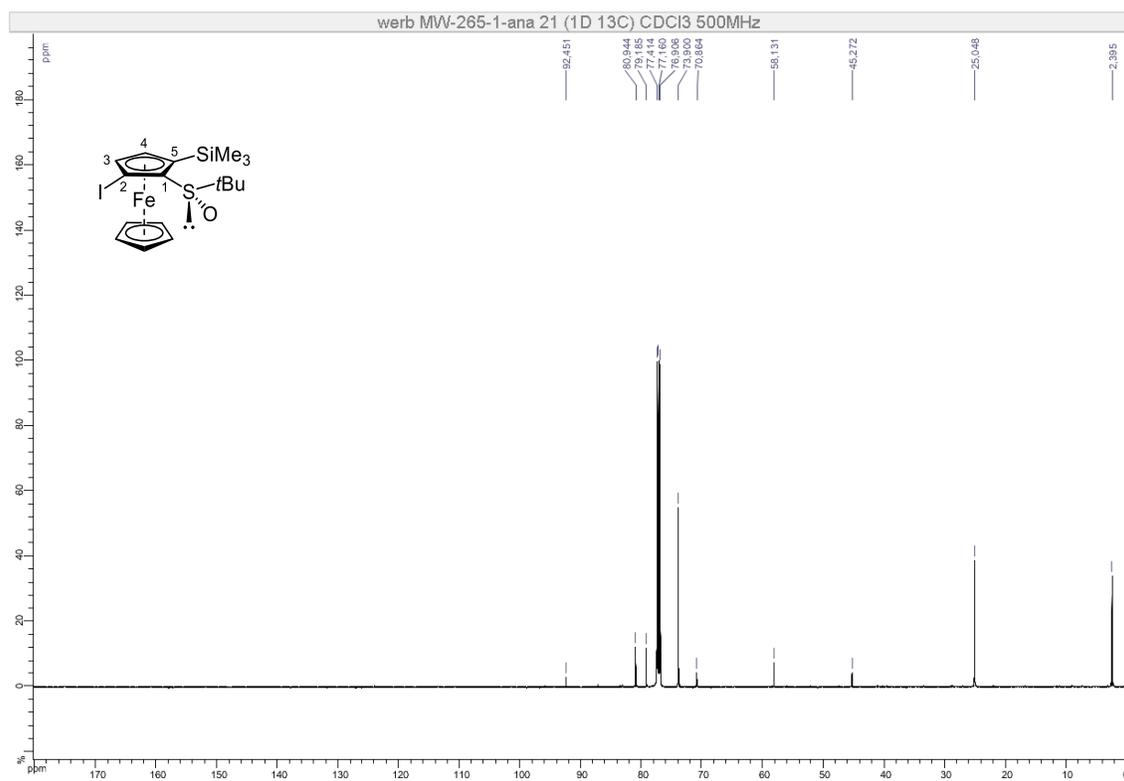


(*S,S*)-*S*-tert-Butyl-2-iodo-5-(trimethylsilyl)ferrocenesulfoxide (*S,S*-2ab)

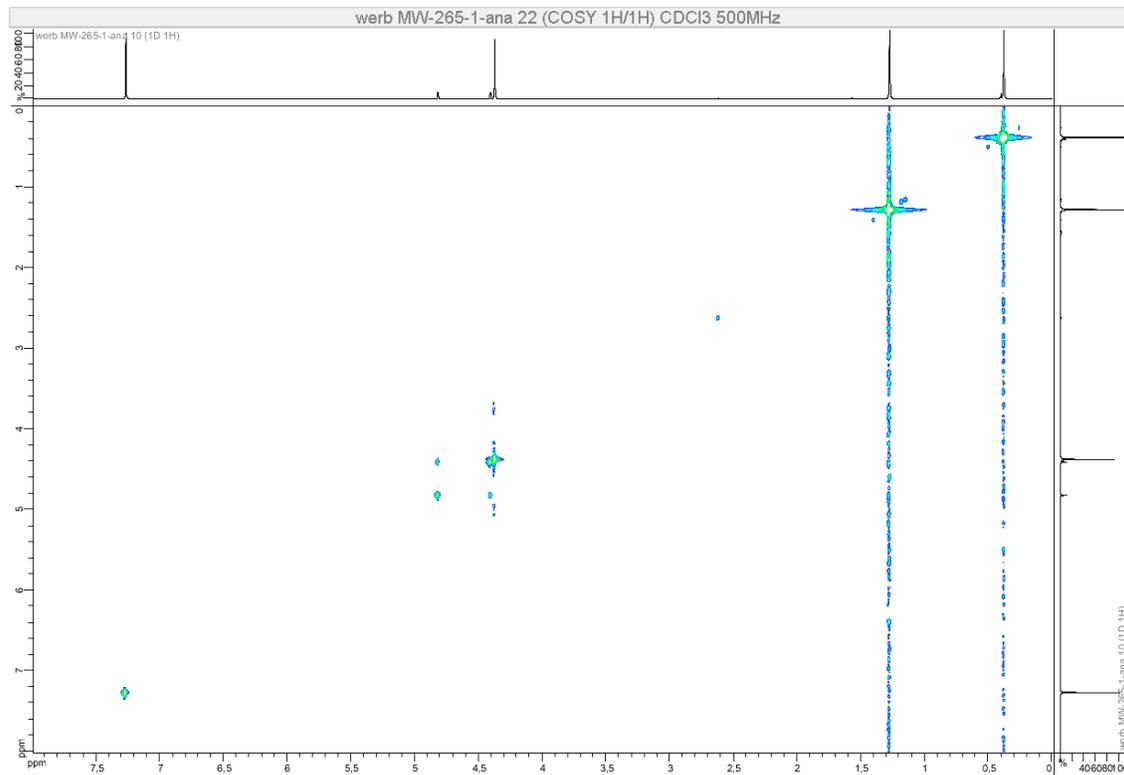
^1H NMR (500 MHz, CDCl_3)



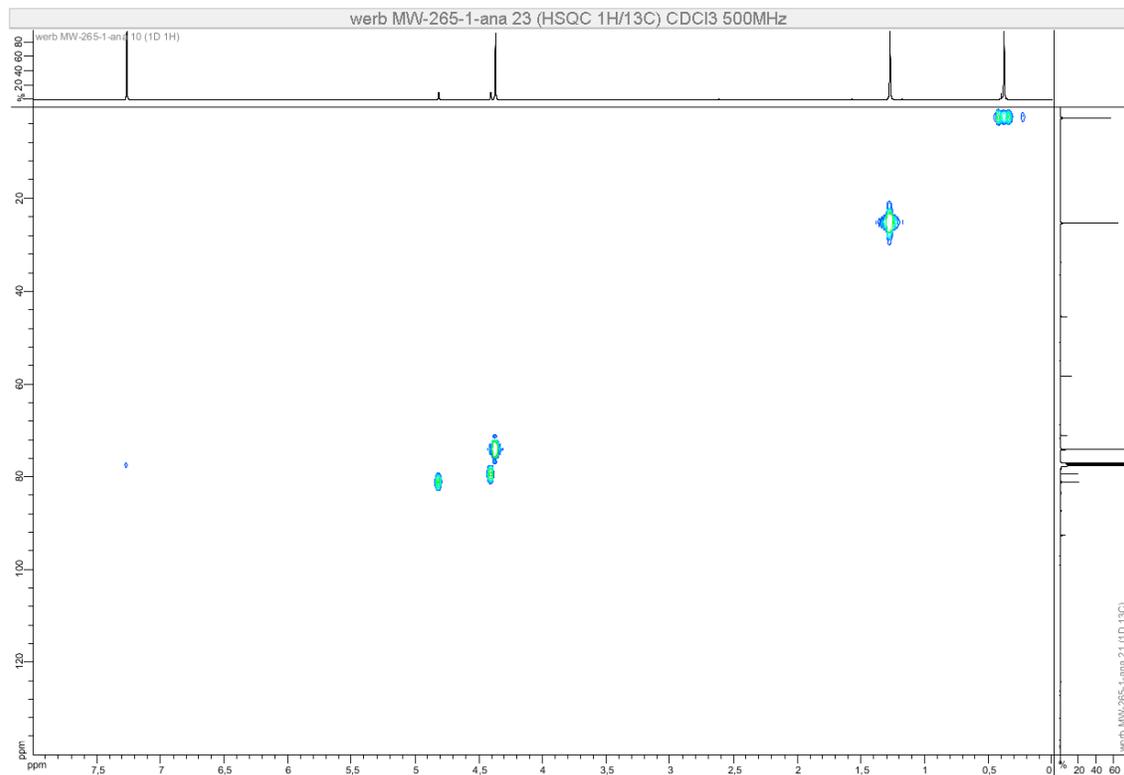
^{13}C NMR (126 MHz, CDCl_3)



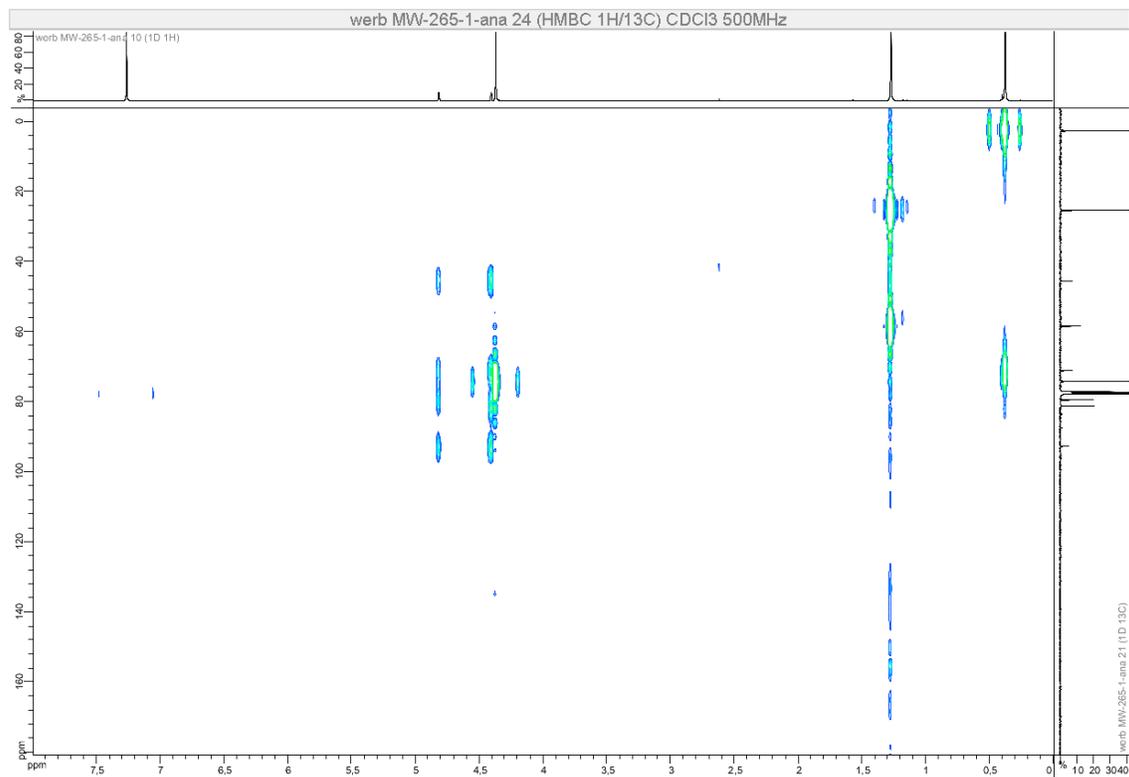
COSY (500 MHz, CDCl₃)



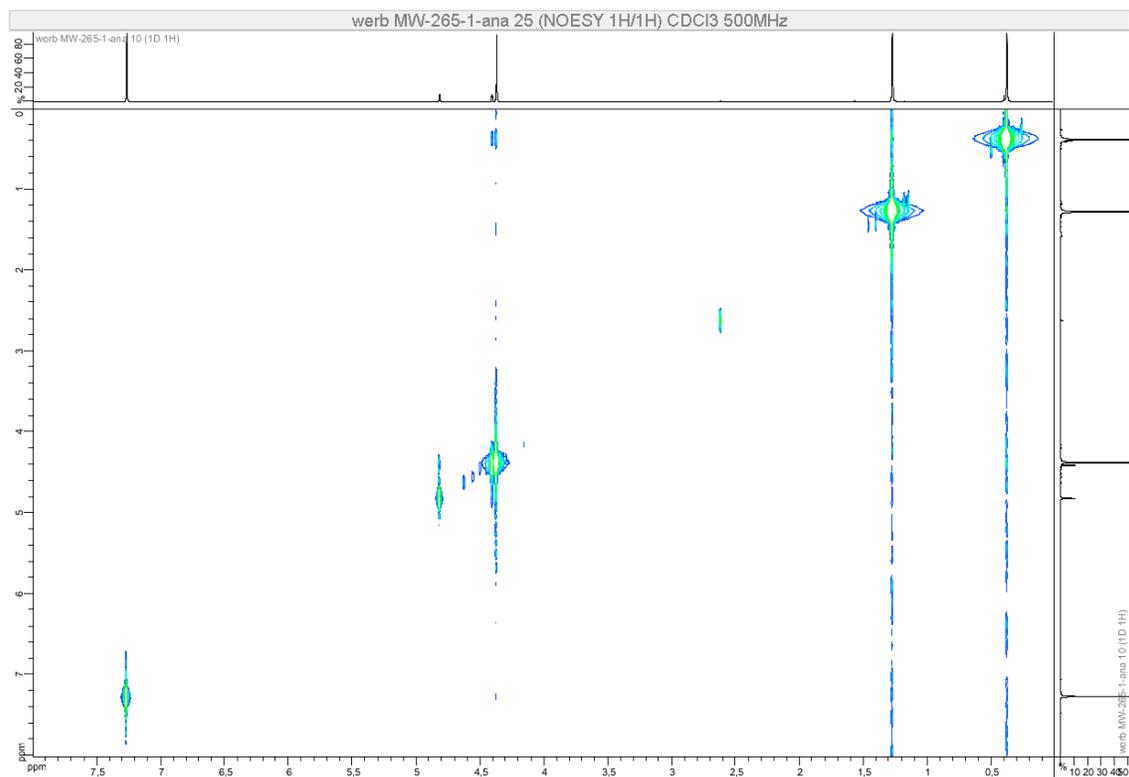
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

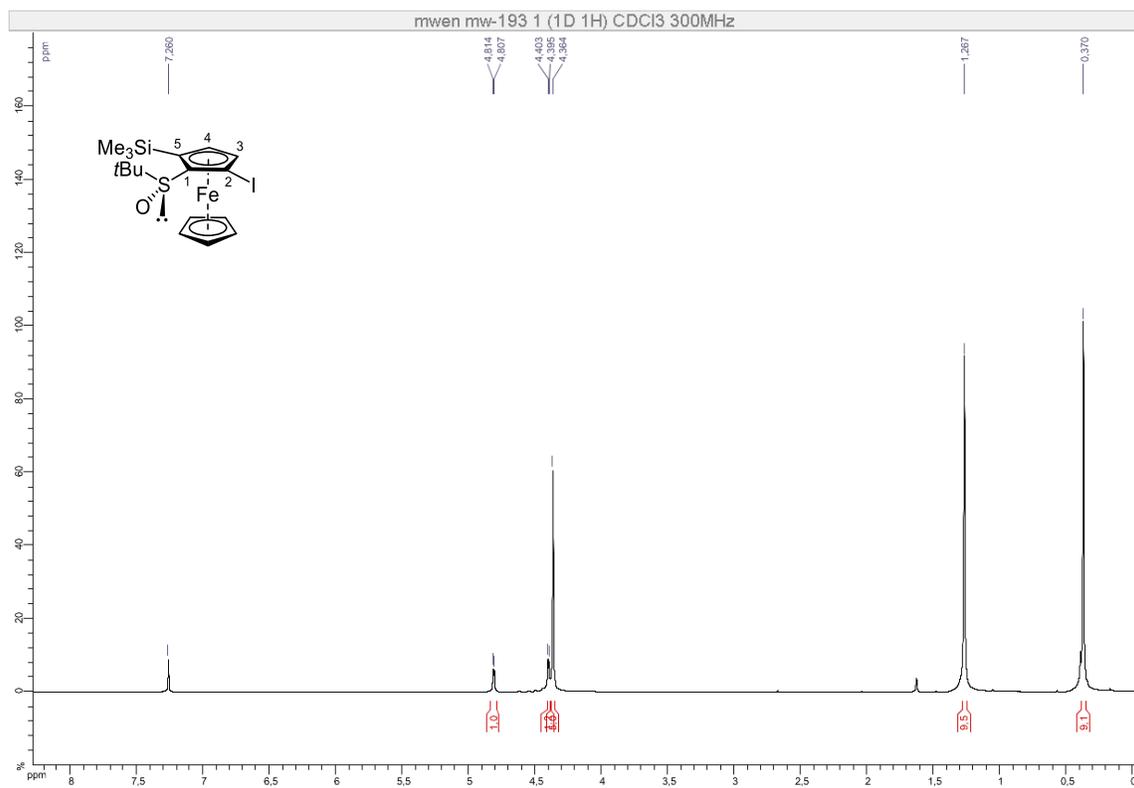


NOESY (500 MHz, CDCl₃)



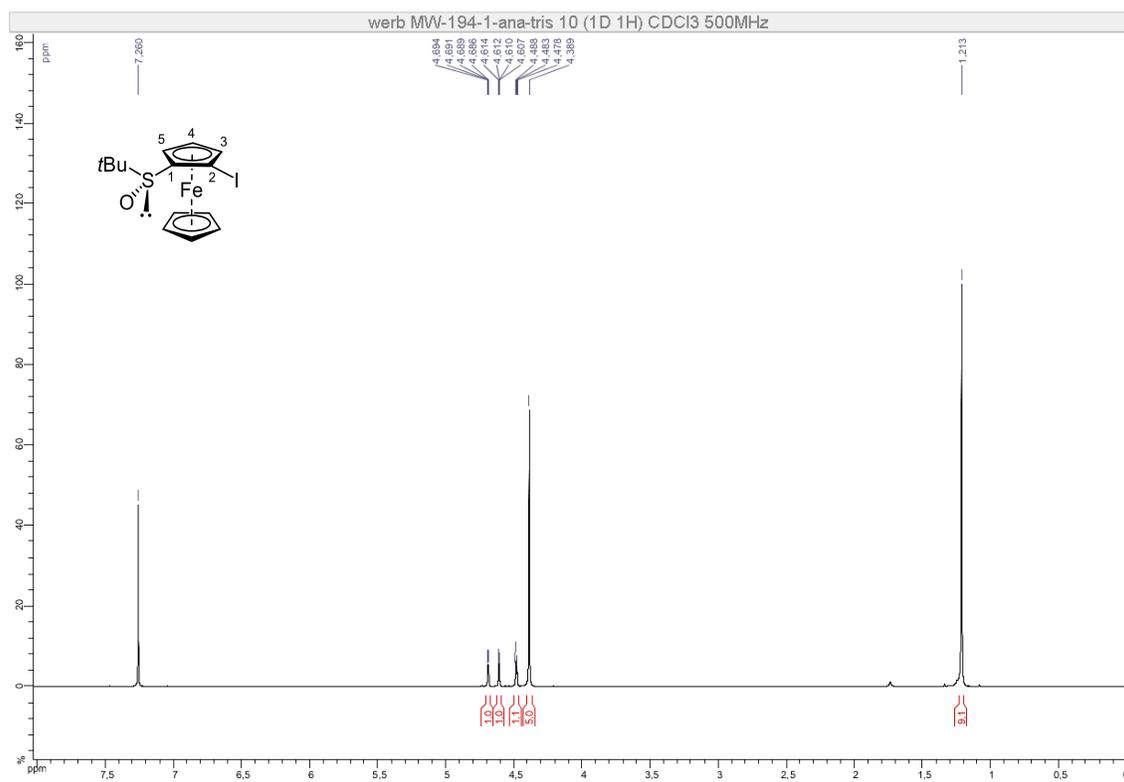
(*R,R*)-*S*-tert-Butyl-2-iodo-5-(trimethylsilyl)ferrocenesulfoxide (*R,R*-2ab)

¹H NMR (500 MHz, CDCl₃)

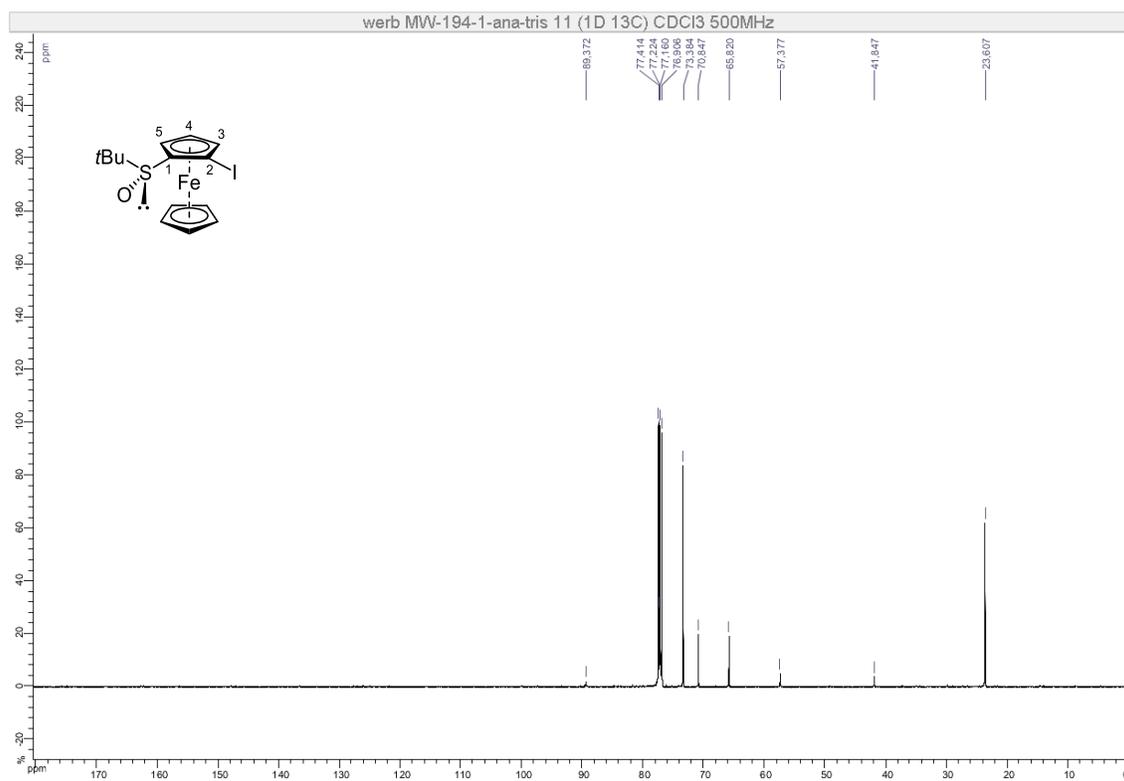


(*R,R*)-*S*-tert-Butyl-2-iodoferrocenesulfoxide (*R,R*-1b)

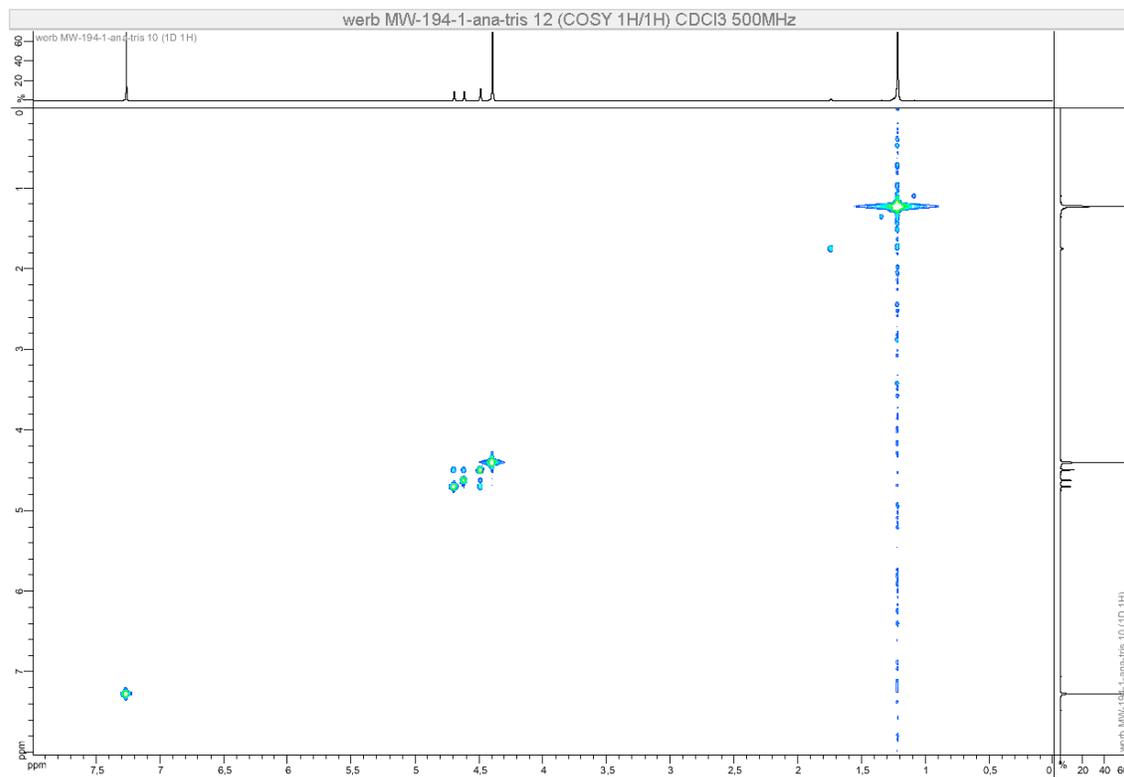
^1H NMR (500 MHz, CDCl_3)



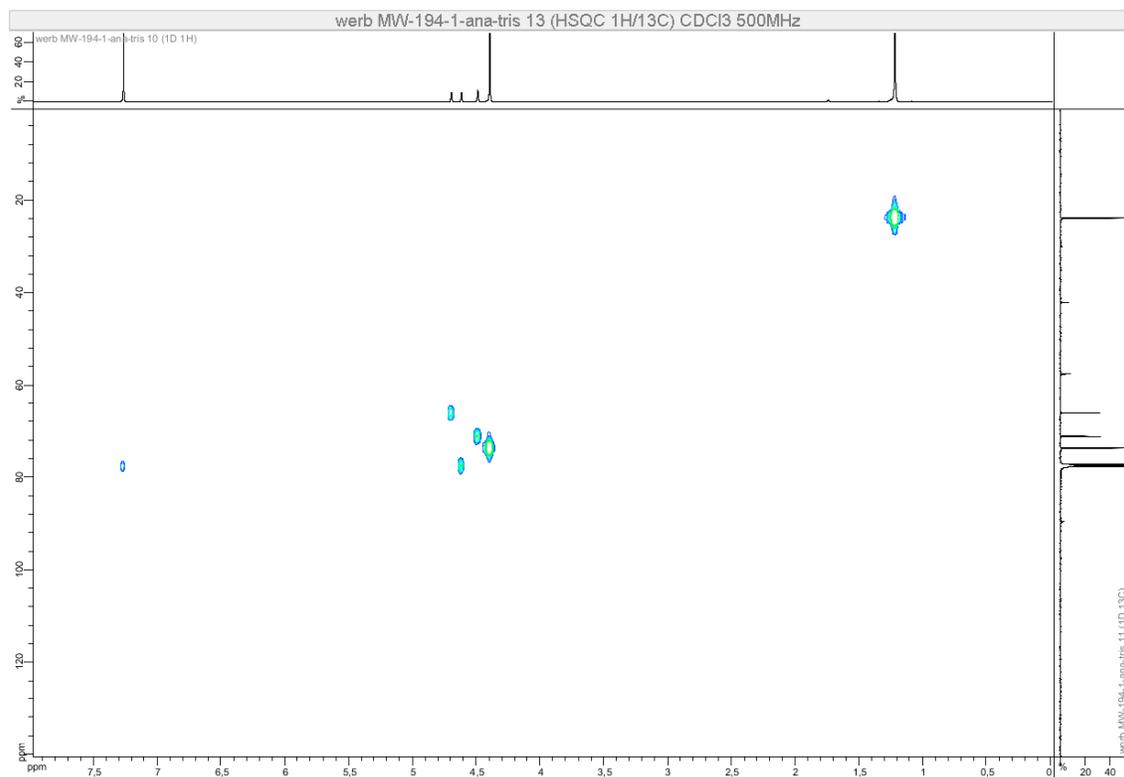
^{13}C NMR (126 MHz, CDCl_3)



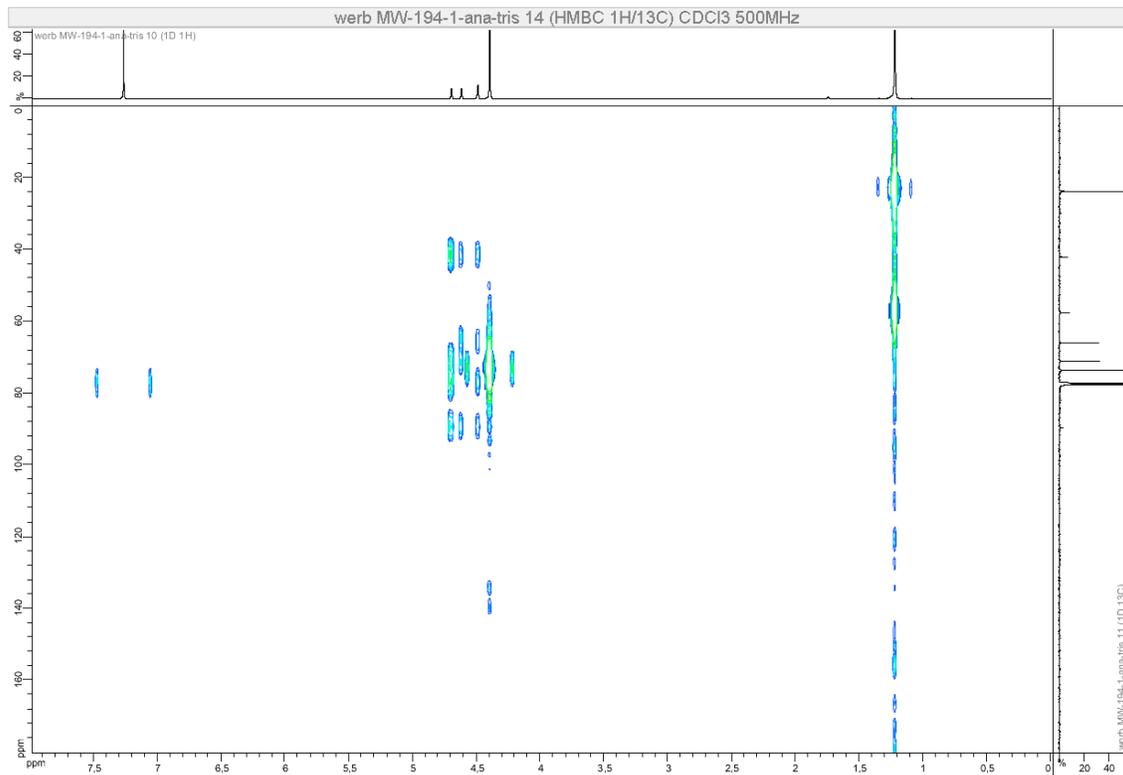
COSY (500 MHz, CDCl₃)



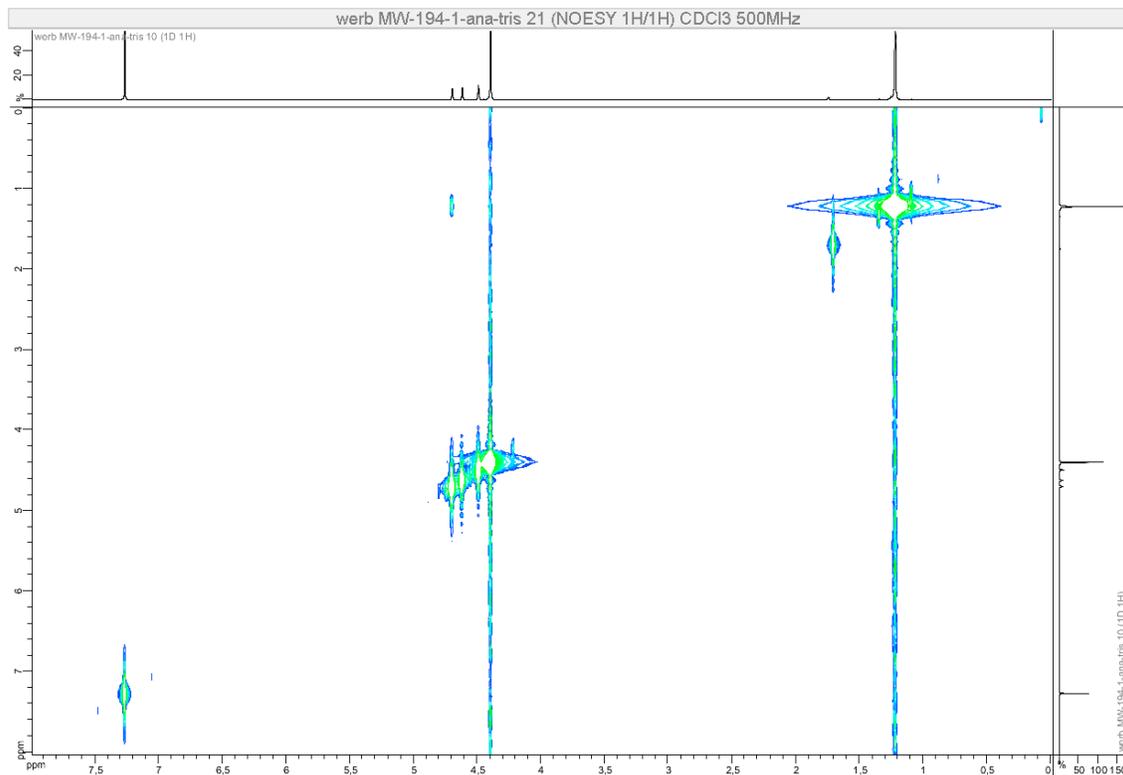
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

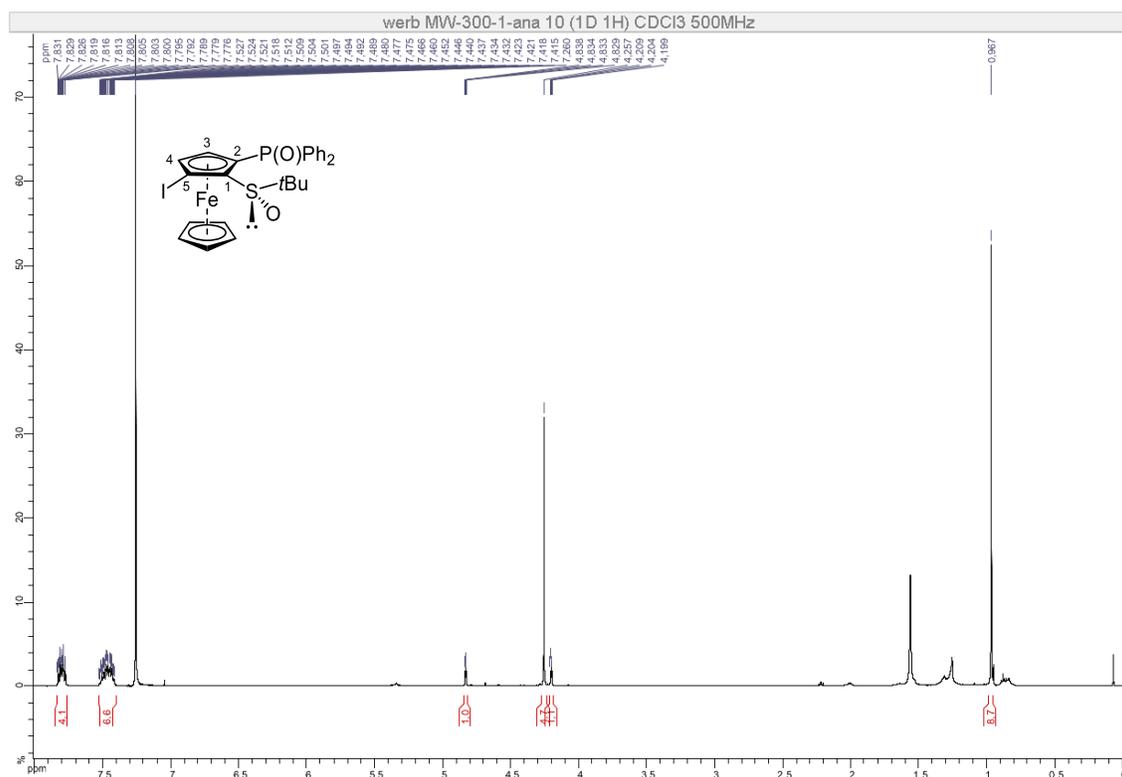


NOESY (500 MHz, CDCl₃)

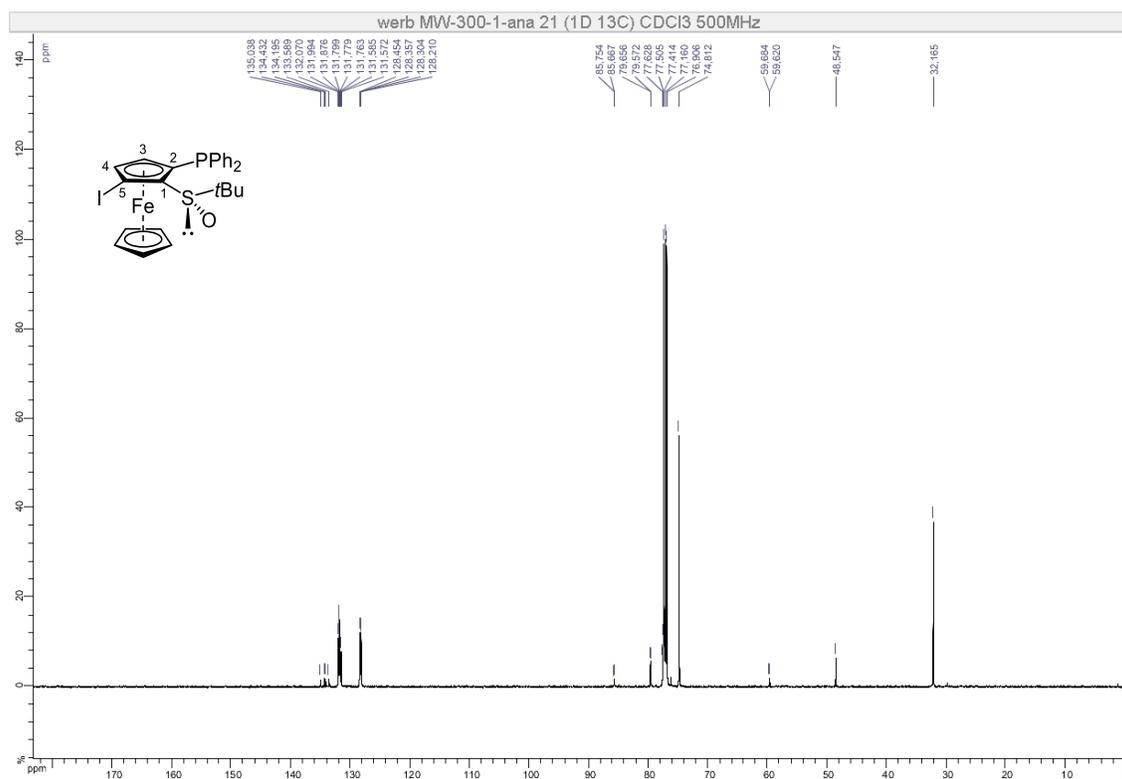


(*S,S*)-*S*-tert-Butyl-2-(diphenylphosphiny)-5-iodoferrocenesulfoxide (*S,S*P-2eb)

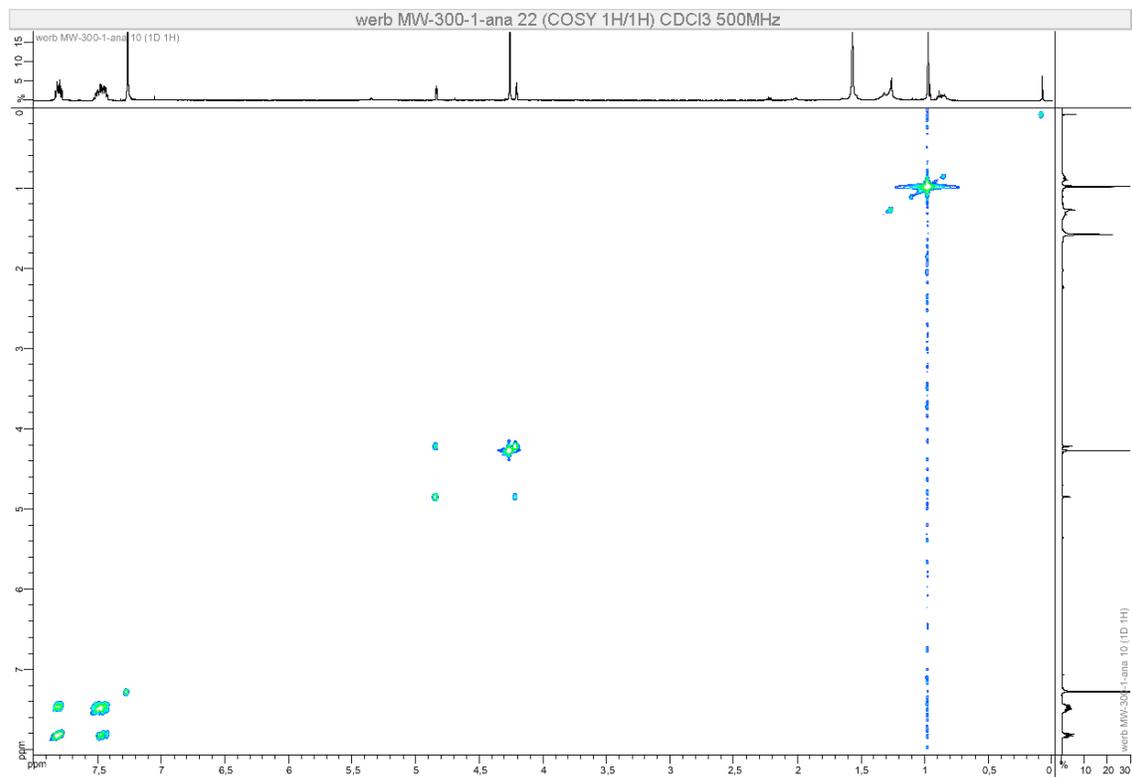
^1H NMR (500 MHz, CDCl_3)



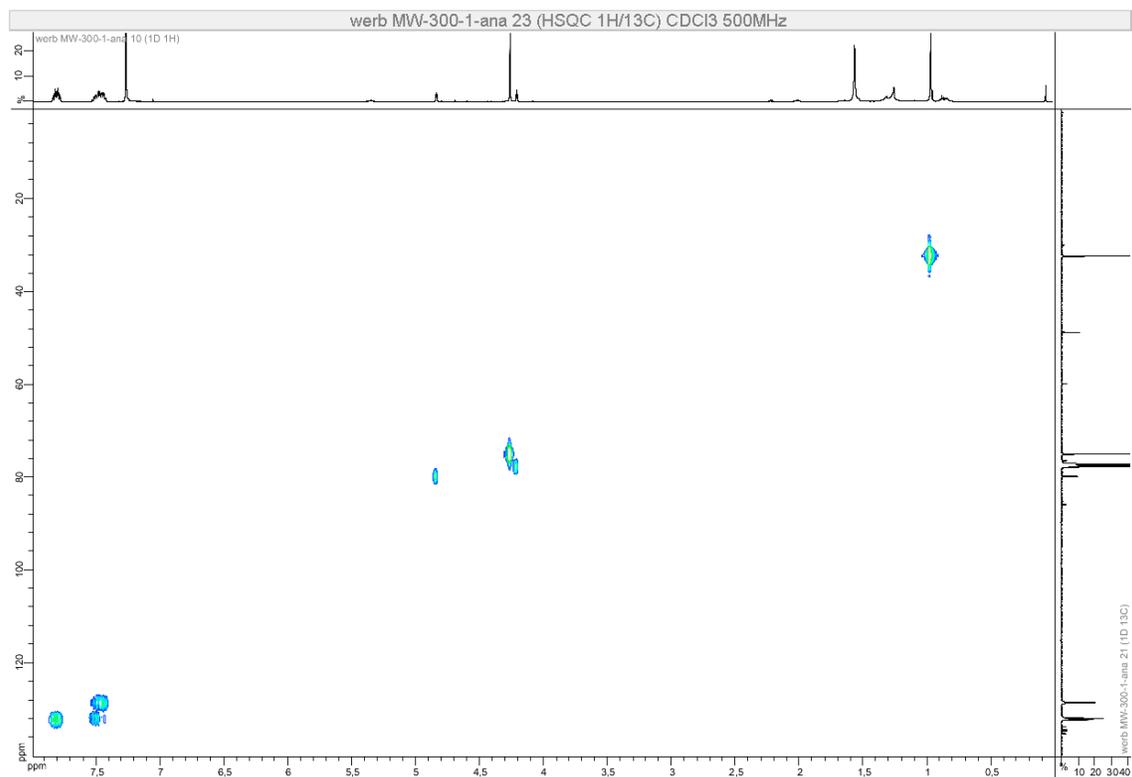
^{13}C NMR (126 MHz, CDCl_3)



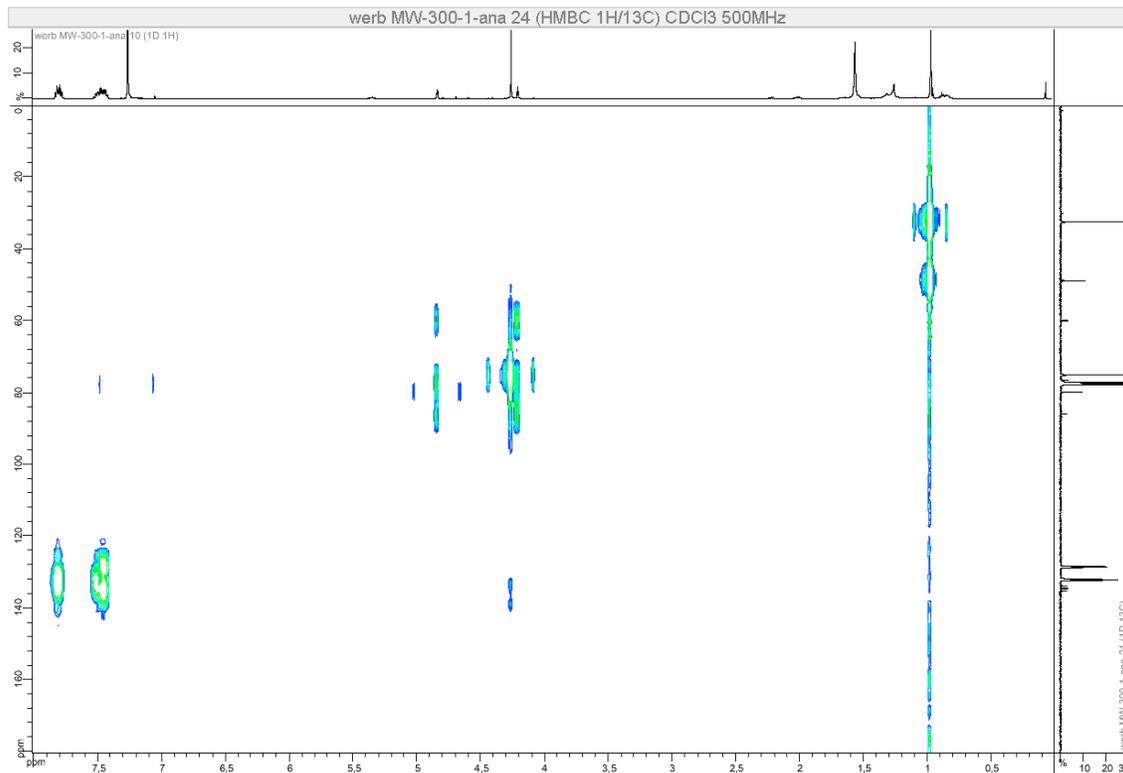
COSY (500 MHz, CDCl₃)



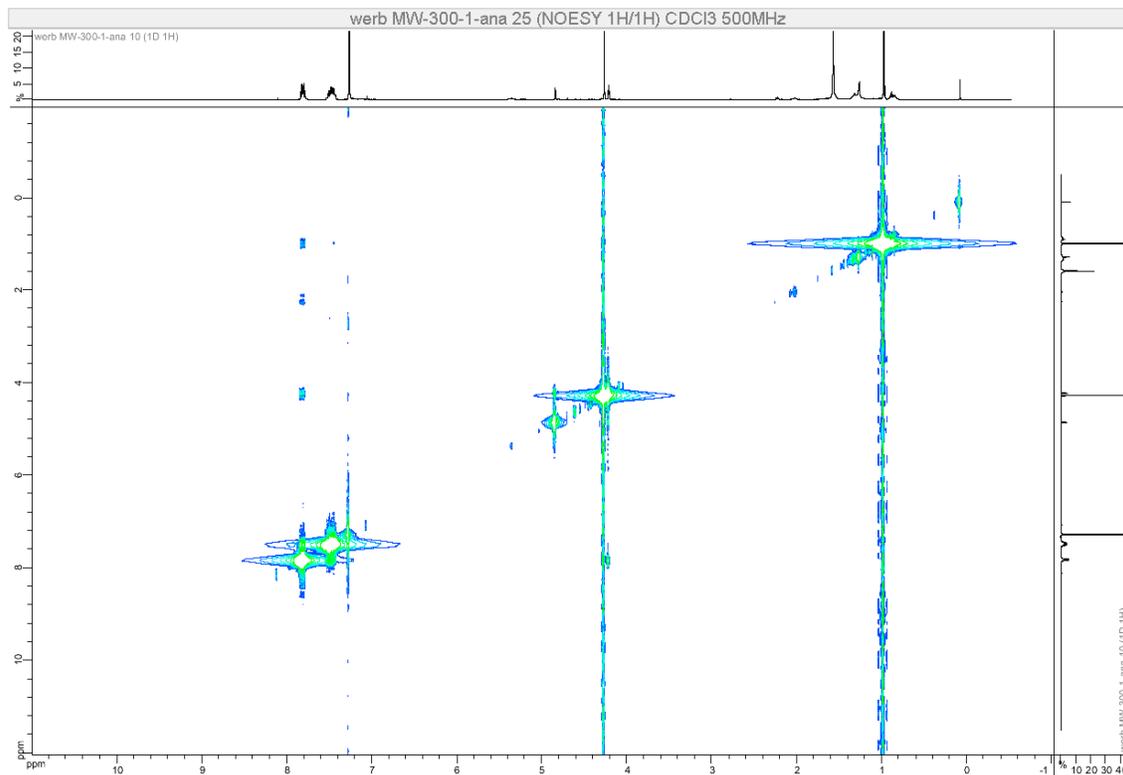
HSQC (500 MHz, CDCl₃)



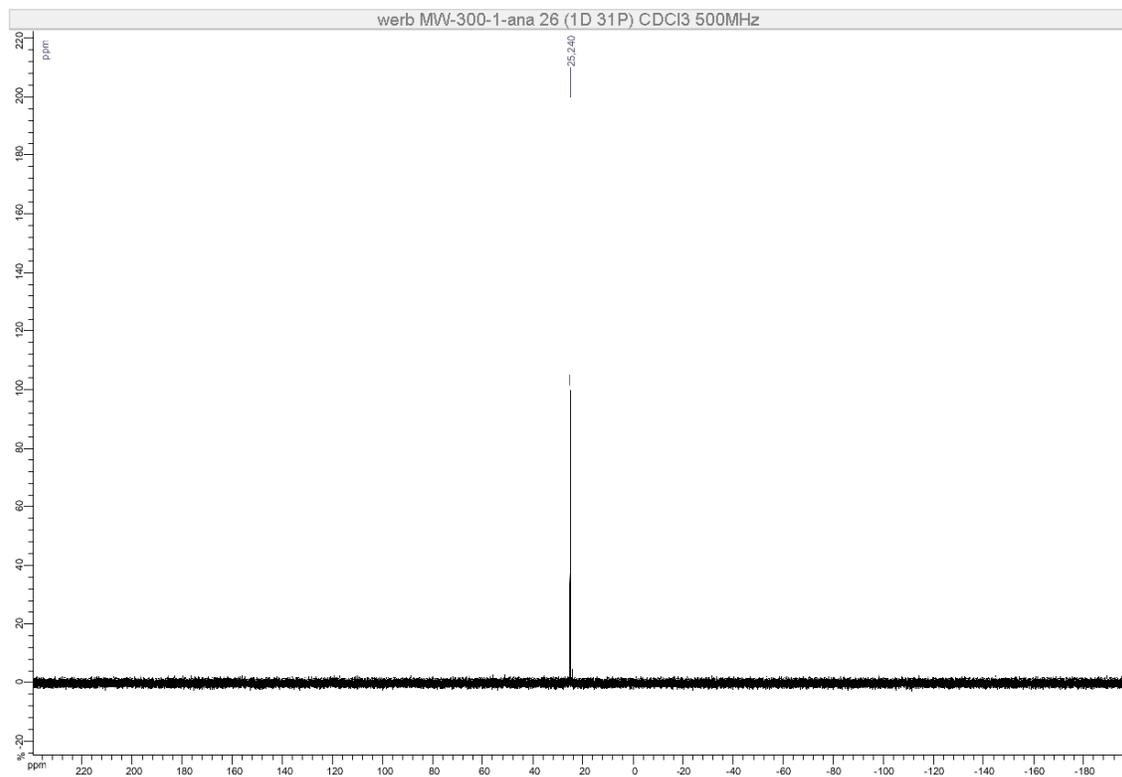
HMBC (500 MHz, CDCl₃)



NOESY (500 MHz, CDCl₃)

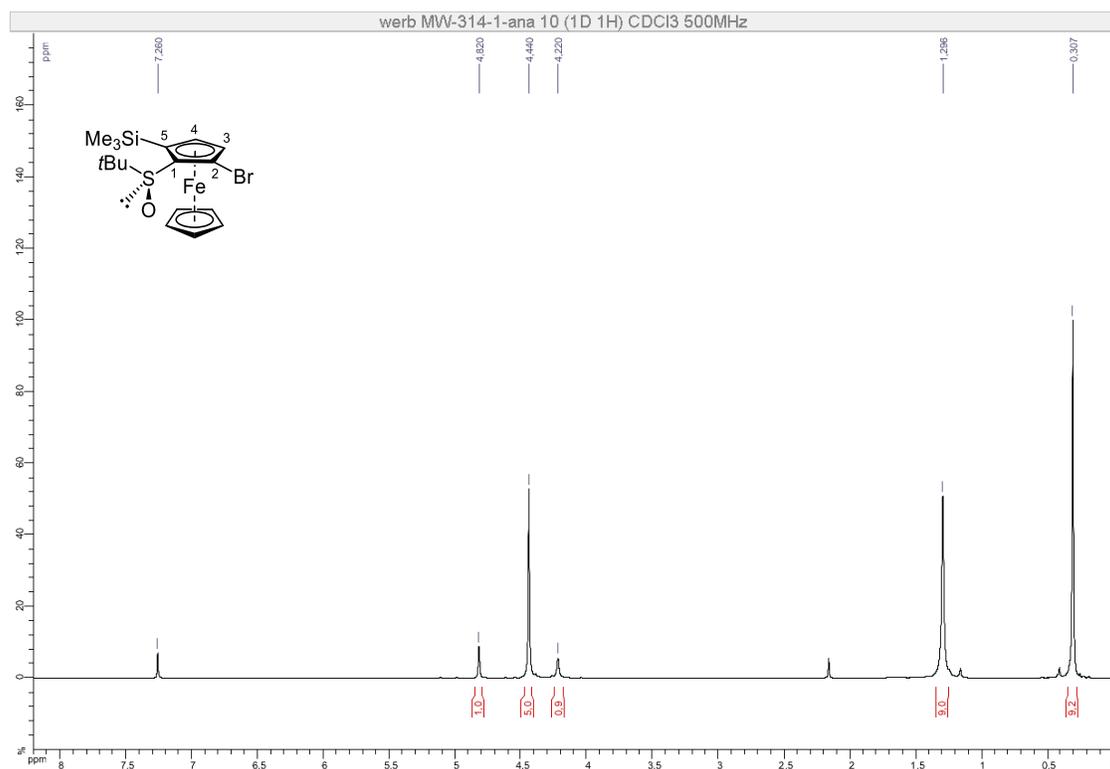


^{31}P NMR (202 MHz, CDCl_3)

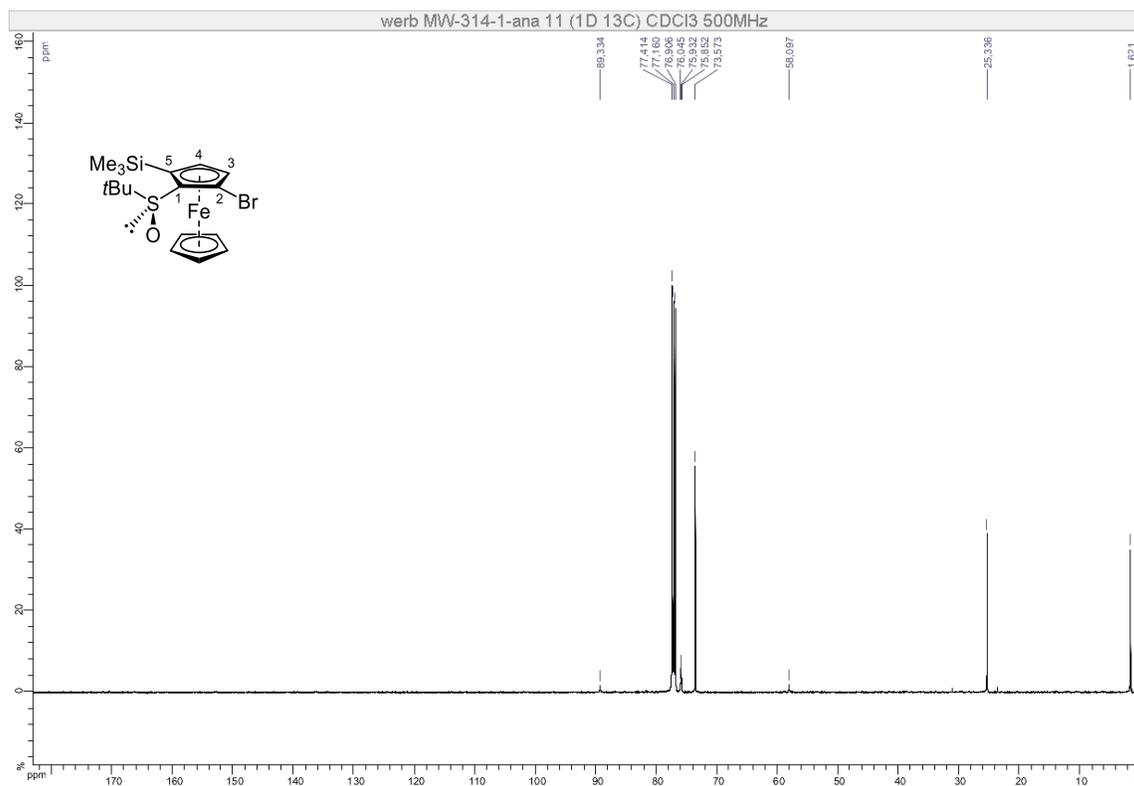


(*S,R*_P)-2-Bromo-*S-tert*-butyl-5-(trimethylsilyl)ferrocenesulfoxide (*S,R*_P-2ja)

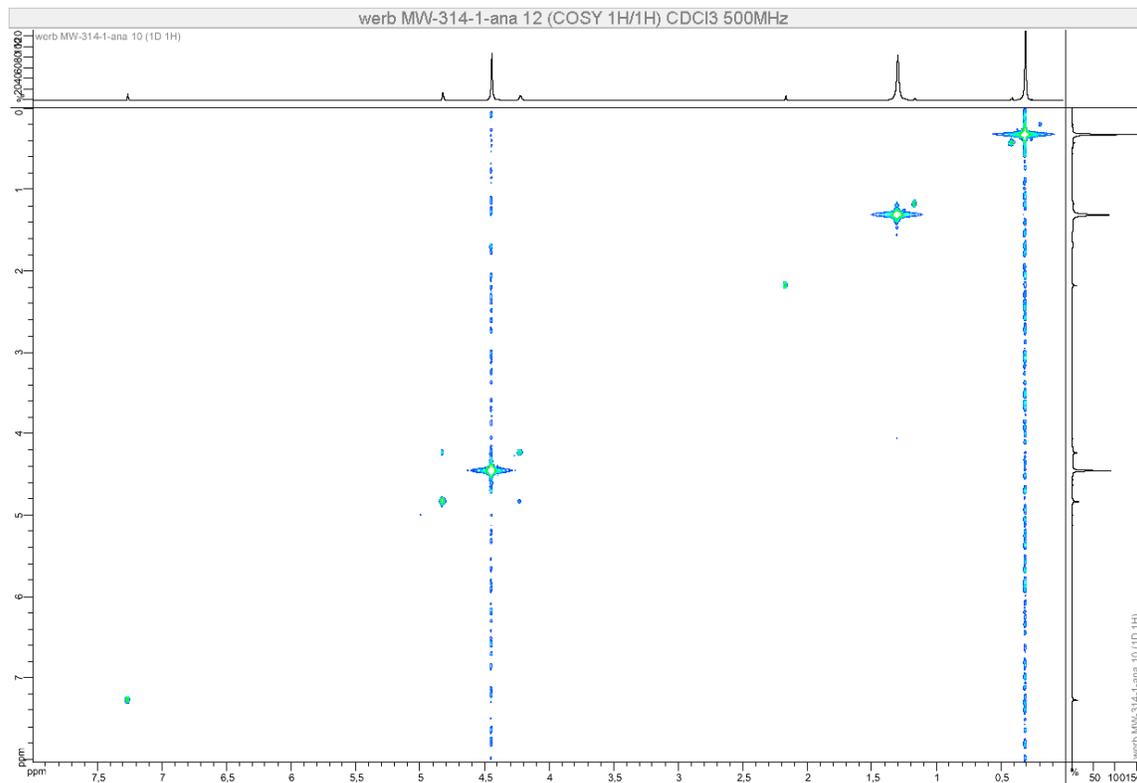
¹H NMR (500 MHz, CDCl₃)



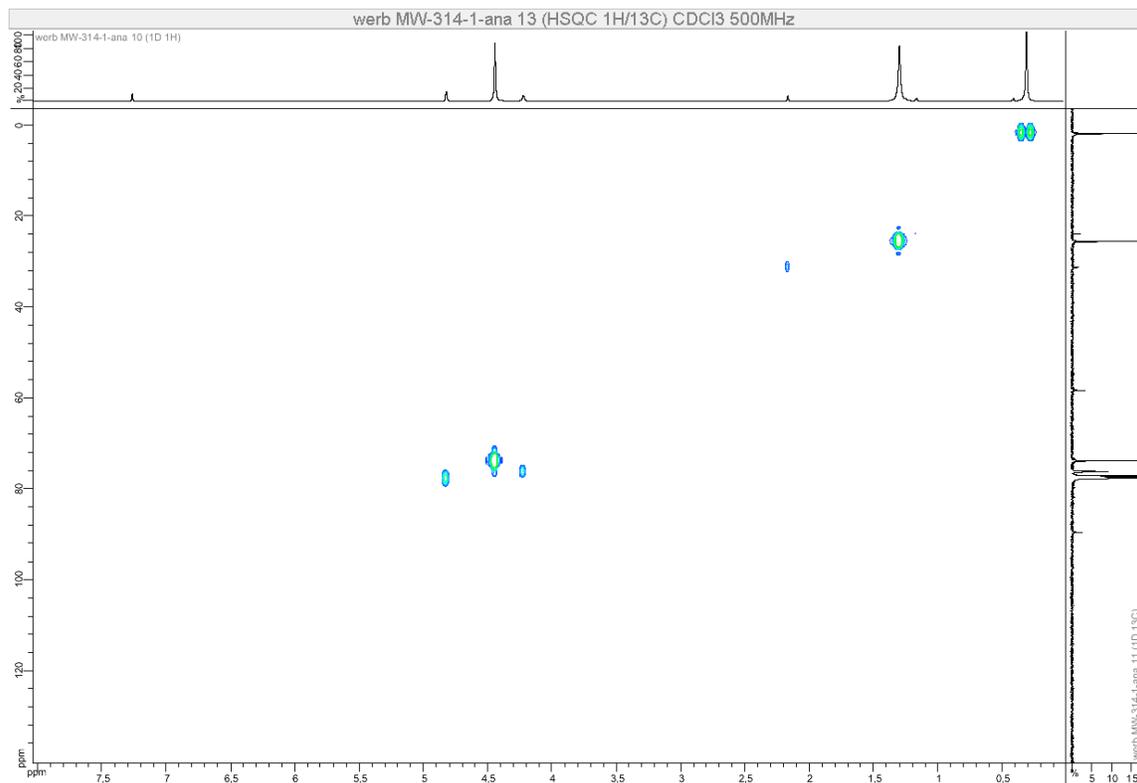
¹³C NMR (126 MHz, CDCl₃)



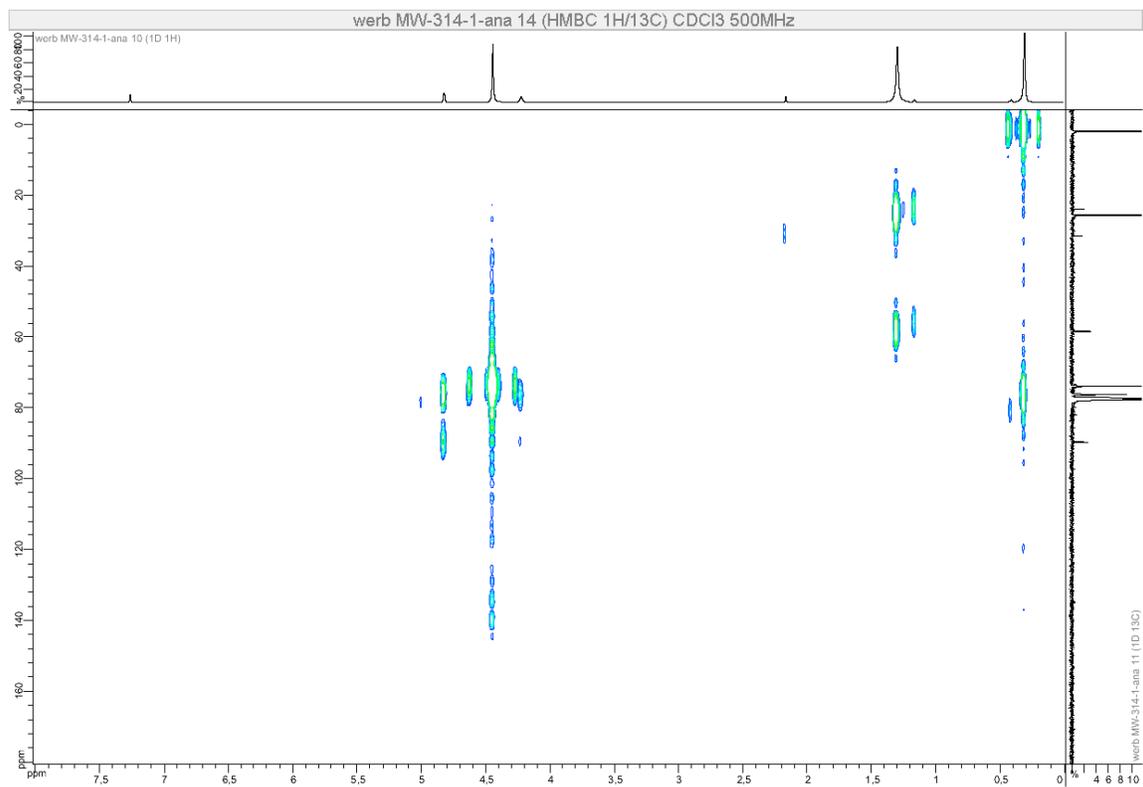
COSY (500 MHz, CDCl₃)



HSQC (500 MHz, CDCl₃)

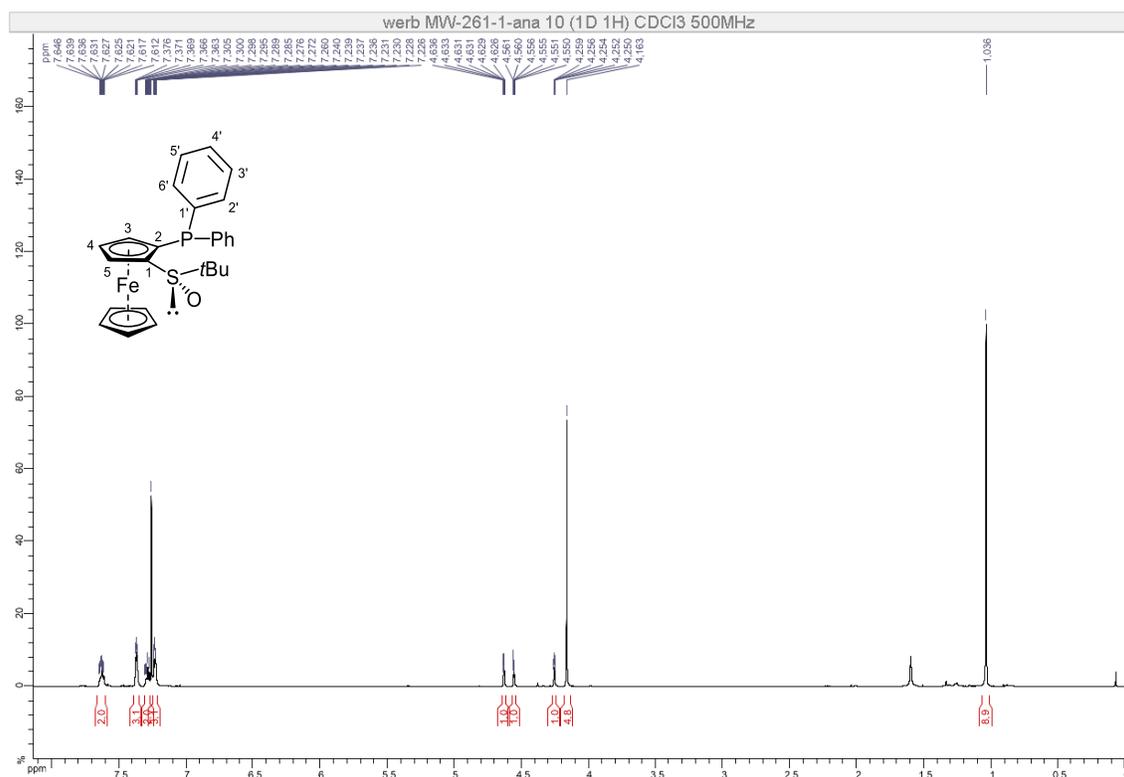


HMBC (500 MHz, CDCl₃)

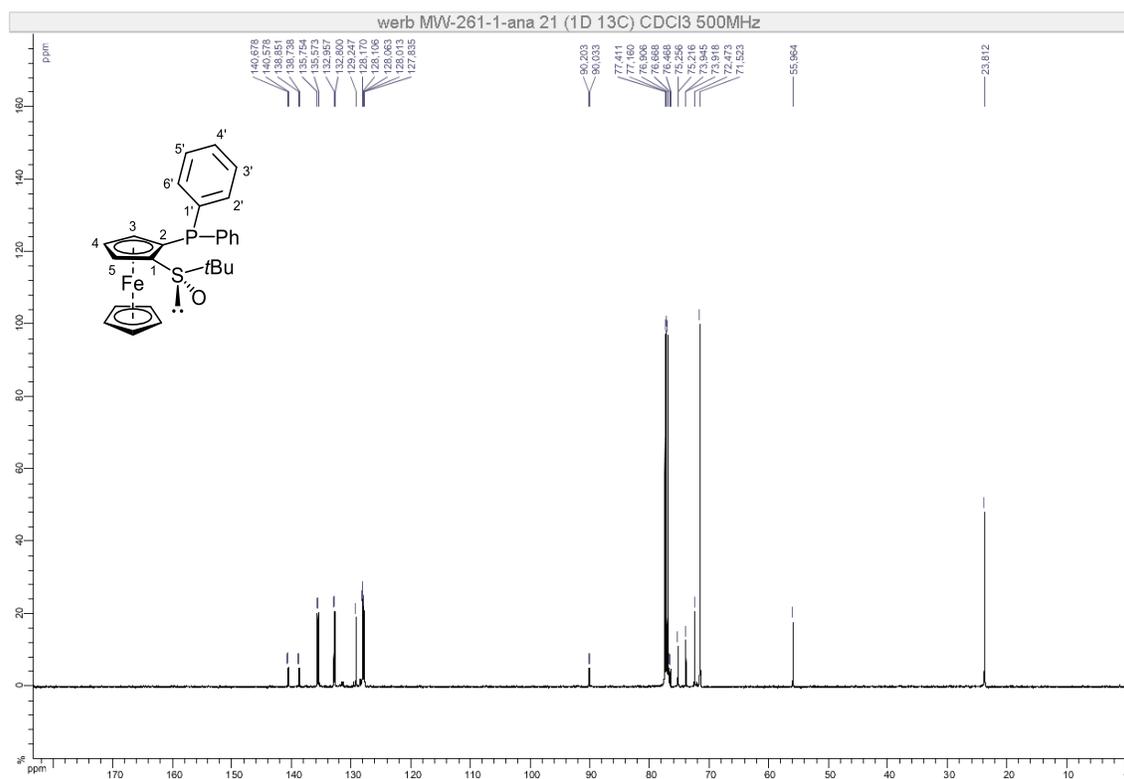


(*S,S*)-*S*-*tert*-Butyl-2-(diphenylphosphino)ferrocenesulfoxide (*S,S*-1e)

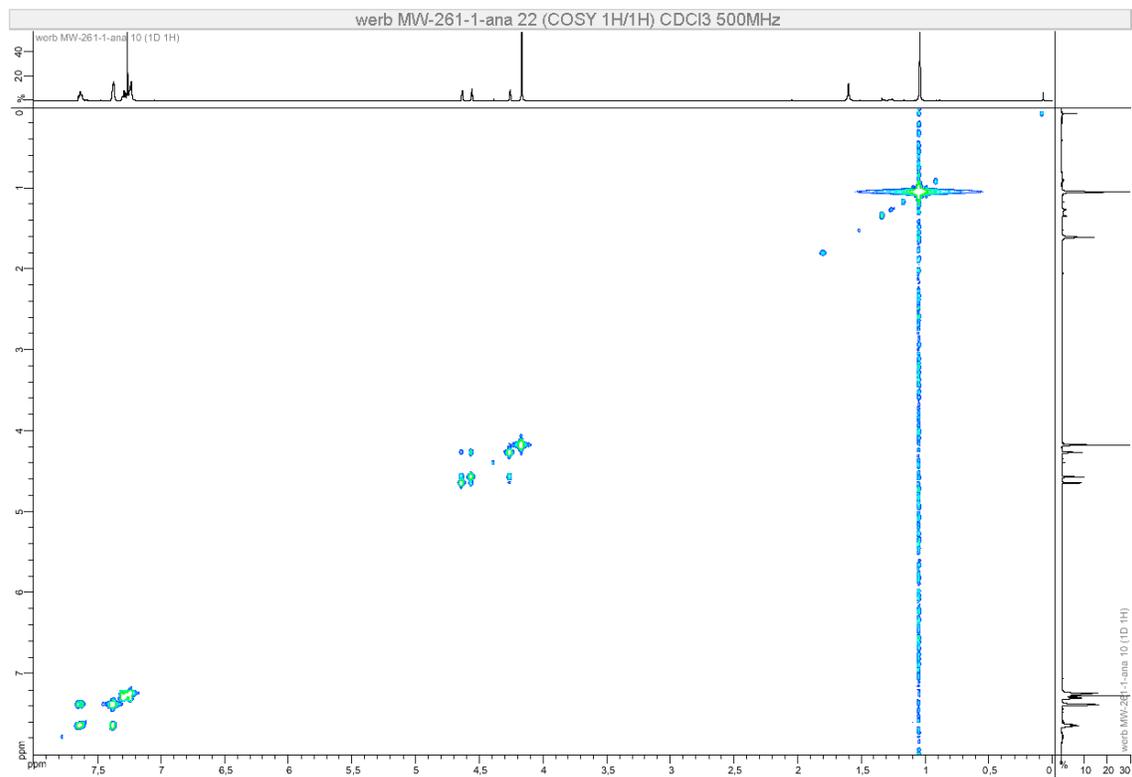
^1H NMR (500 MHz, CDCl_3)



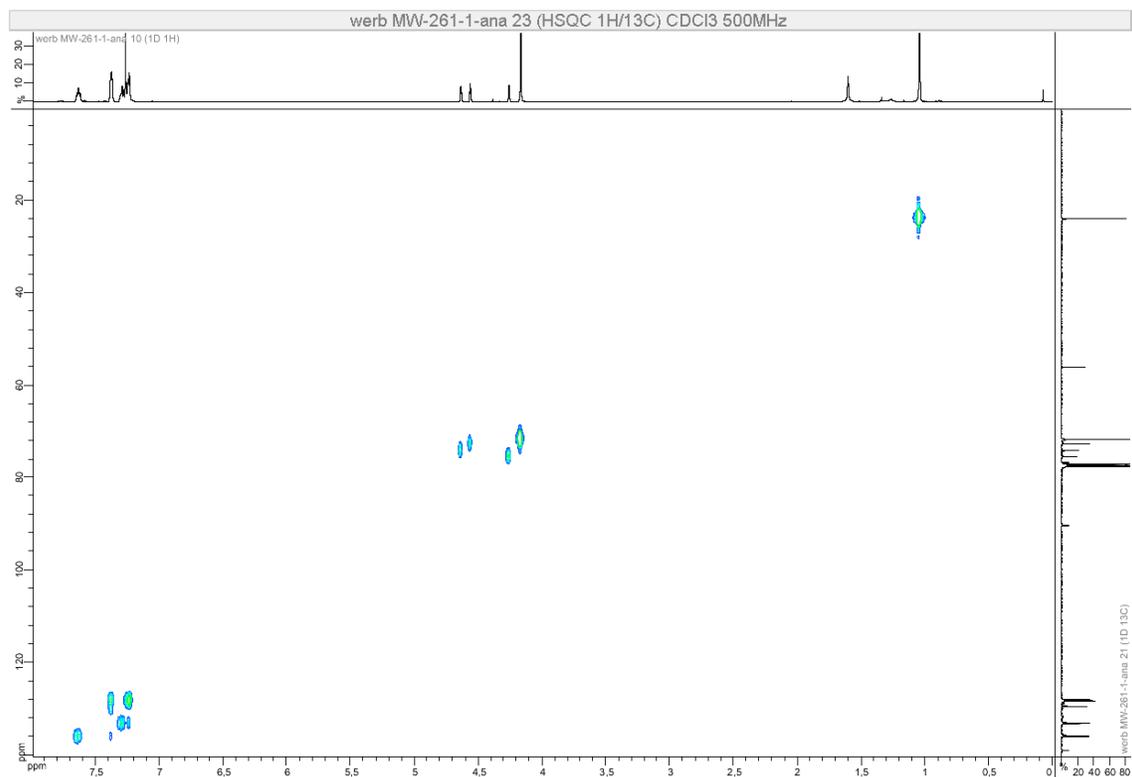
^{13}C NMR (126 MHz, CDCl_3)



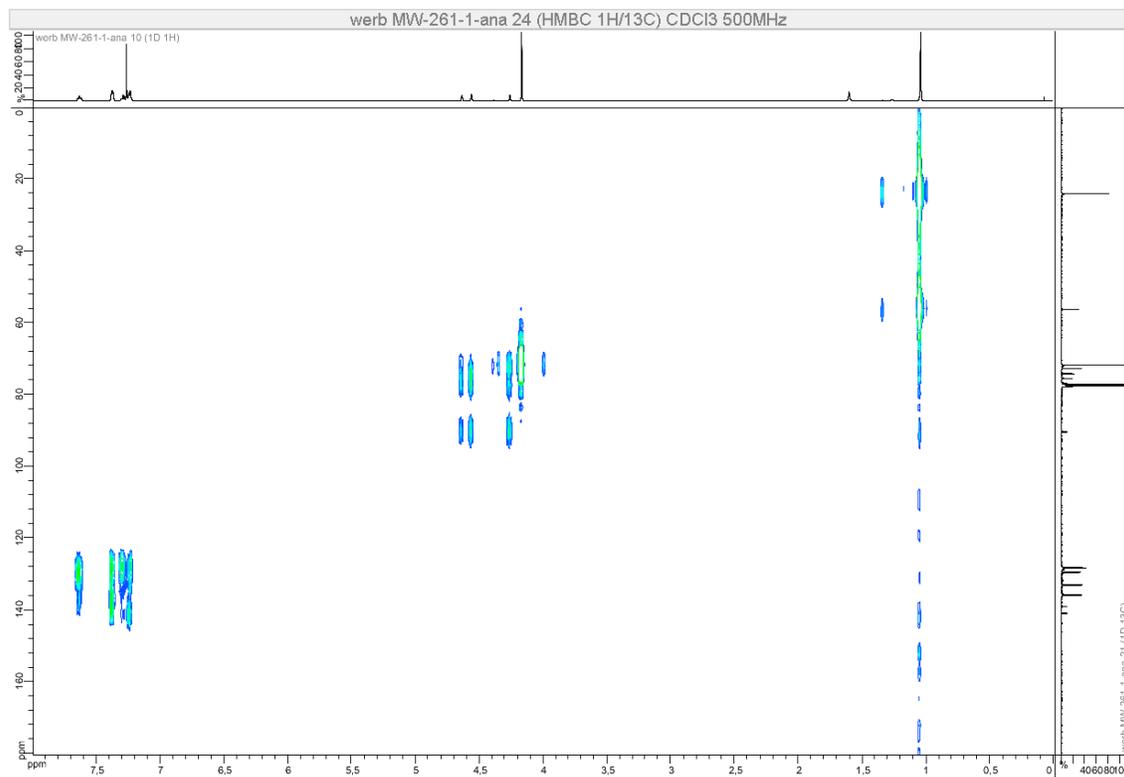
COSY (500 MHz, CDCl₃)



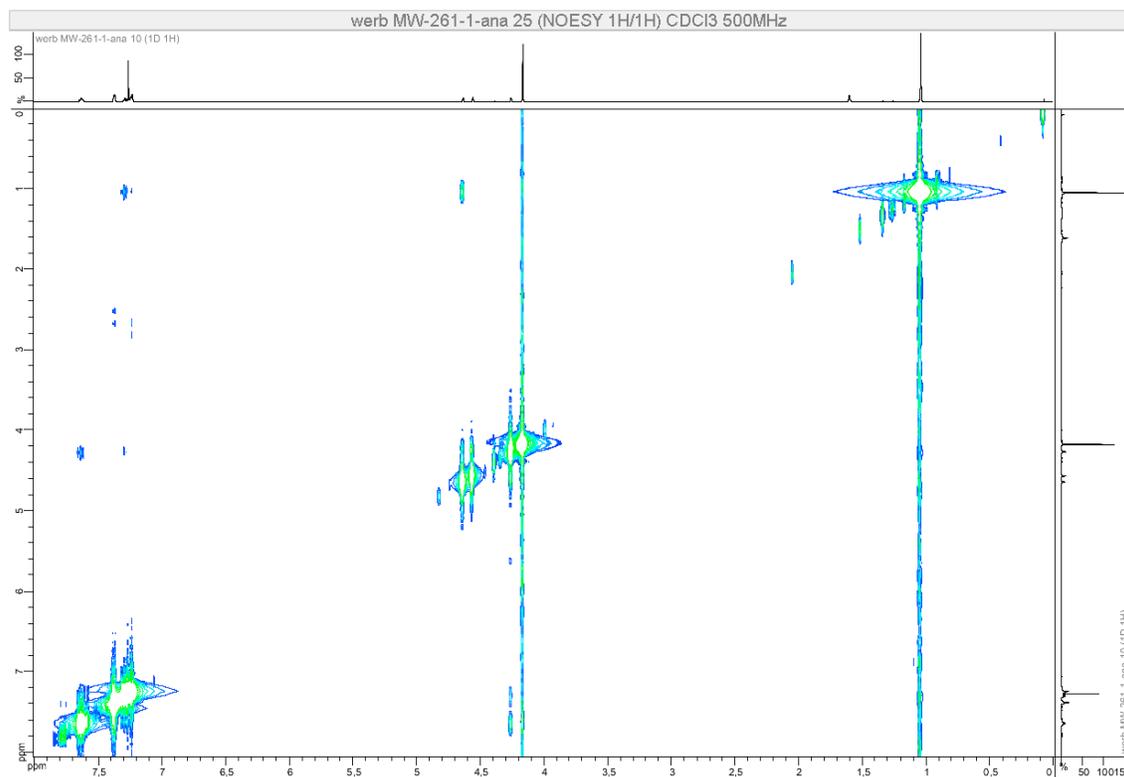
HSQC (500 MHz, CDCl₃)



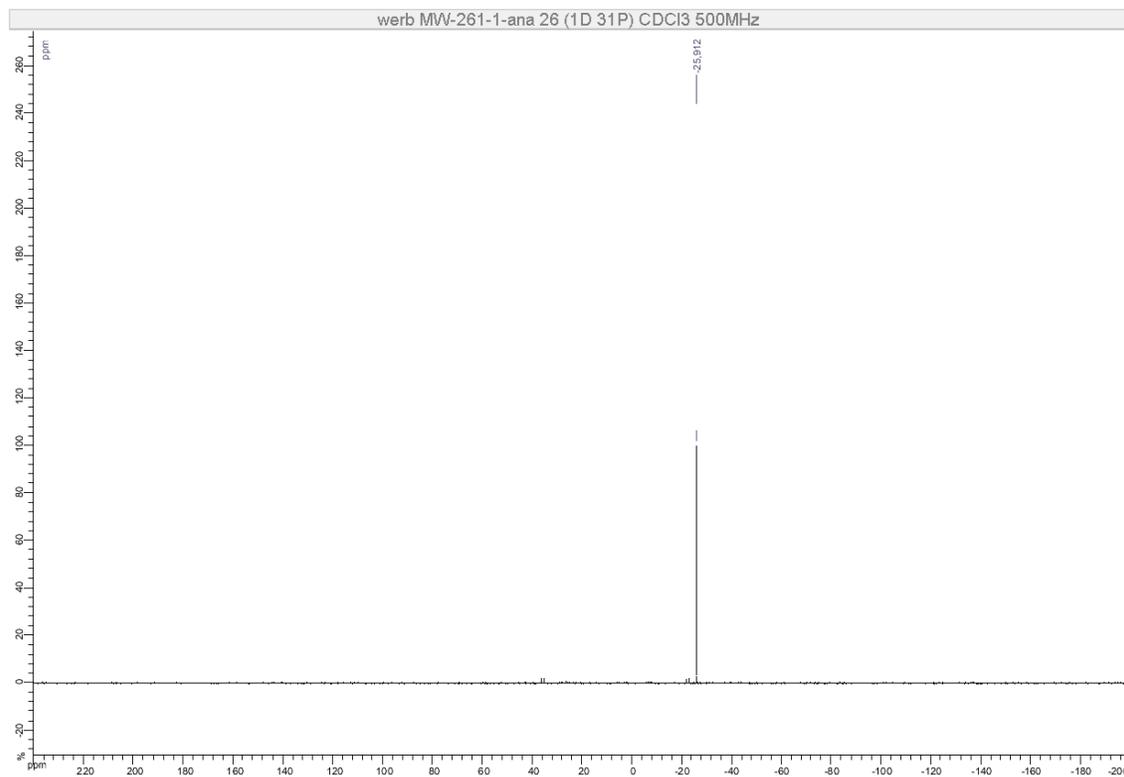
HMBC (500 MHz, CDCl₃)



NOESY (500 MHz, CDCl₃)

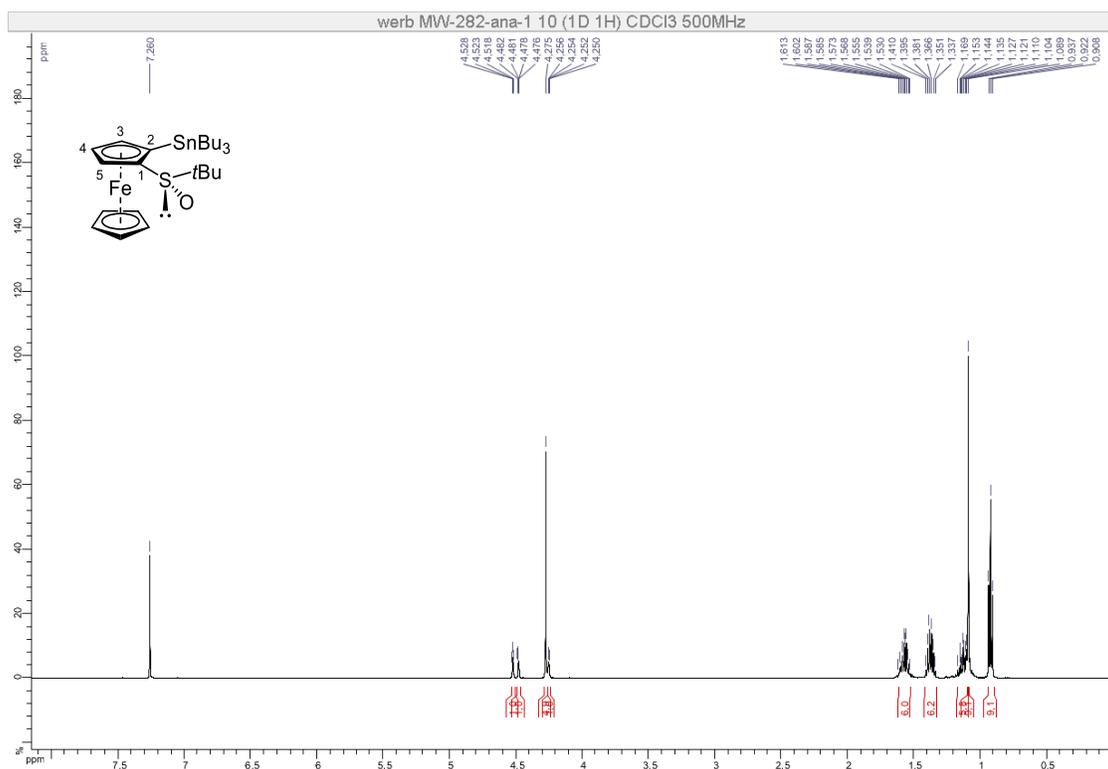


^{31}P NMR (202 MHz, CDCl_3)

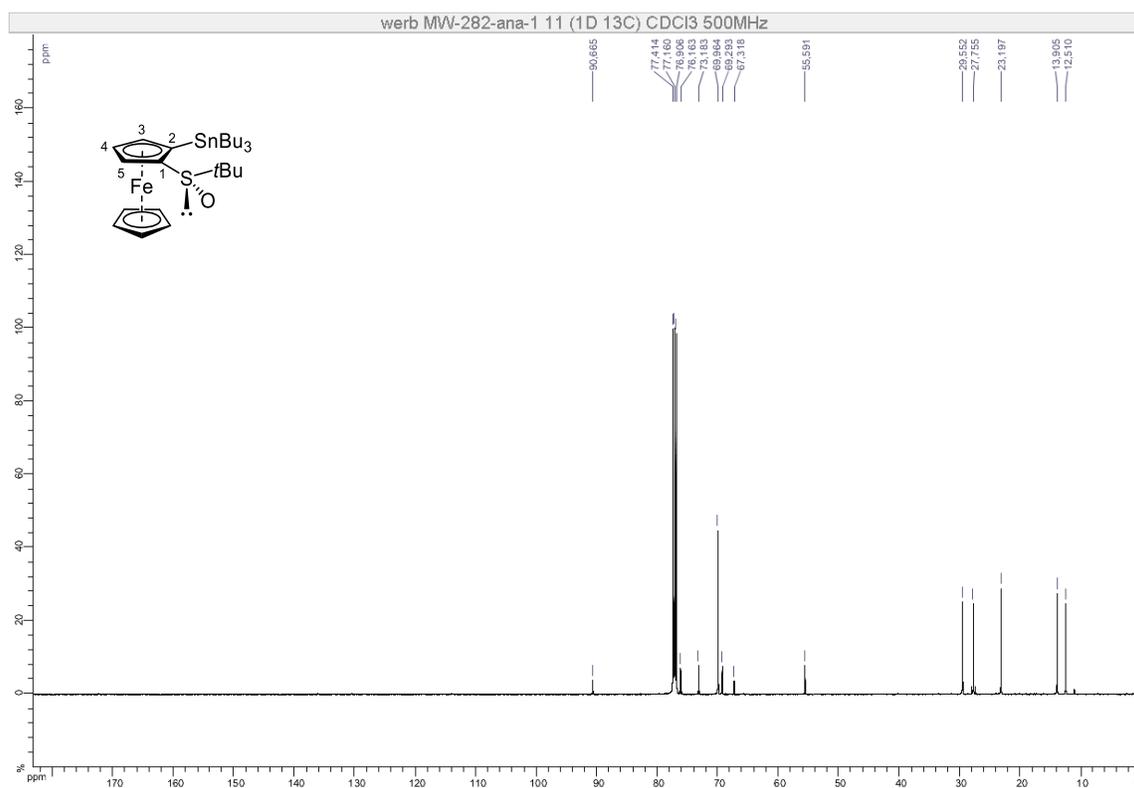


(*S,R_P*)-*S-tert*-Butyl-2-(tributylstannyl)ferrocenesulfoxide (*S,R_P*-1f)

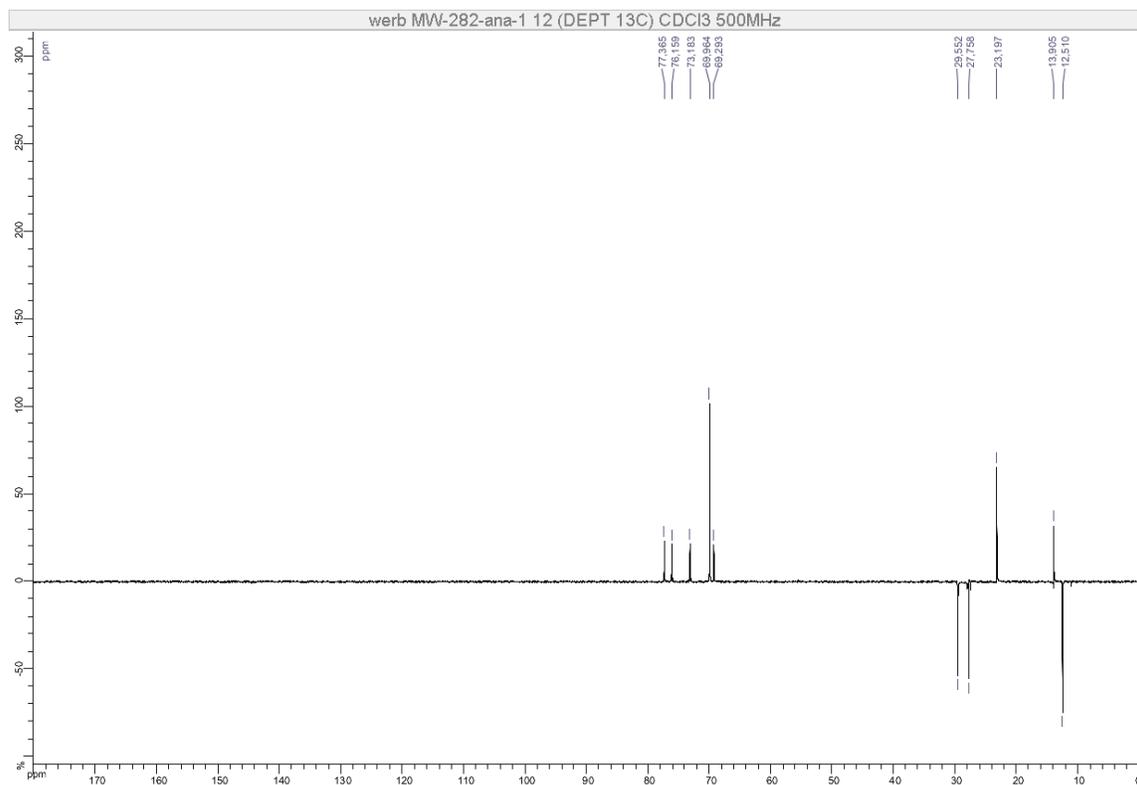
^1H NMR (500 MHz, CDCl_3)



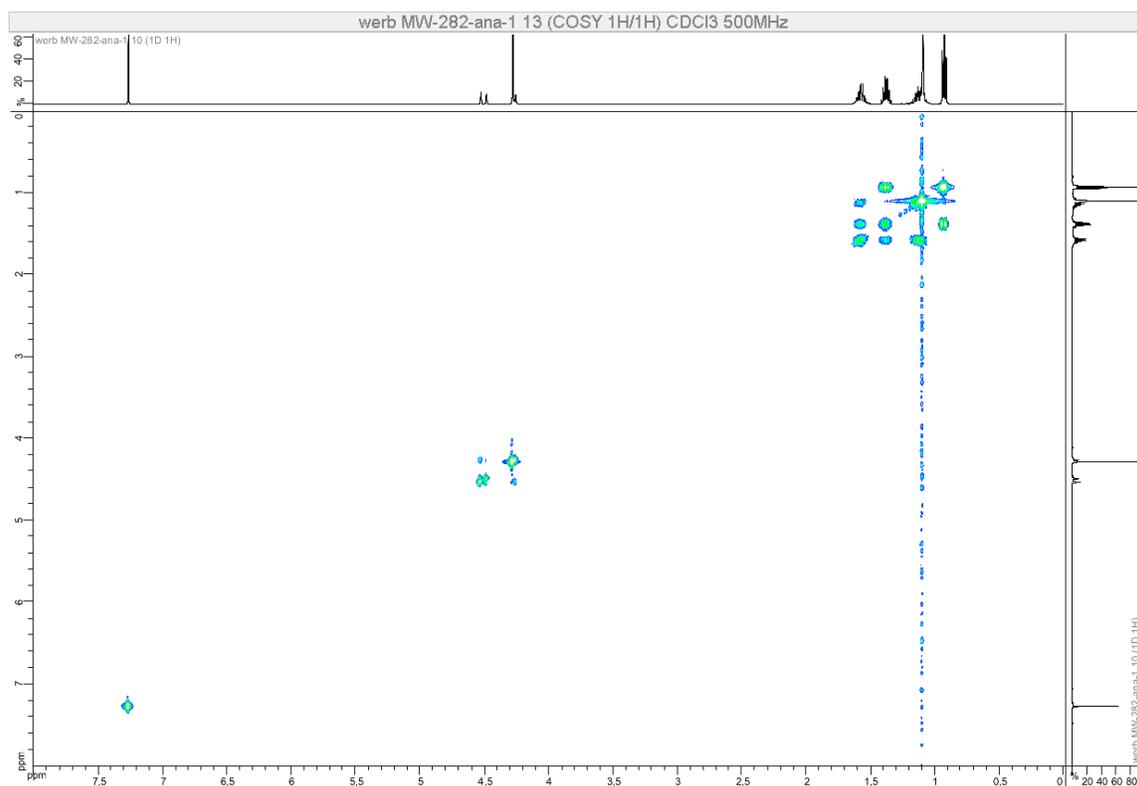
^{13}C NMR (126 MHz, CDCl_3)



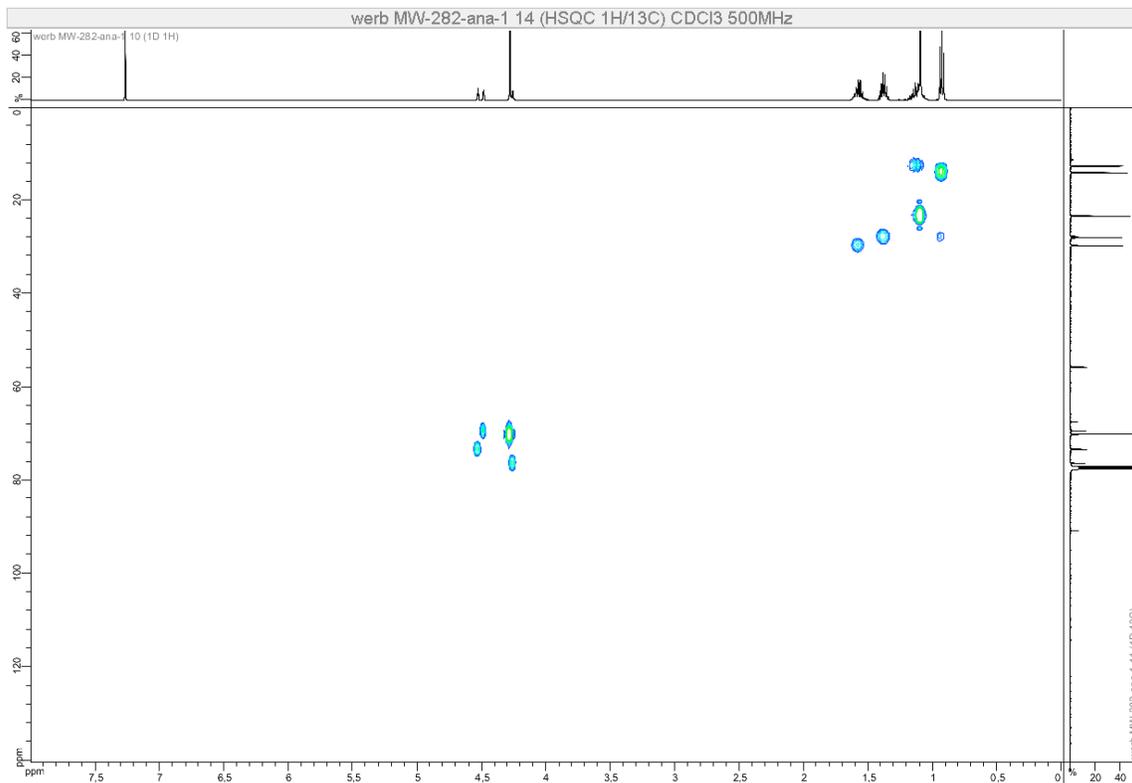
DEPT 135 (126 MHz, CDCl₃)



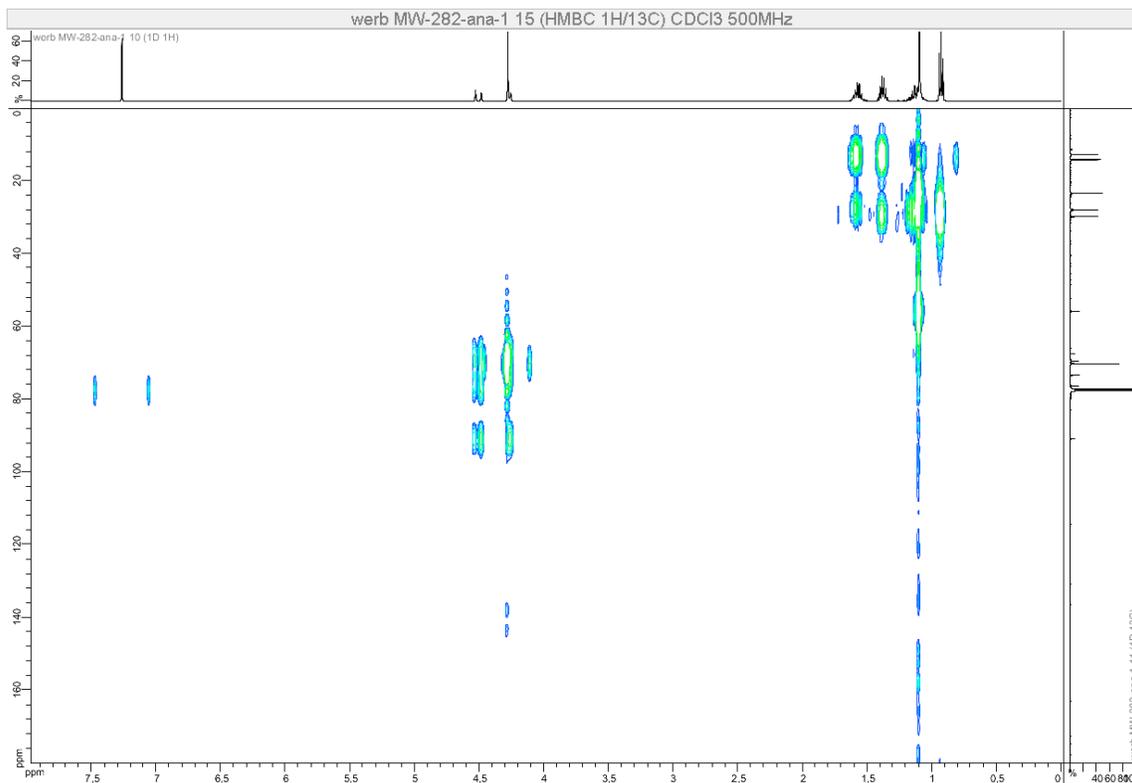
COSY (500 MHz, CDCl₃)



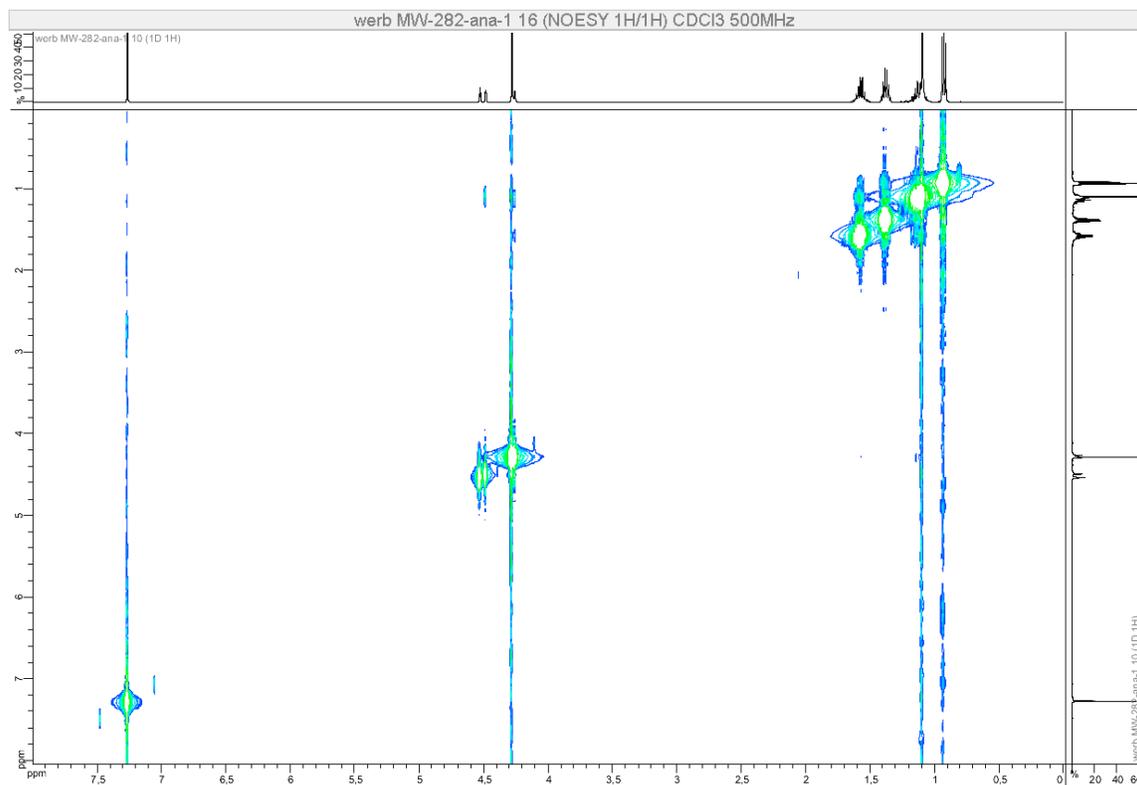
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

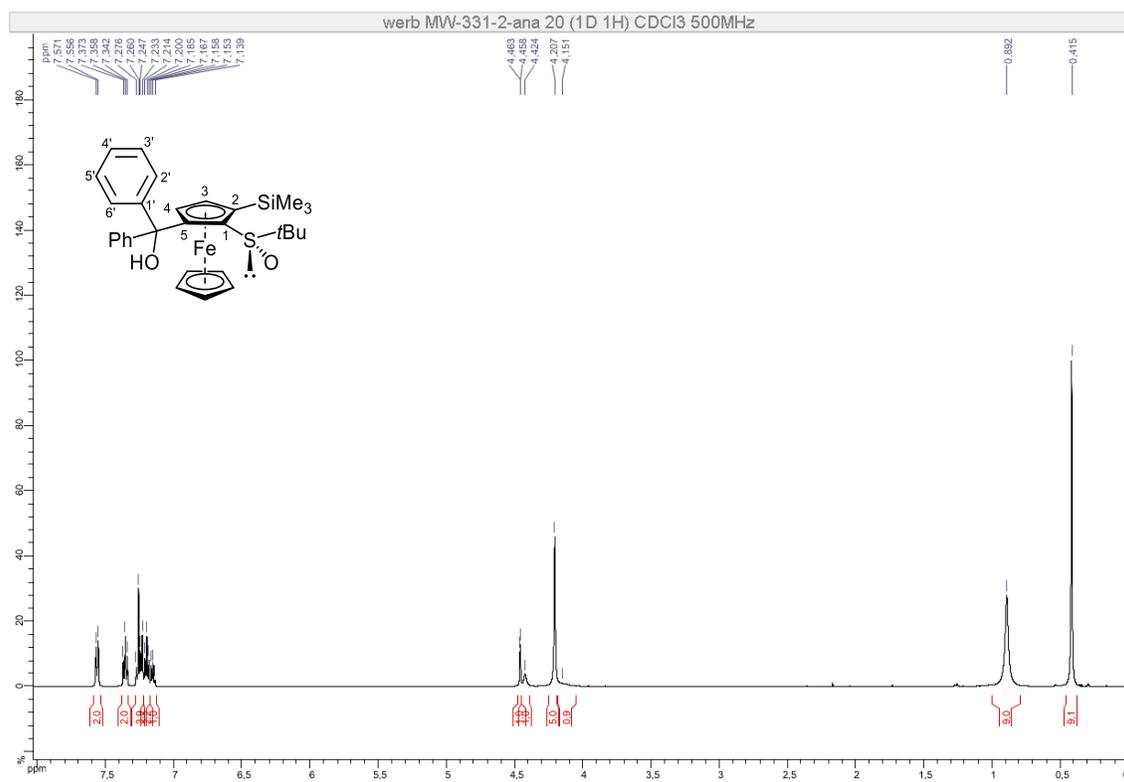


NOESY (500 MHz, CDCl₃)

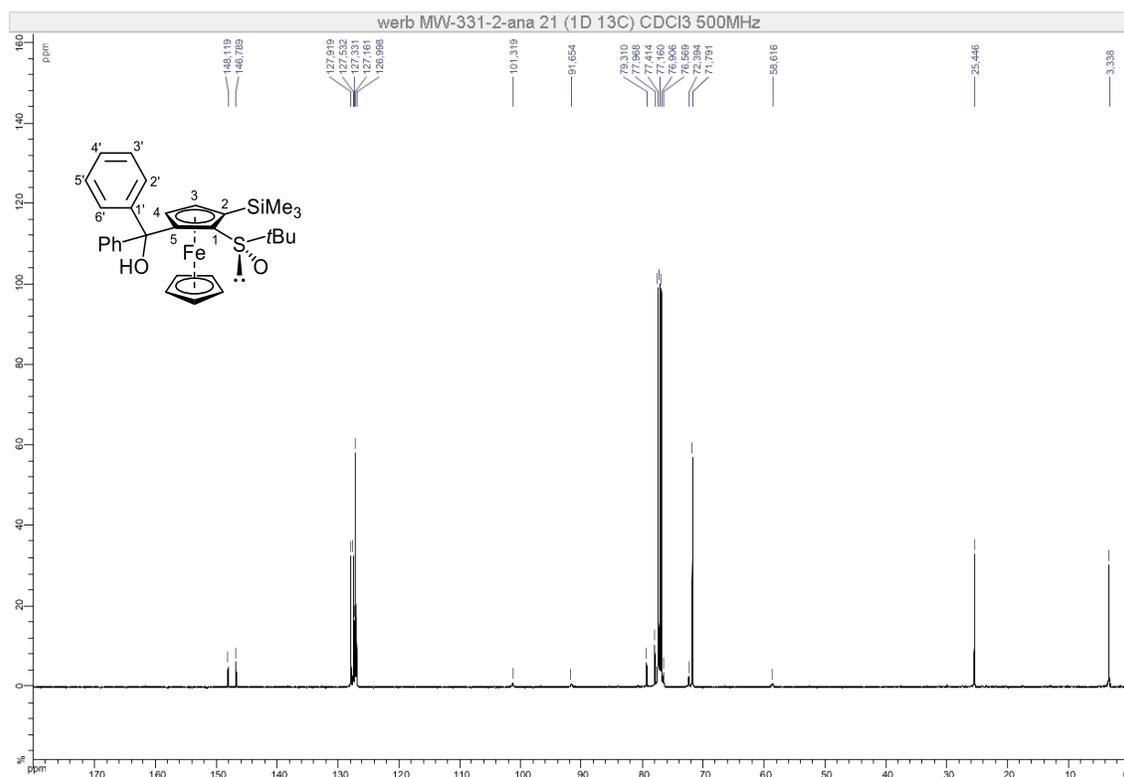


(*S,S*)-*S*-tert-Butyl-2-[(α,α -diphenyl)hydroxymethyl]-5-(trimethylsilyl)ferrocenesulfoxide (*S,S*P-2ag)

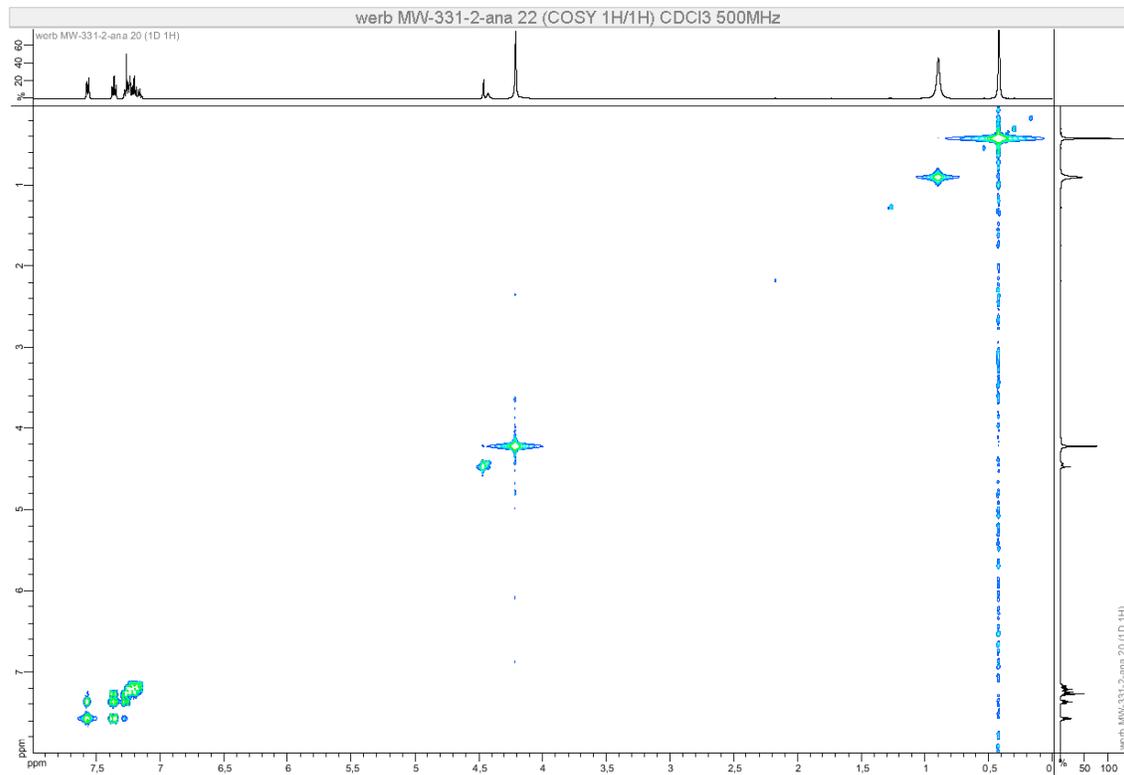
^1H NMR (500 MHz, CDCl_3)



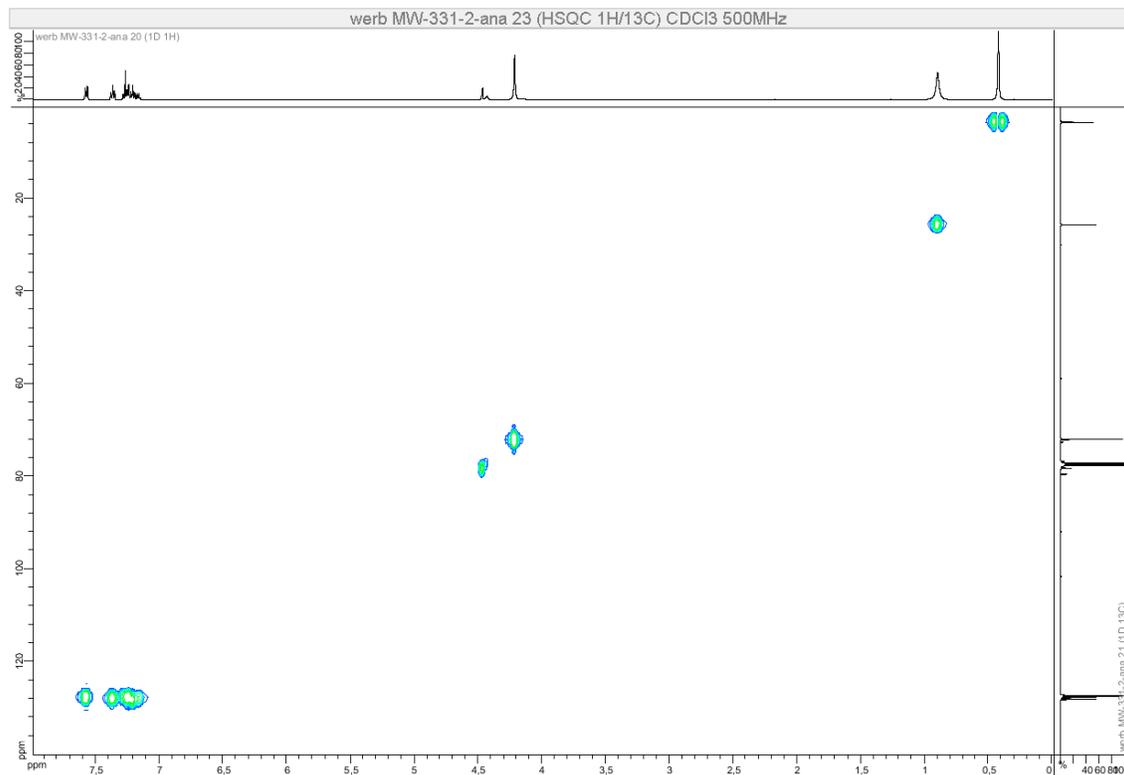
^{13}C NMR (126 MHz, CDCl_3)



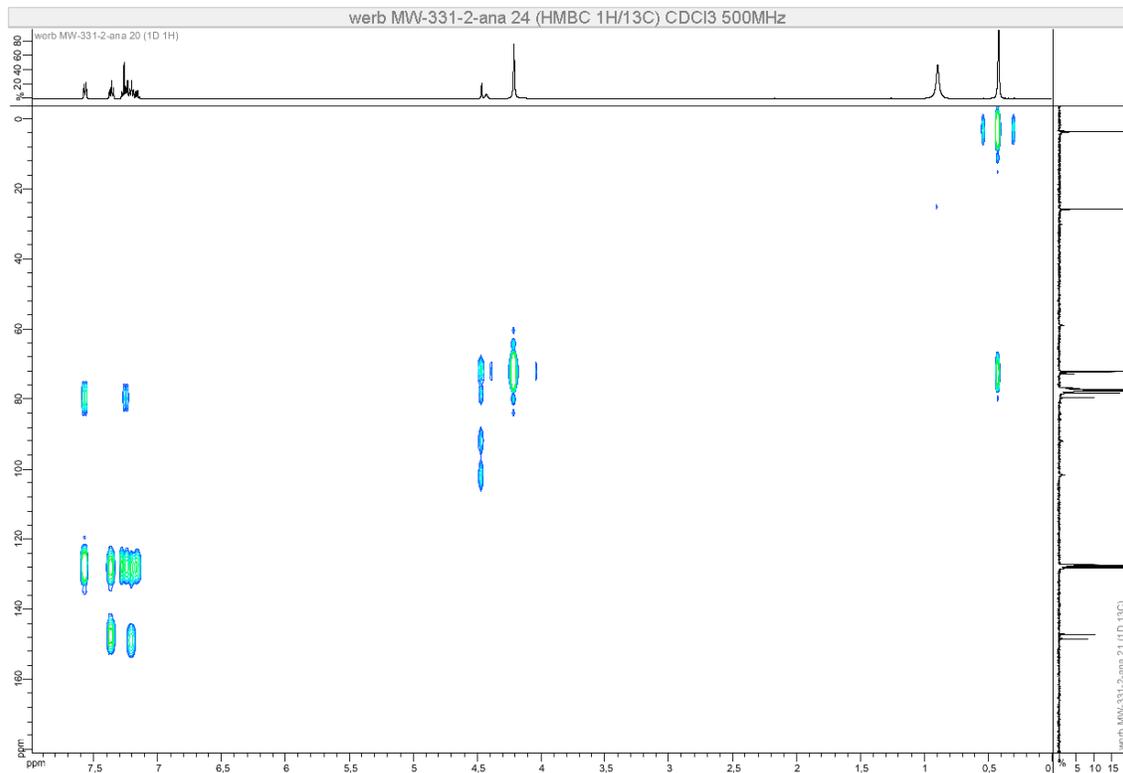
COSY (500 MHz, CDCl₃)



HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

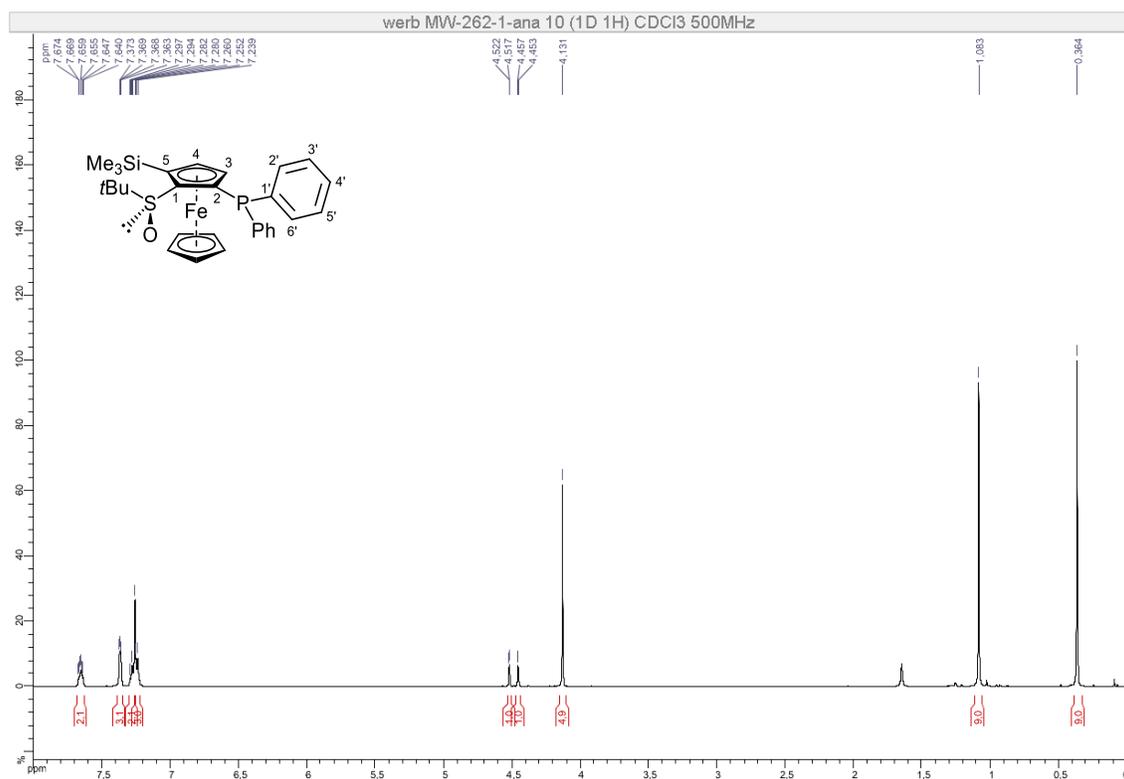


NOESY (500 MHz, CDCl₃)

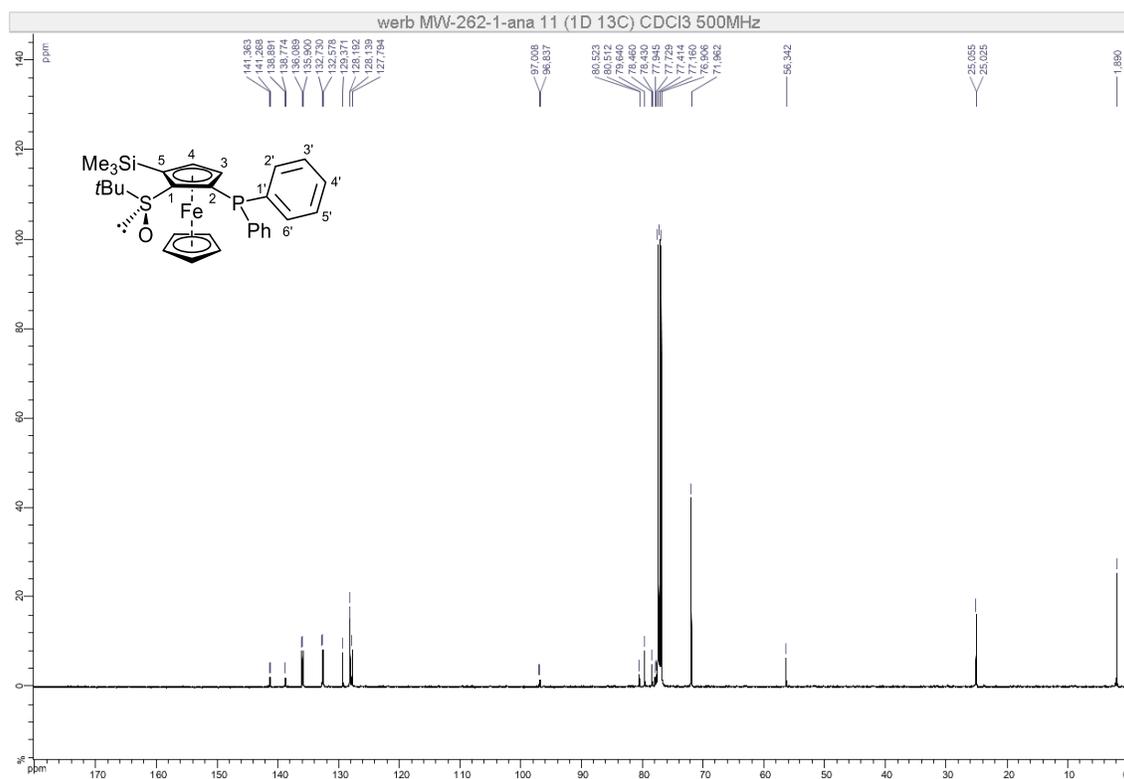


(*S,S*_P)-*S*-tert-Butyl-2-(diphenylphosphino)-5-(trimethylsilyl)ferrocenesulfoxide (*S,S*_P-2ea)

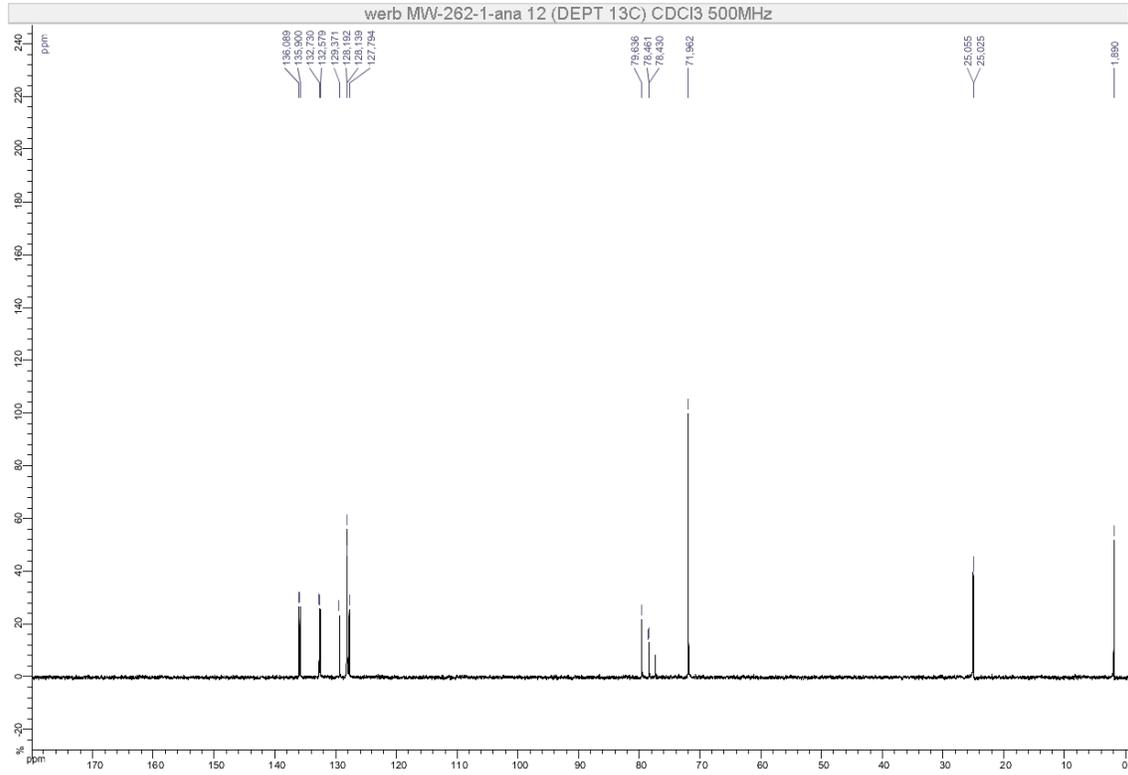
¹H NMR (500 MHz, CDCl₃)



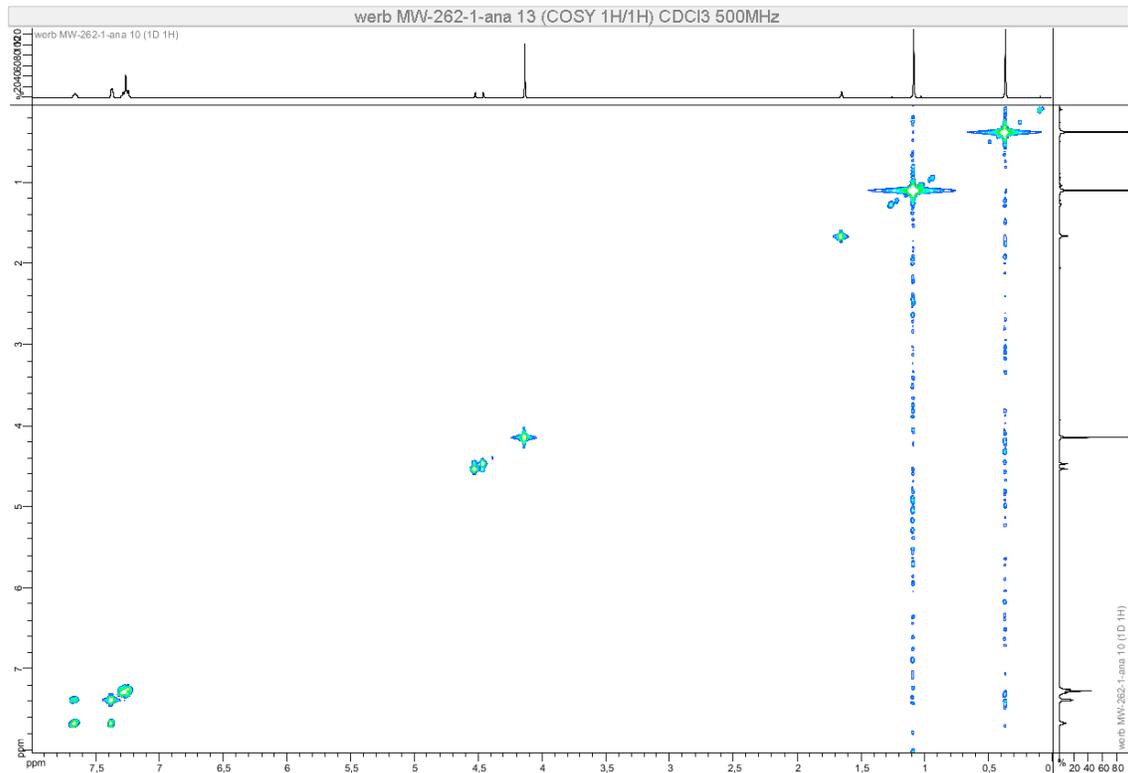
¹³C NMR (126 MHz, CDCl₃)



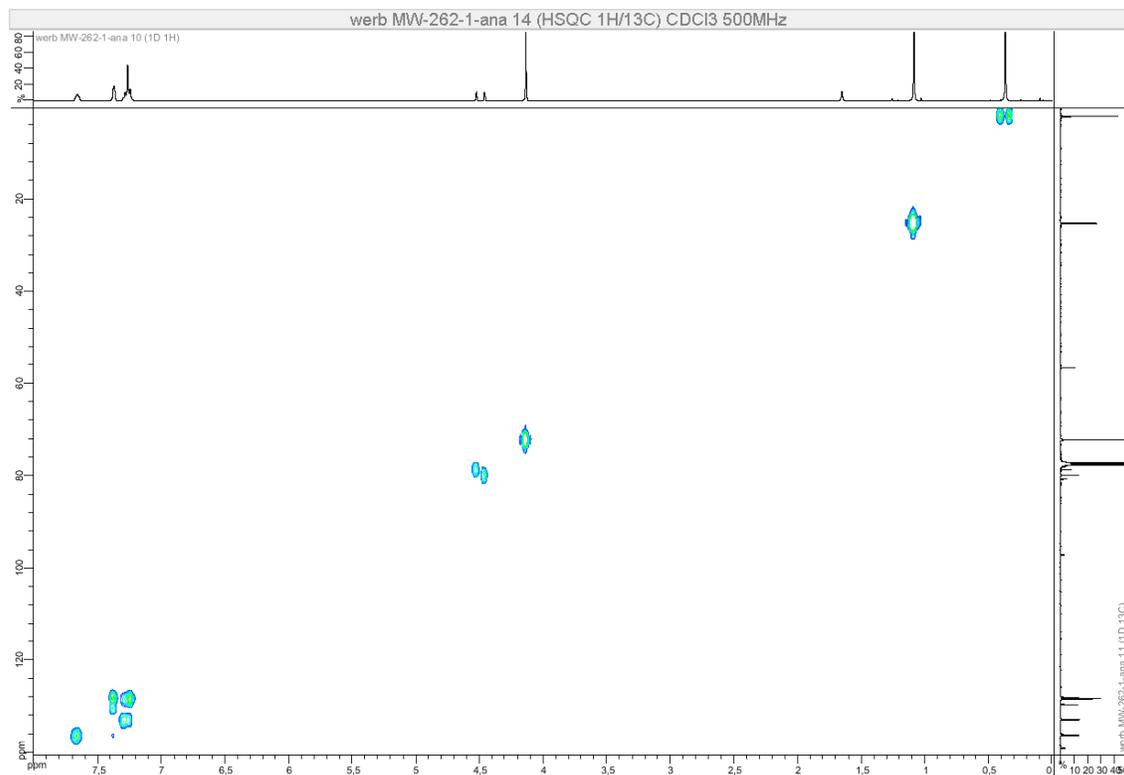
DEPT 135 (126 MHz, CDCl₃)



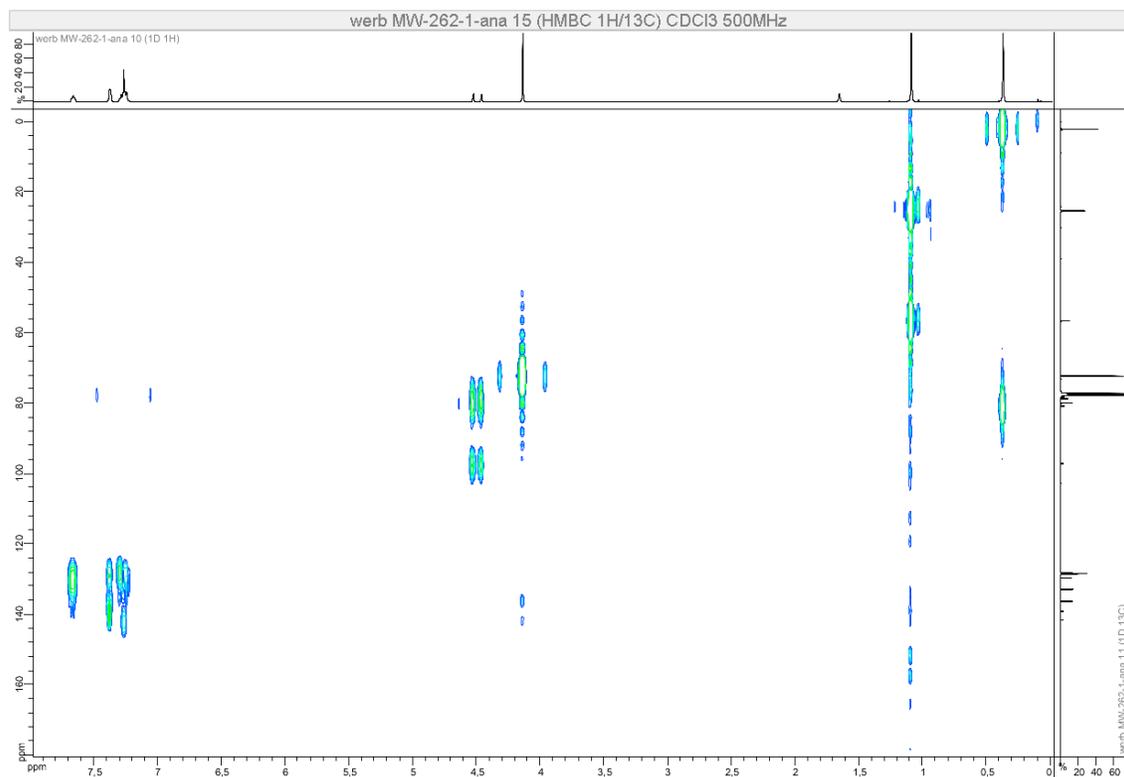
COSY (500 MHz, CDCl₃)



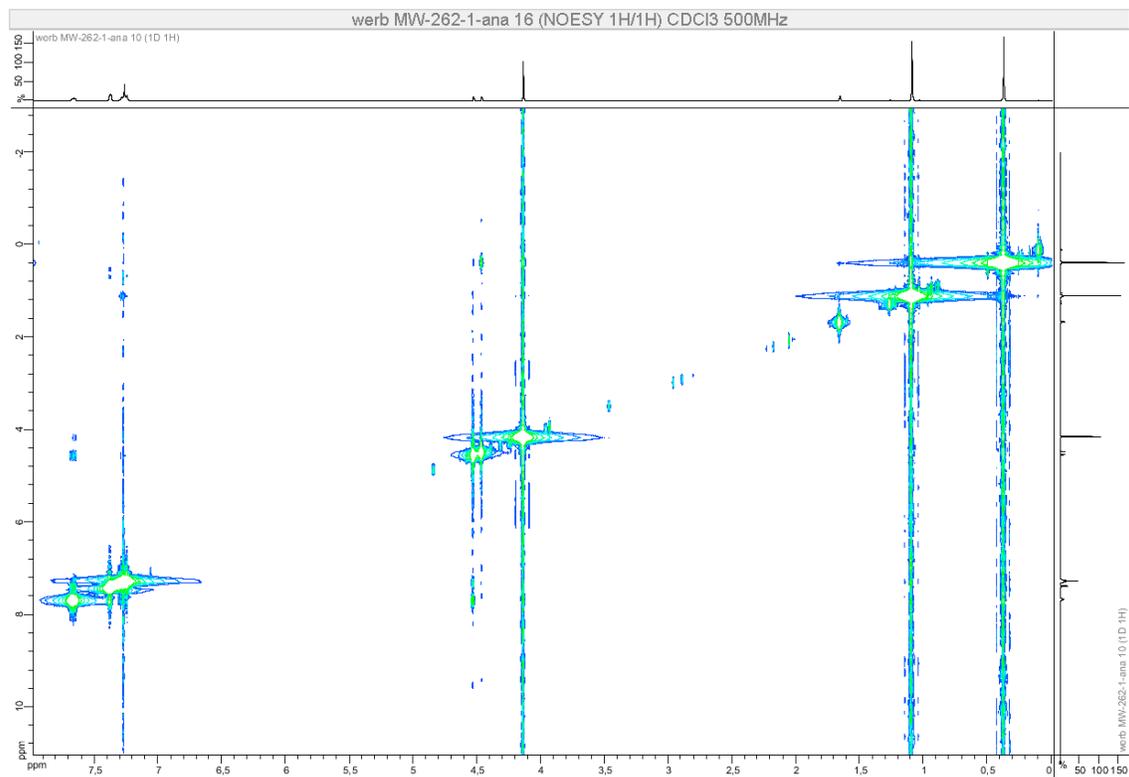
HSQC (500 MHz, CDCl₃)



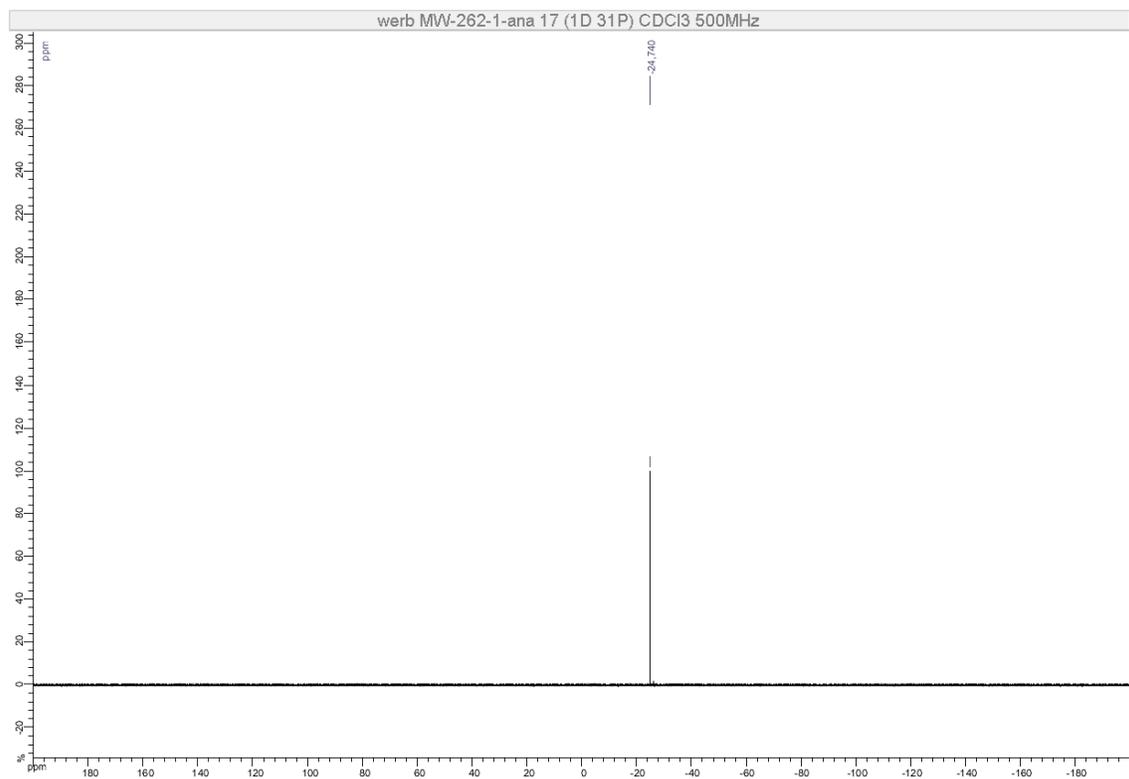
HMBC (500 MHz, CDCl₃)



NOESY (500 MHz, CDCl₃)

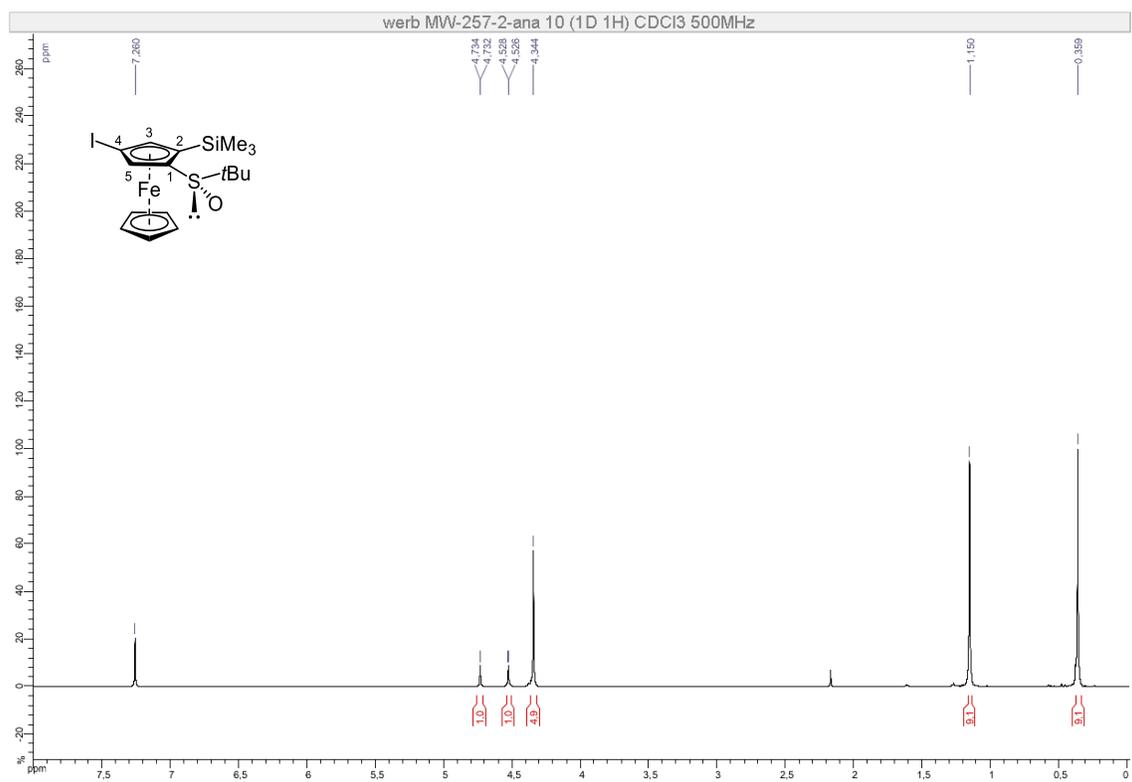


³¹P NMR (202 MHz, CDCl₃)

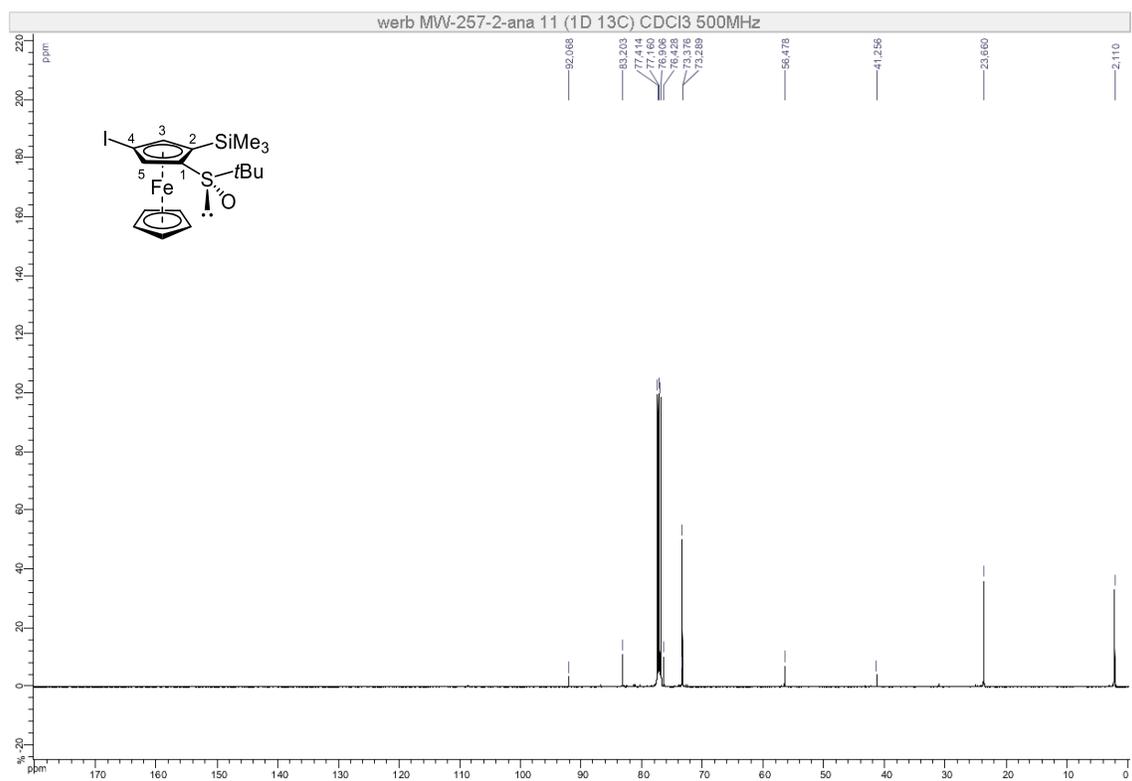


(*S,S*)-*S*-tert-Butyl-4-iodo-2-(trimethylsilyl)ferrocenesulfoxide (*S,S*p-7)

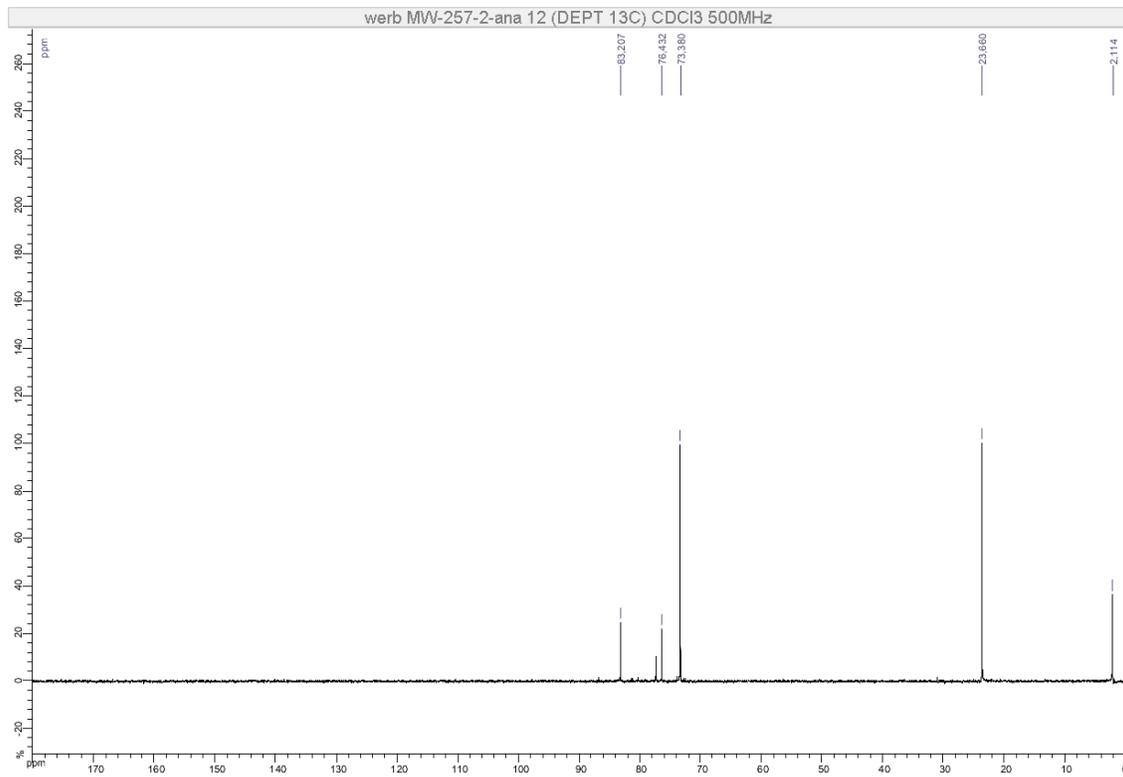
¹H NMR (500 MHz, CDCl₃)



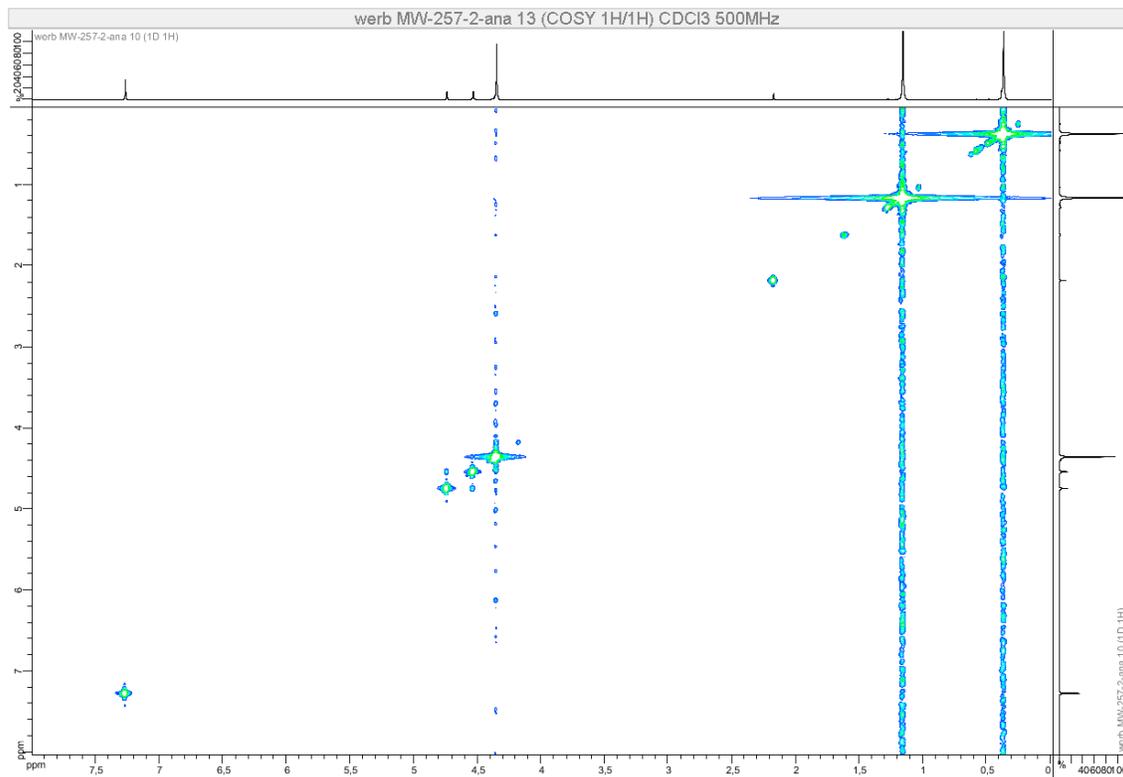
¹³C NMR (126 MHz, CDCl₃)



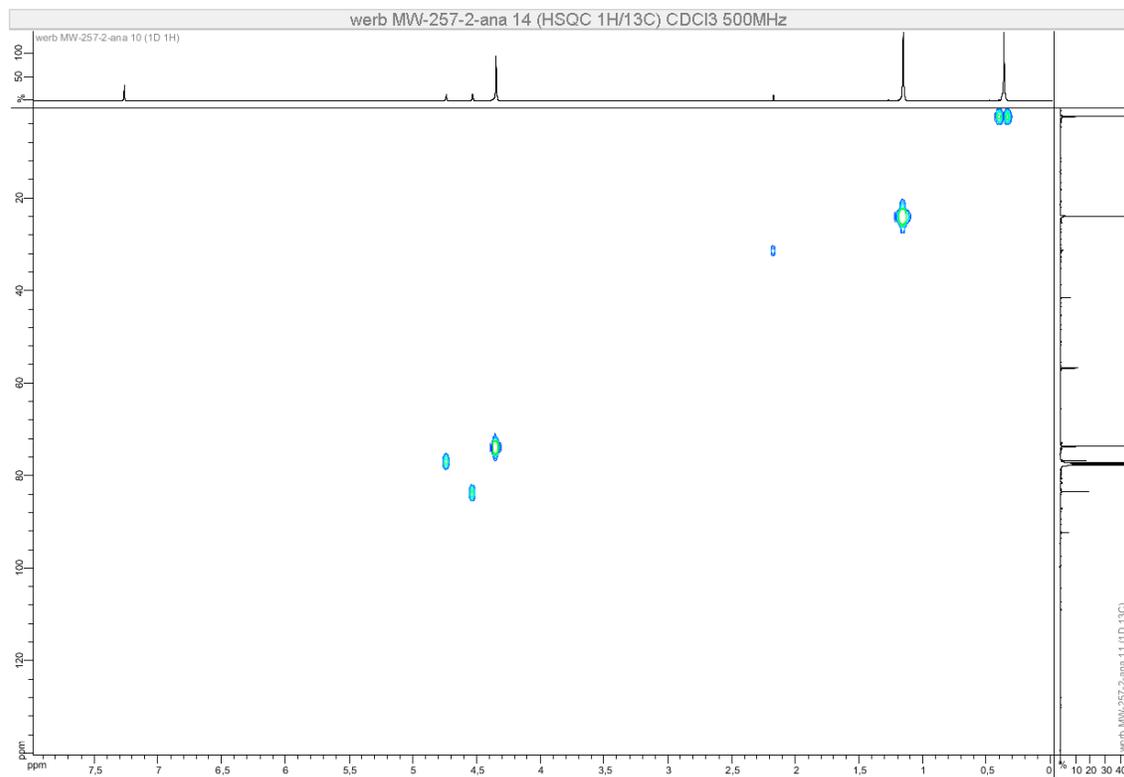
DEPT 135 (126 MHz, CDCl₃)



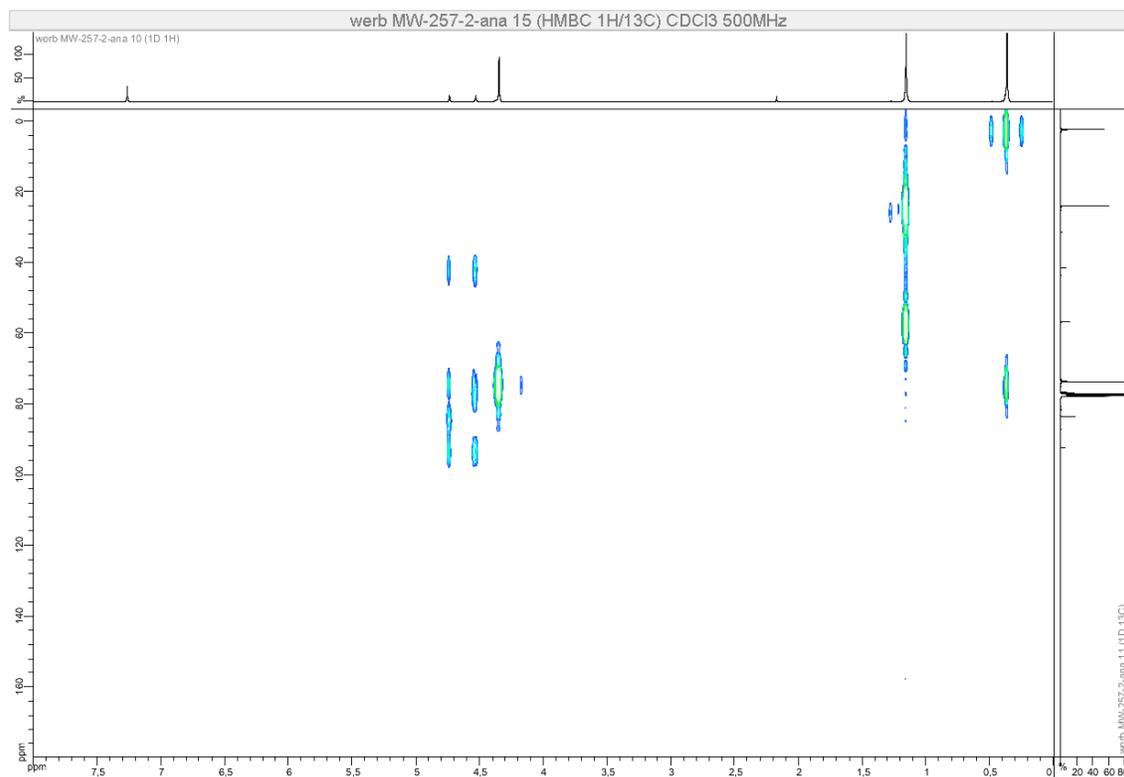
COSY (500 MHz, CDCl₃)



HSQC (500 MHz, CDCl₃)

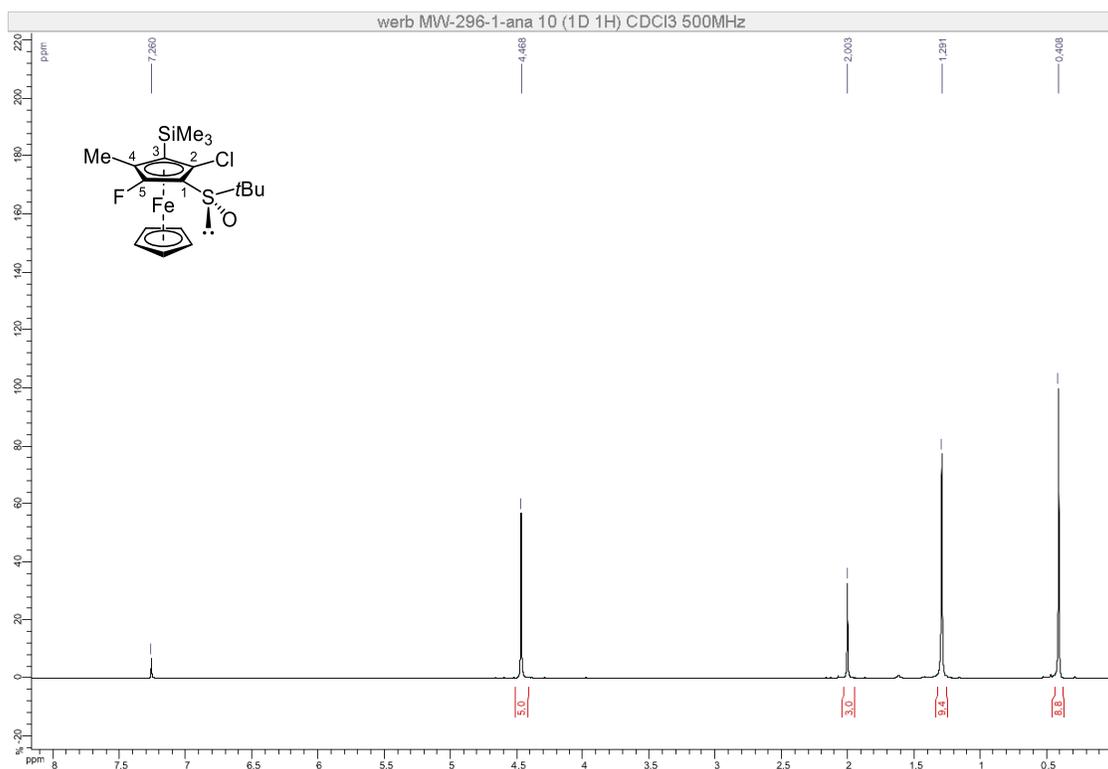


HMBC (500 MHz, CDCl₃)

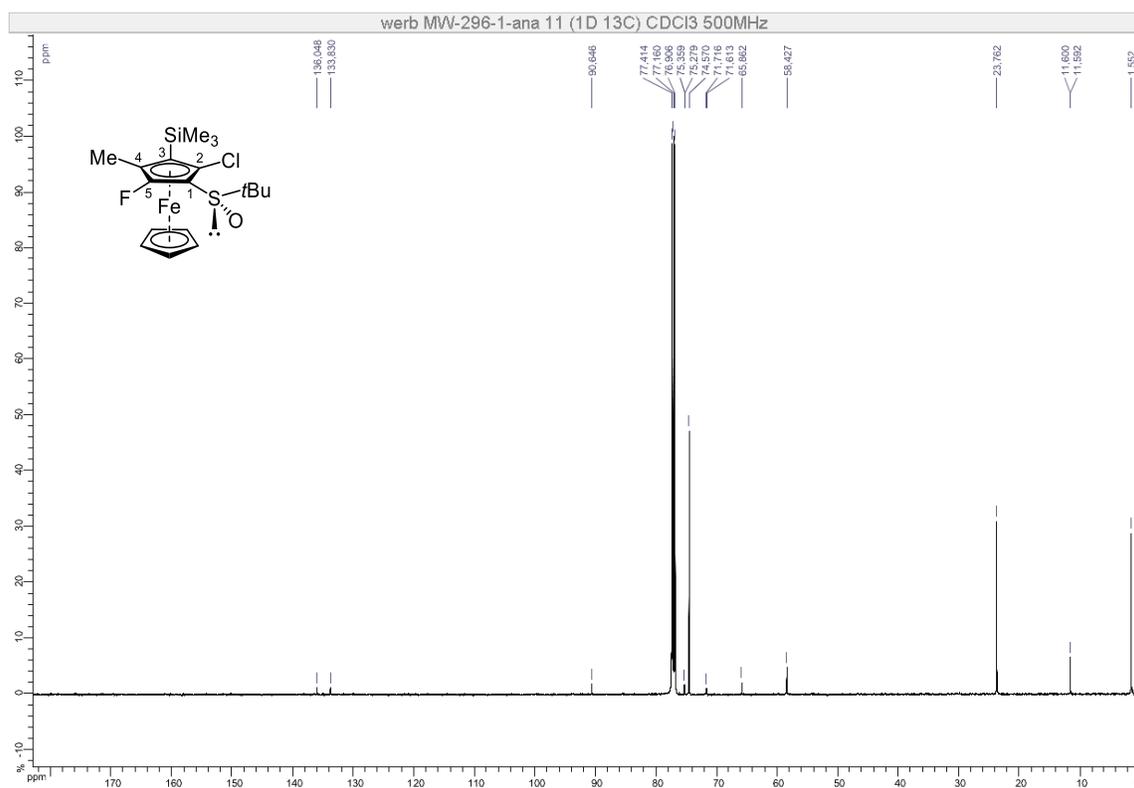


(*S,S*_P)-*S*-tert-Butyl-2-chloro-5-fluoro-4-methyl-3-(trimethylsilyl)ferrocenesulfoxide (*S,S*_P-12)

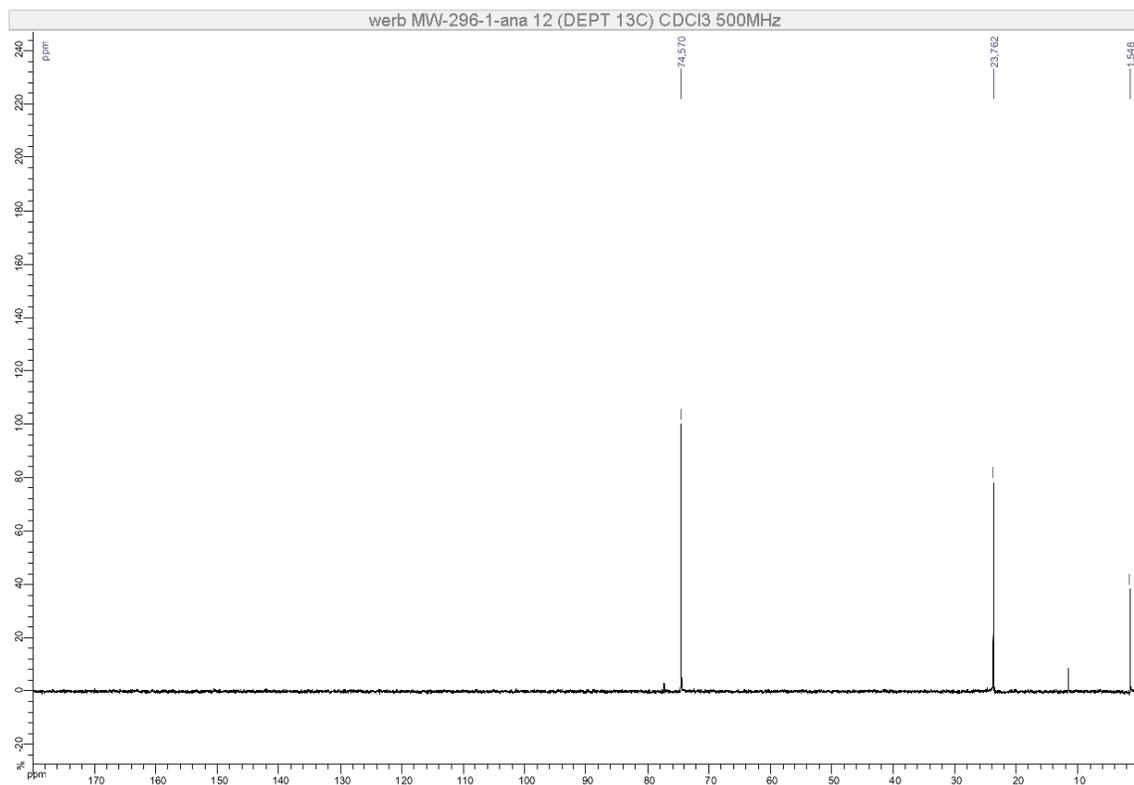
¹H NMR (500 MHz, CDCl₃)



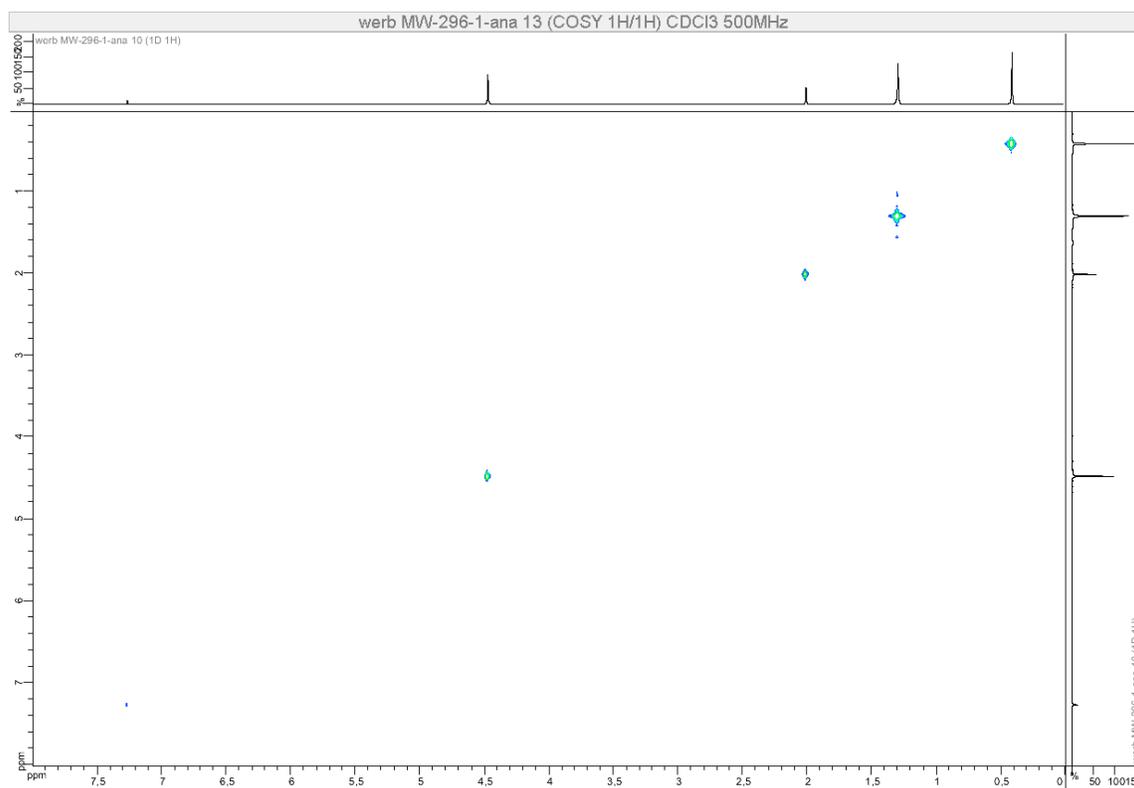
¹³C NMR (126 MHz, CDCl₃)



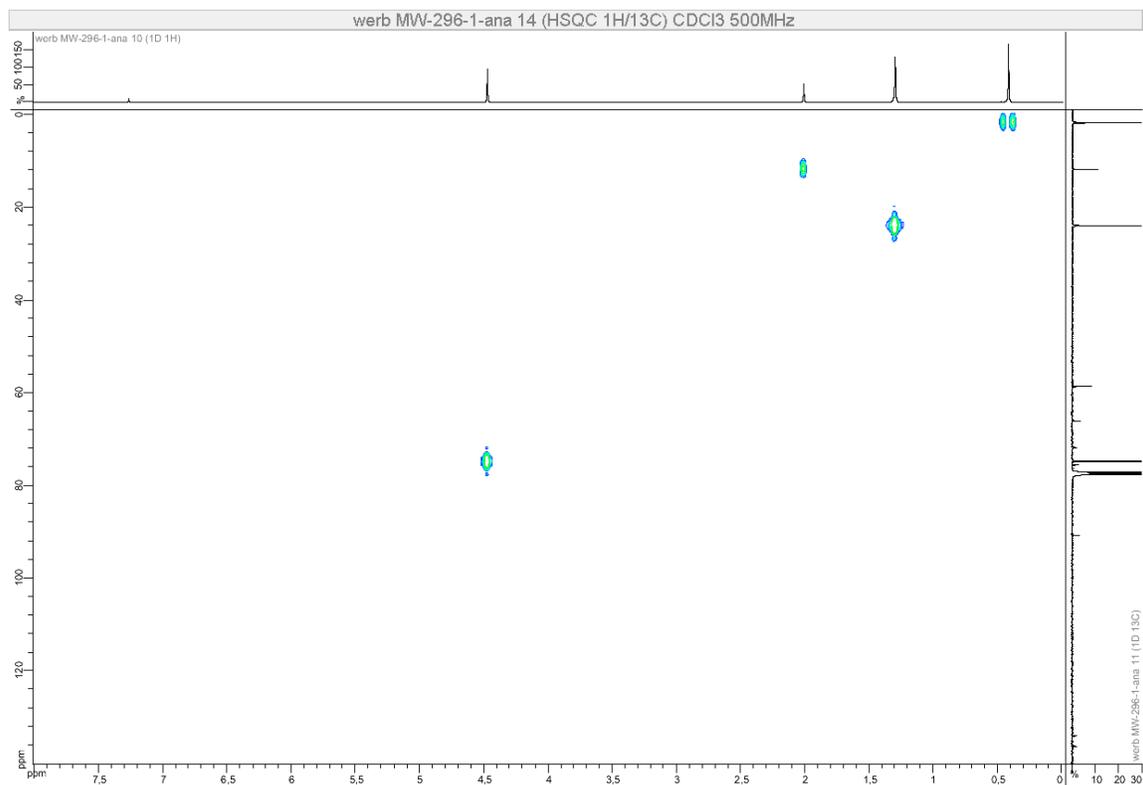
DEPT 135 (126 MHz, CDCl₃)



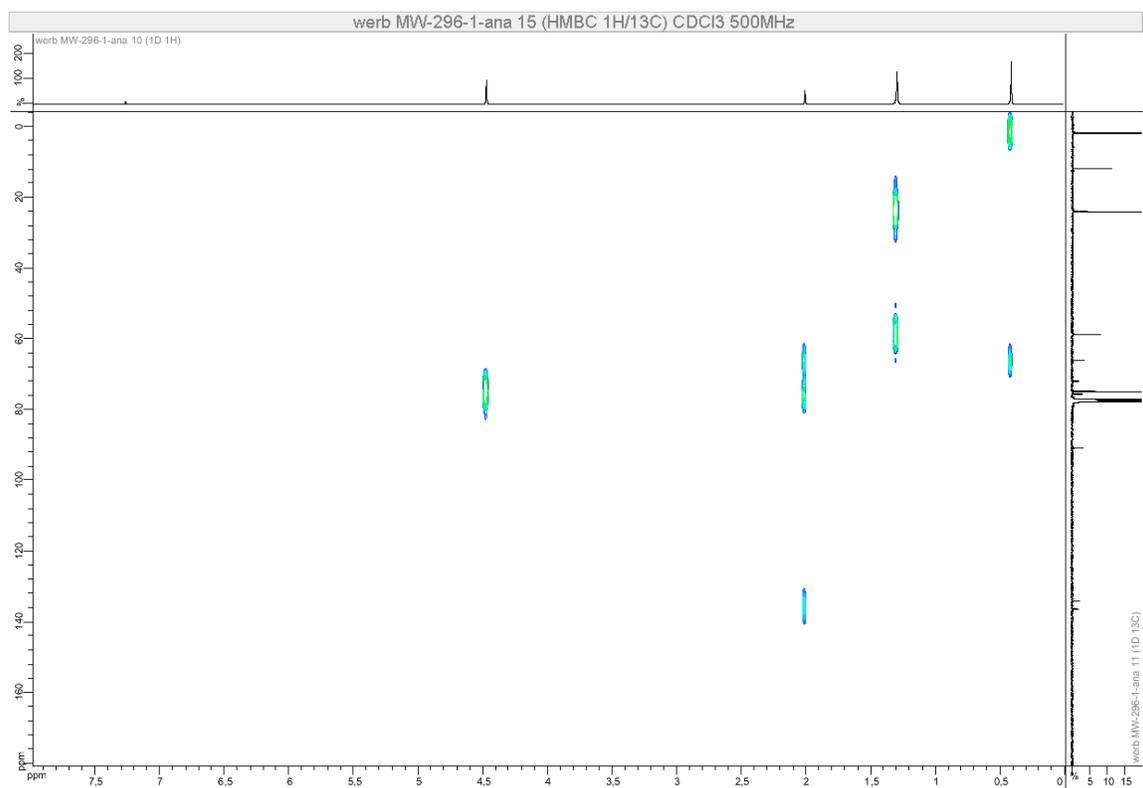
COSY (500 MHz, CDCl₃)



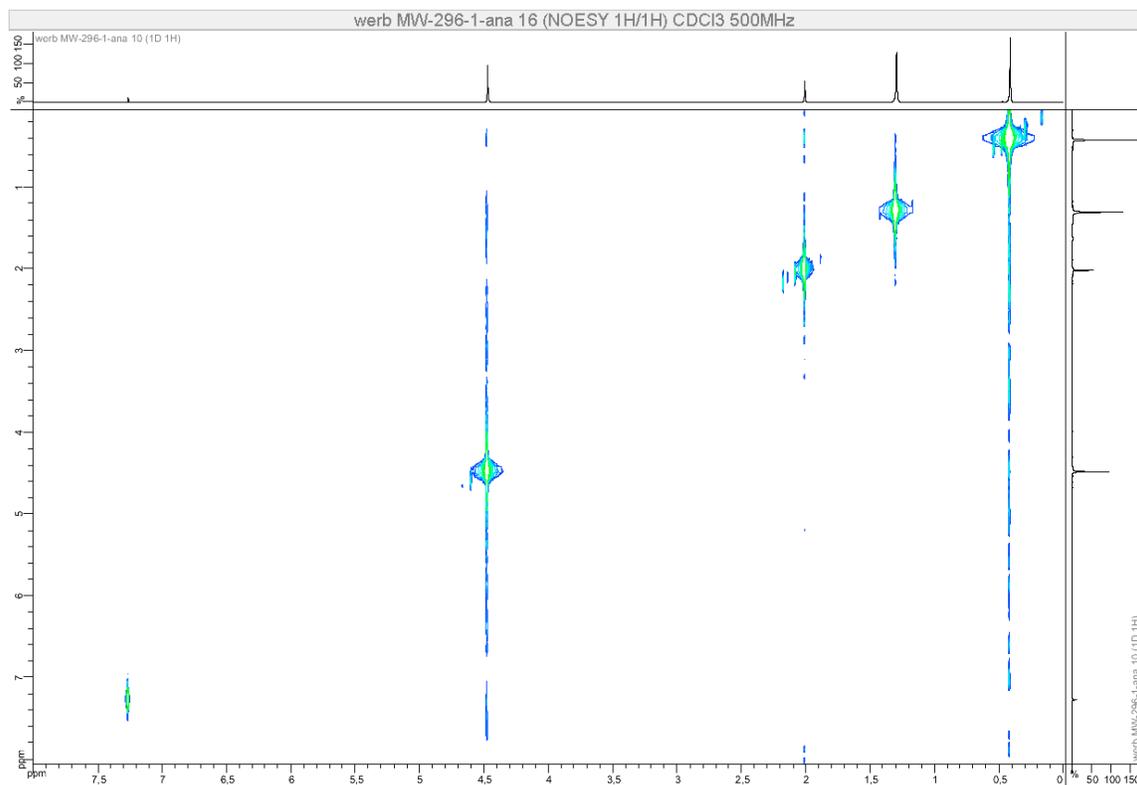
HSQC (500 MHz, CDCl₃)



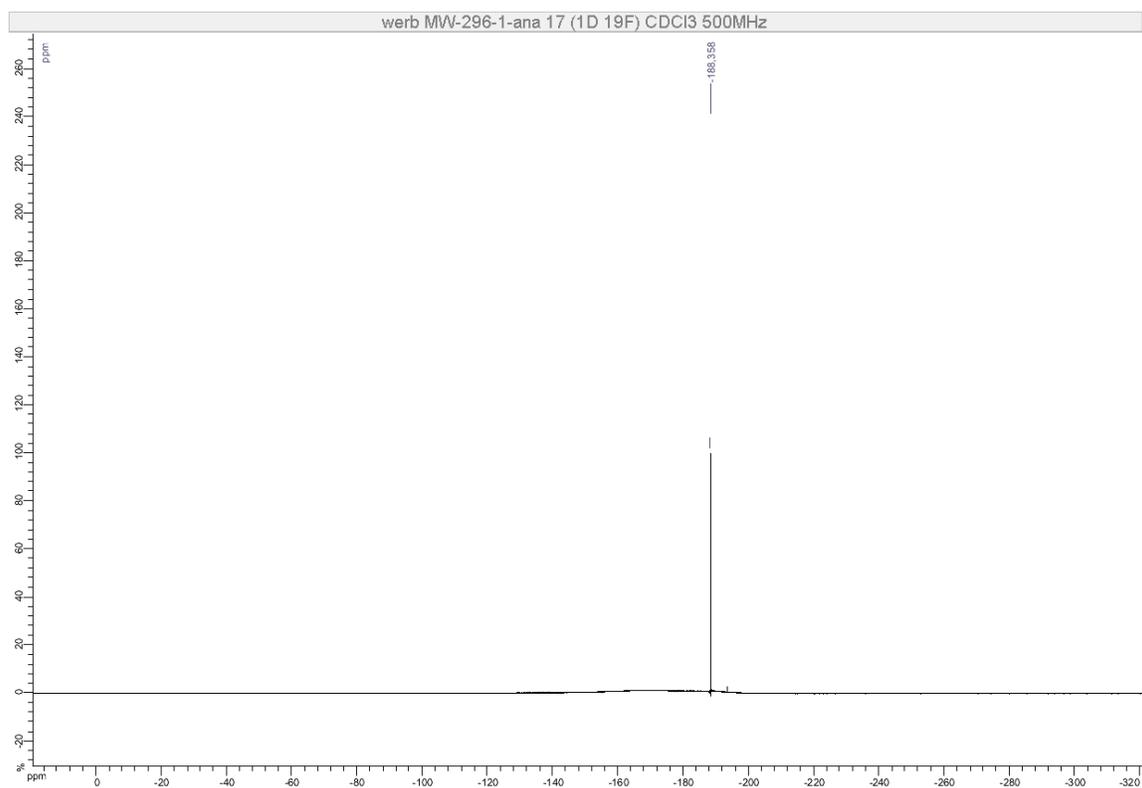
HMBC (500 MHz, CDCl₃)



NOESY (500 MHz, CDCl₃)

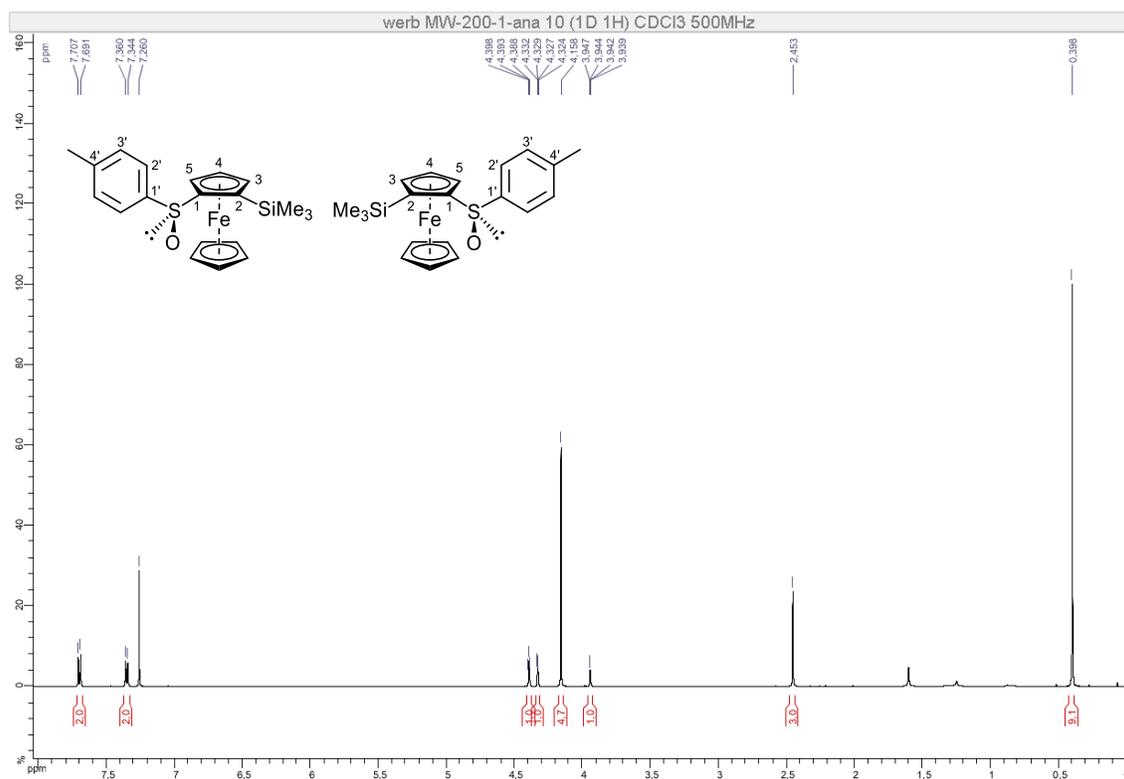


¹⁹F NMR (471 MHz, CDCl₃)

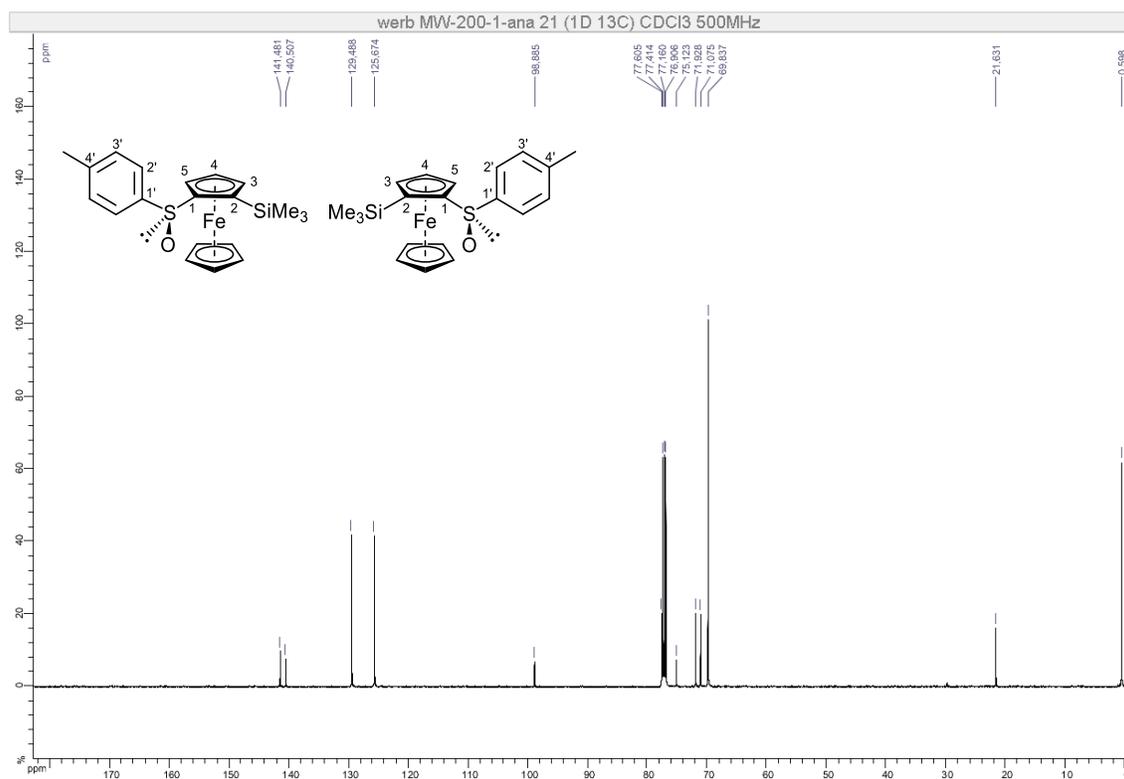


(R,R_P)- and (S,S_P)-S-(4-Tolyl)-2-(trimethylsilyl)ferrocenesulfoxide (R,R_P/S,S_P-3a)

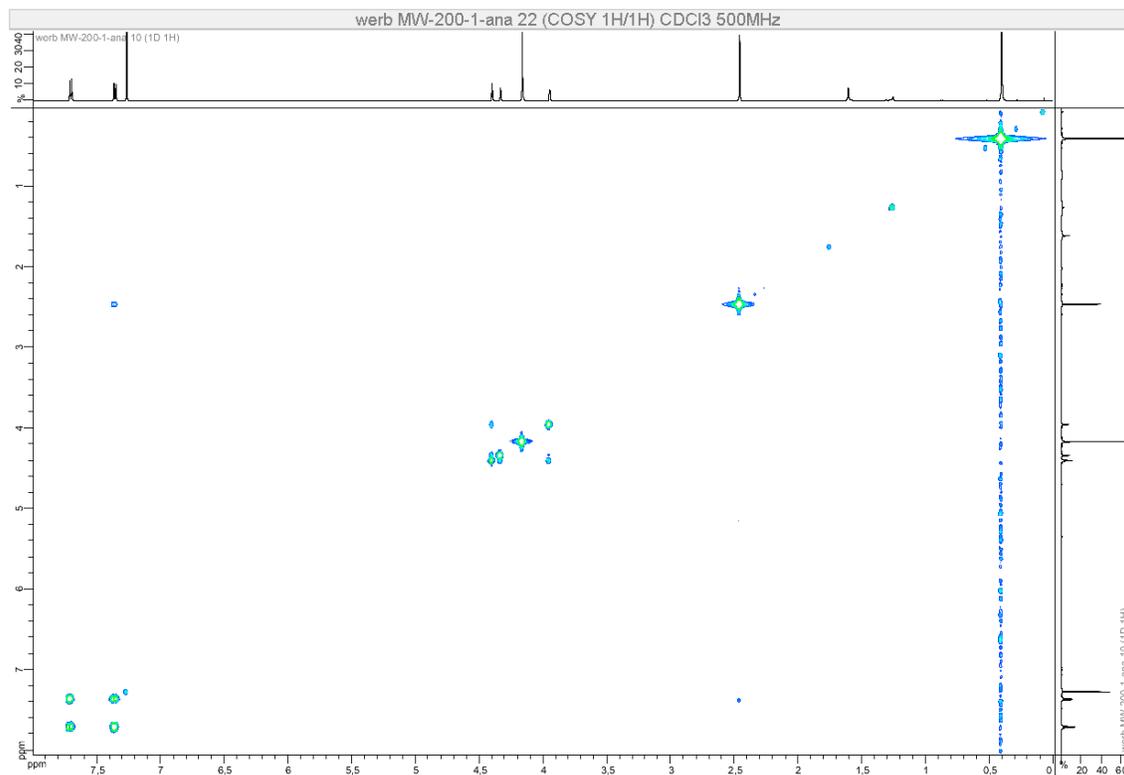
¹H NMR (500 MHz, CDCl₃)



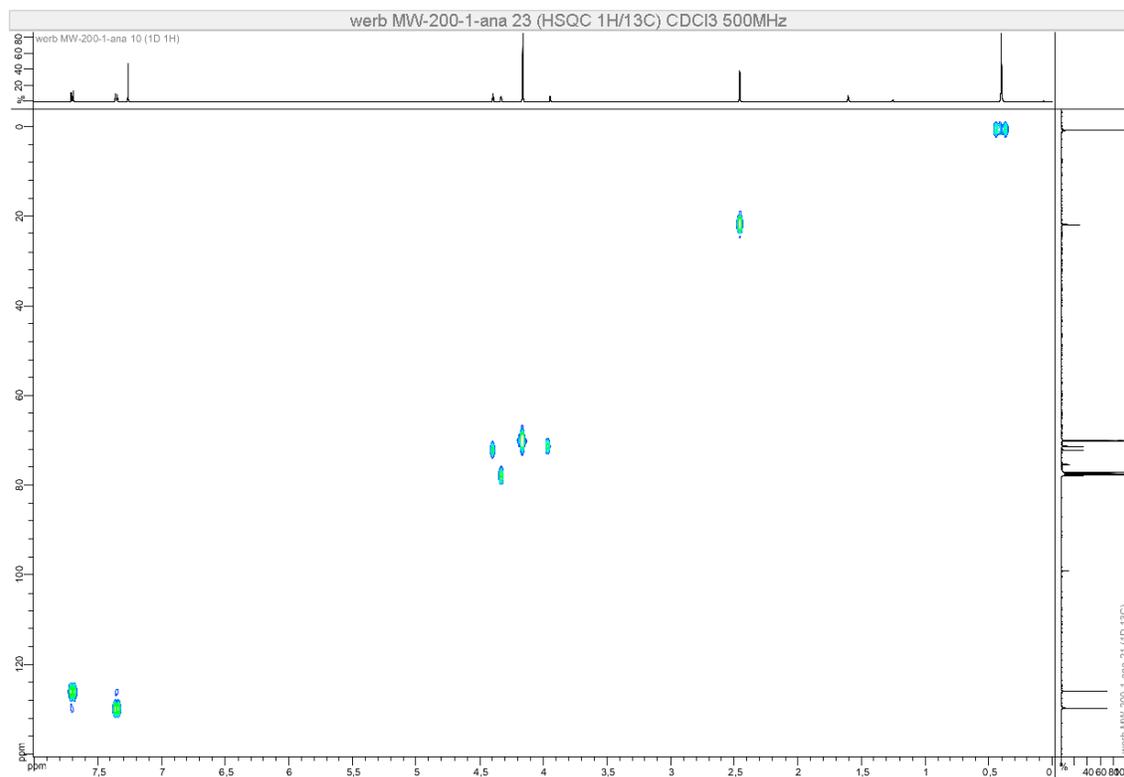
¹³C NMR (126 MHz, CDCl₃)



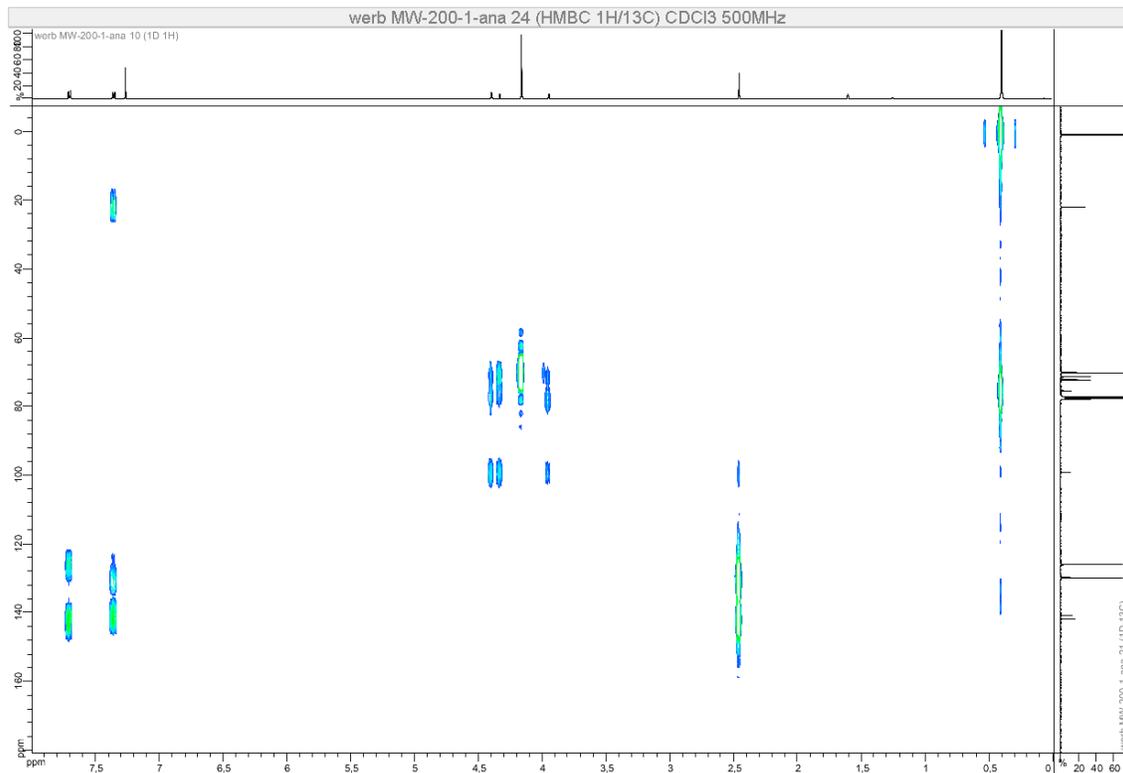
COSY (500 MHz, CDCl₃)



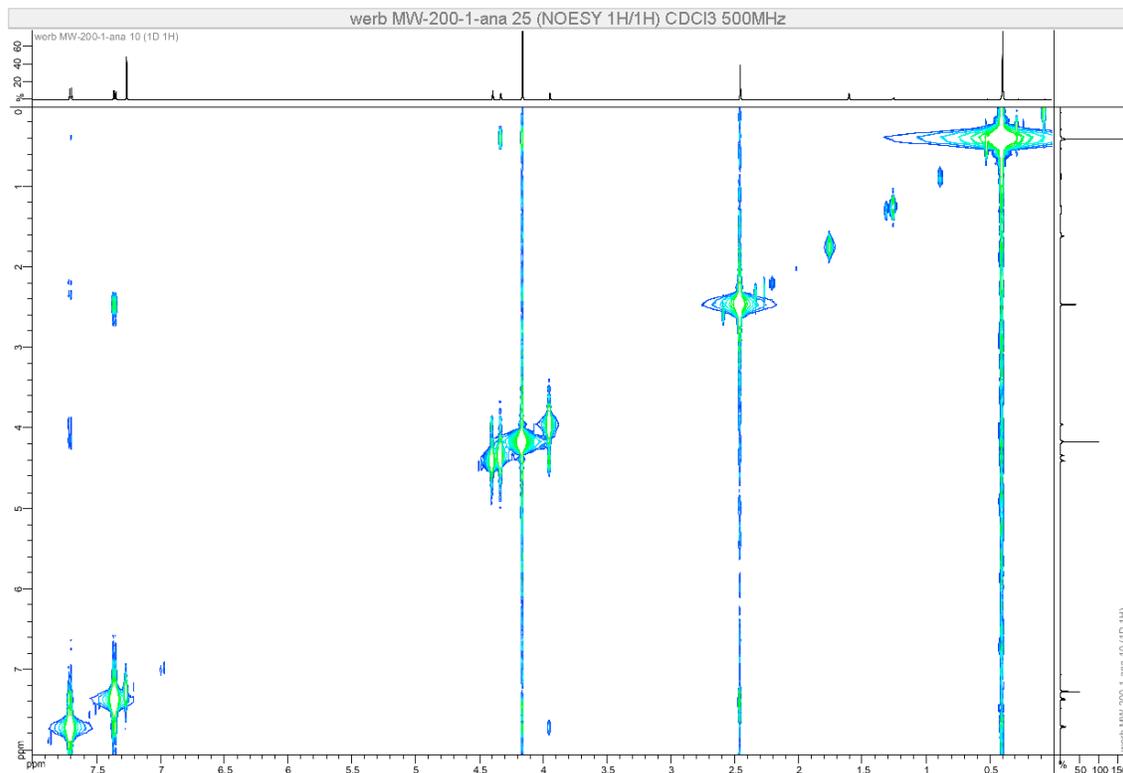
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

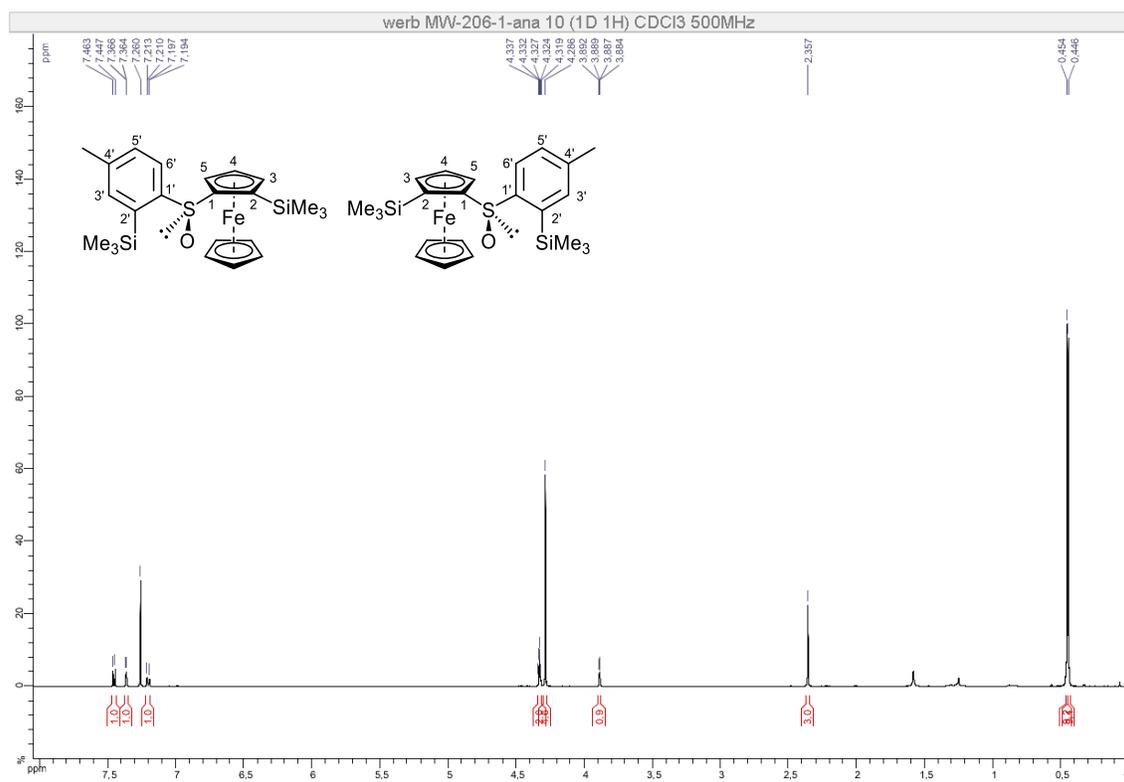


NOESY (500 MHz, CDCl₃)

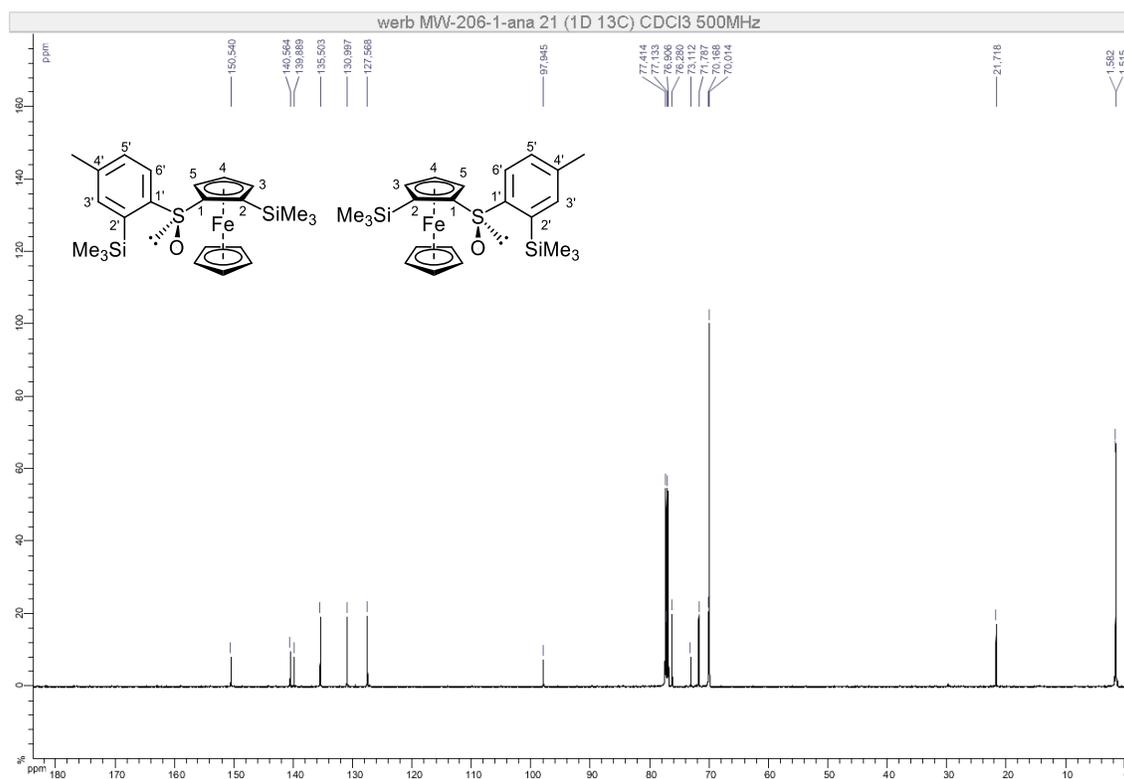


(*R,R*)- and (*S,S*)-*S*-[4-Methyl-2-(trimethylsilyl)phenyl]-2-(trimethylsilyl)ferrocenesulfoxide (*R,R*/*S,S*-3a'**)**

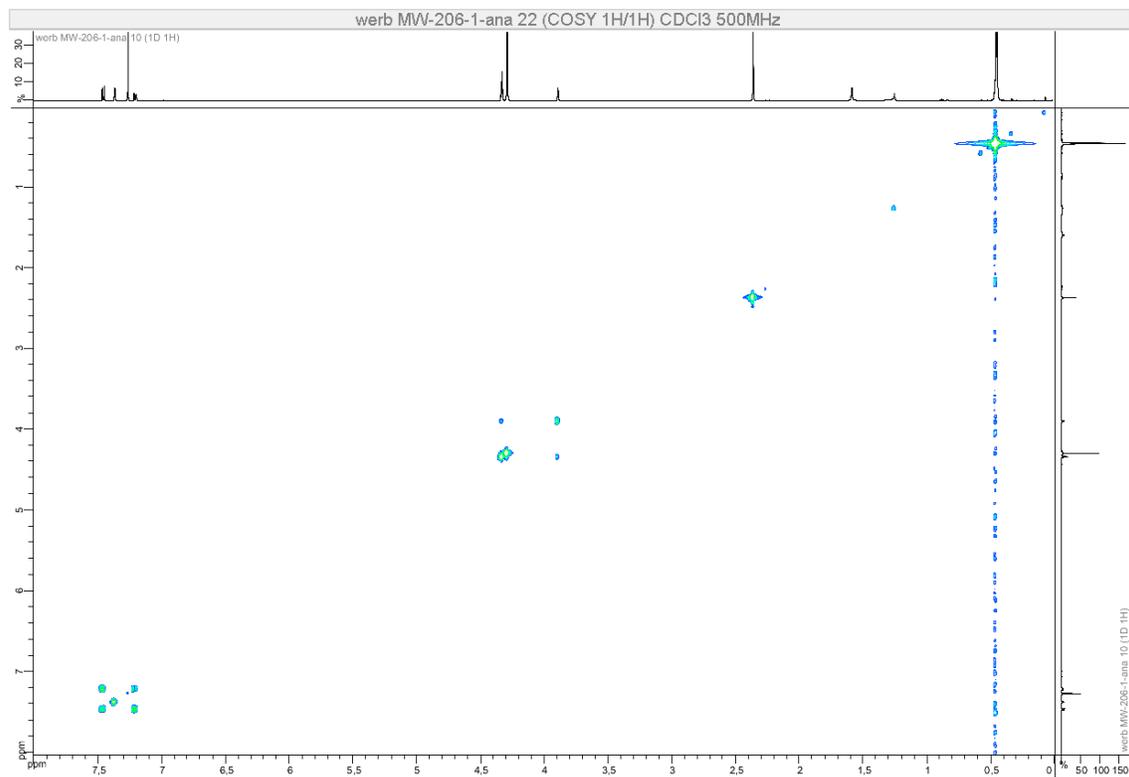
^1H NMR (500 MHz, CDCl_3)



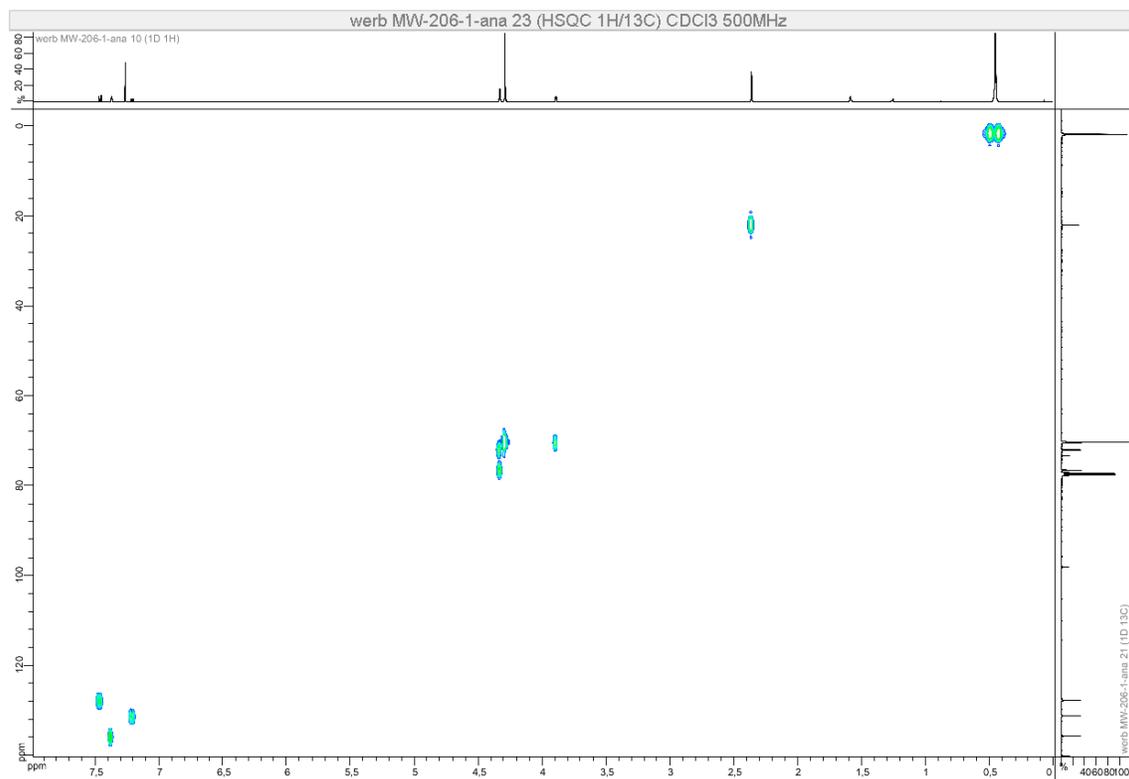
^{13}C NMR (126 MHz, CDCl_3)



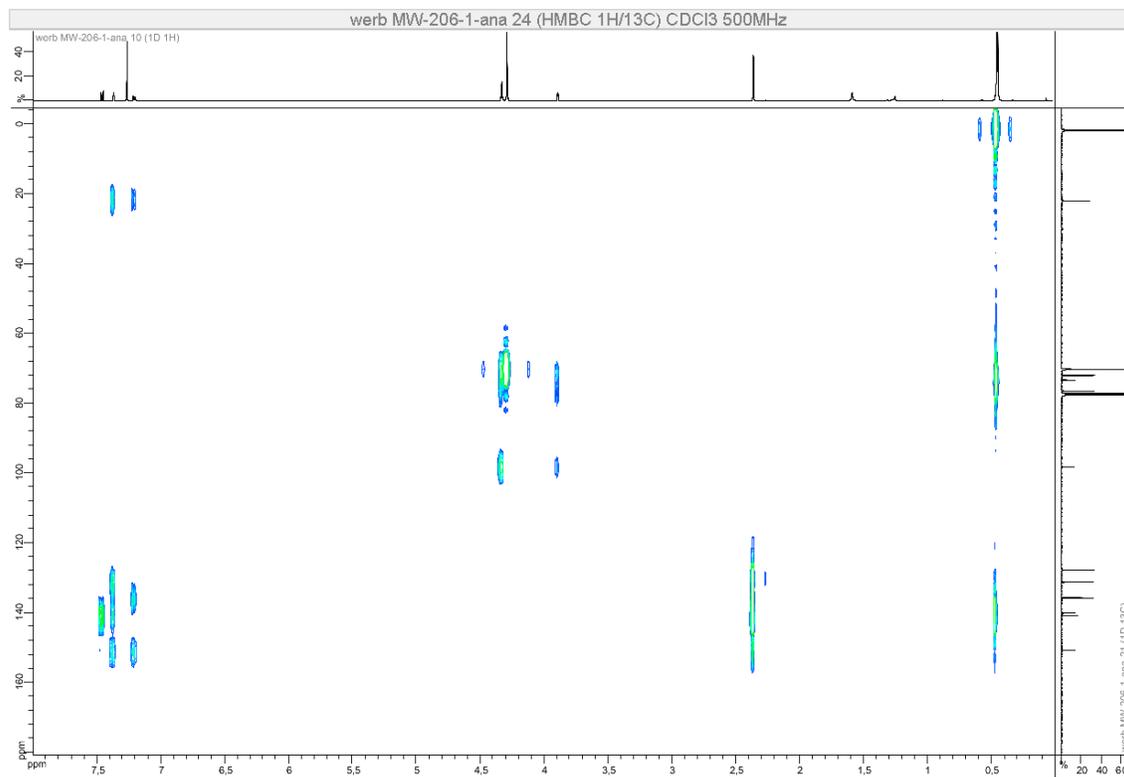
COSY (500 MHz, CDCl₃)



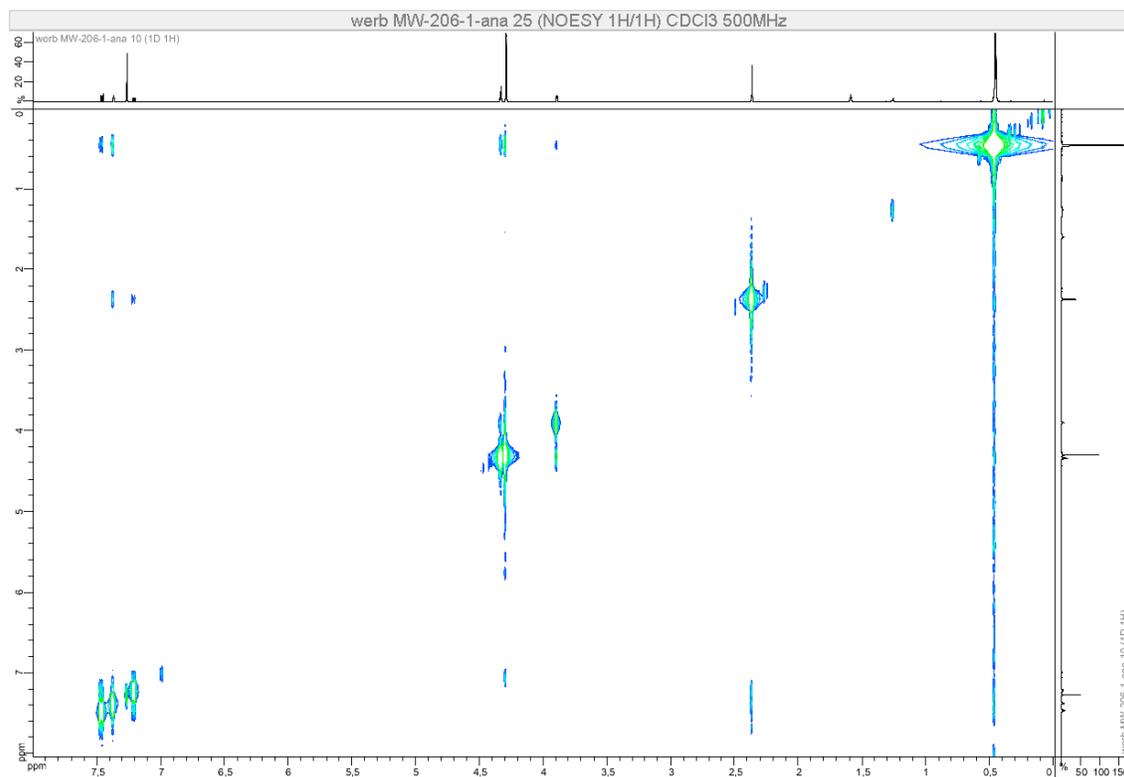
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

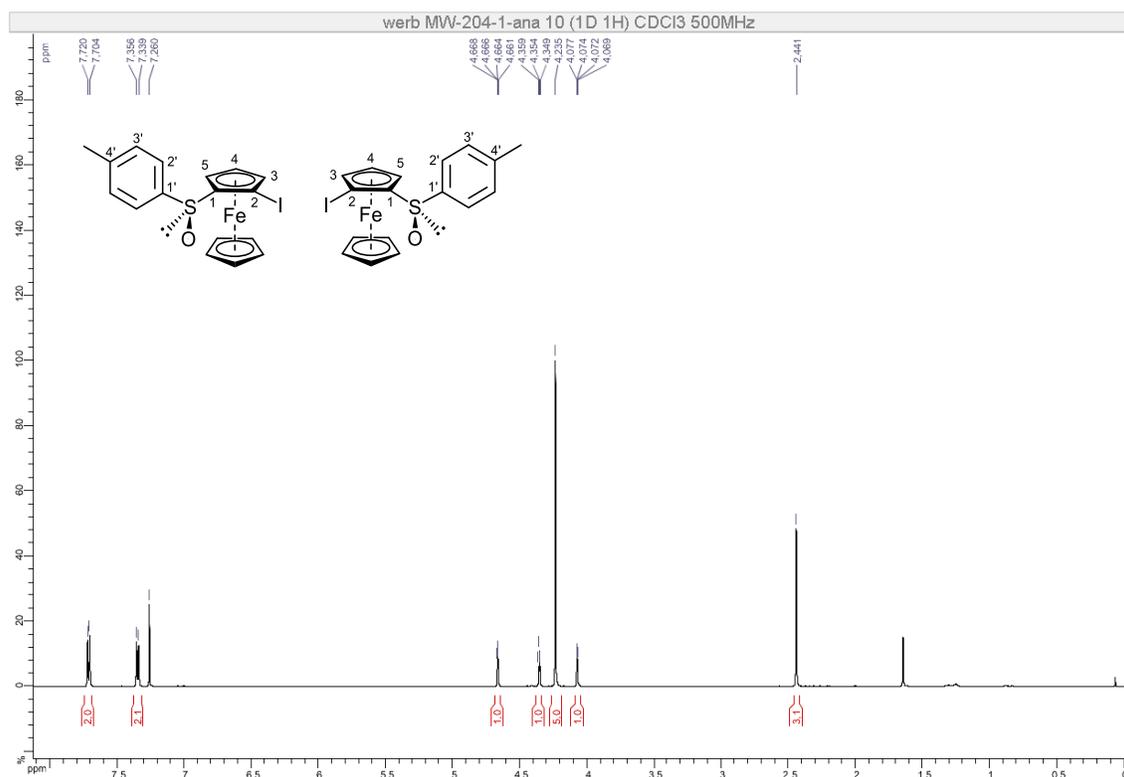


NOESY (500 MHz, CDCl₃)

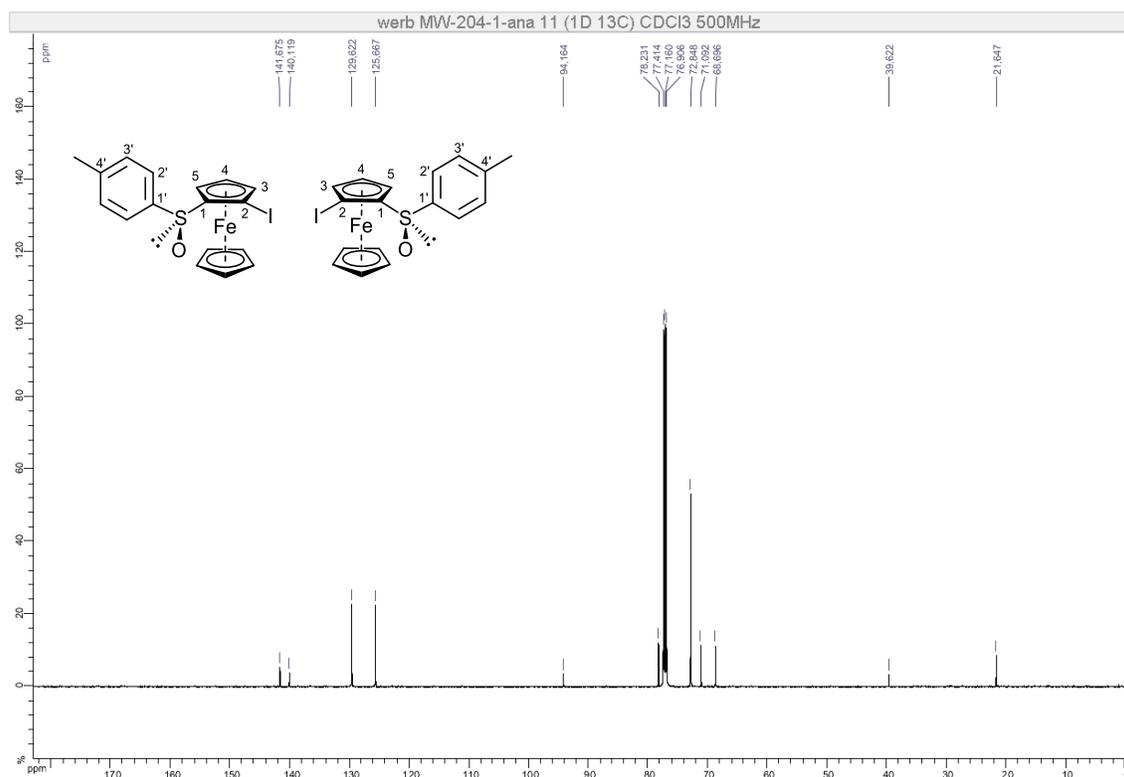


(*R,S*)- and (*S,R*)-2-Iodo-*S*-(4-tolyl)ferrocenesulfoxide (*R,S*/*S,R*-3b)

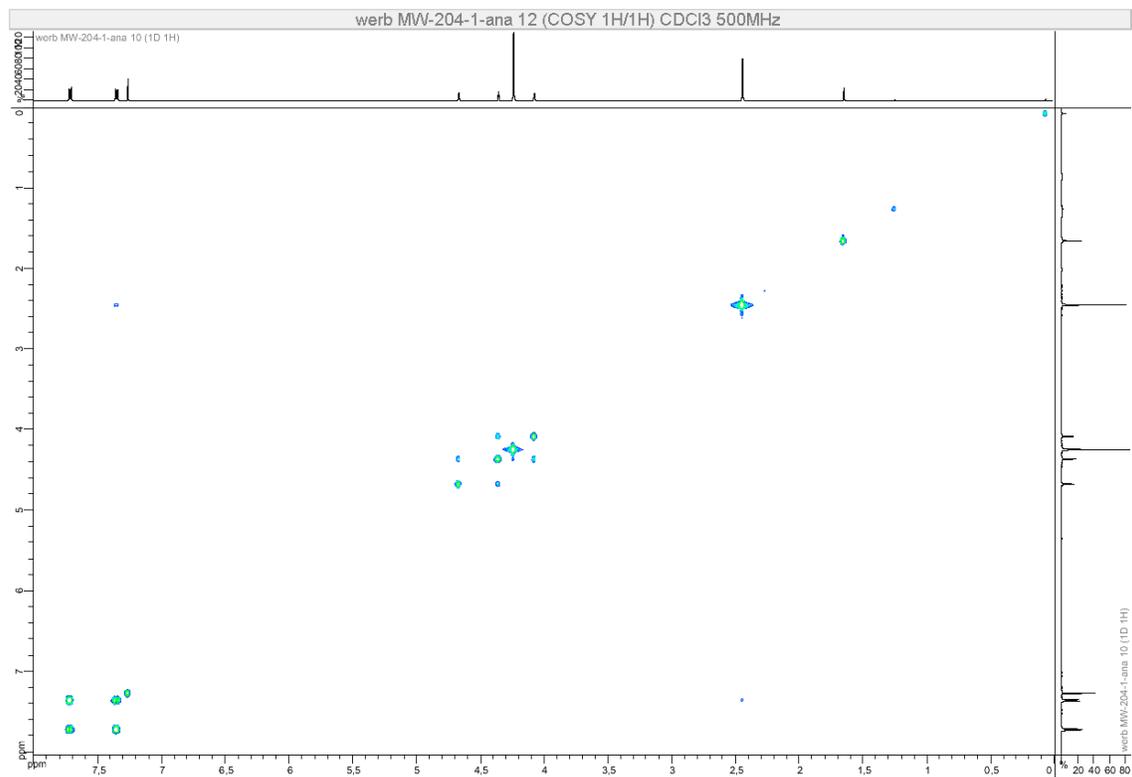
¹H NMR (500 MHz, CDCl₃)



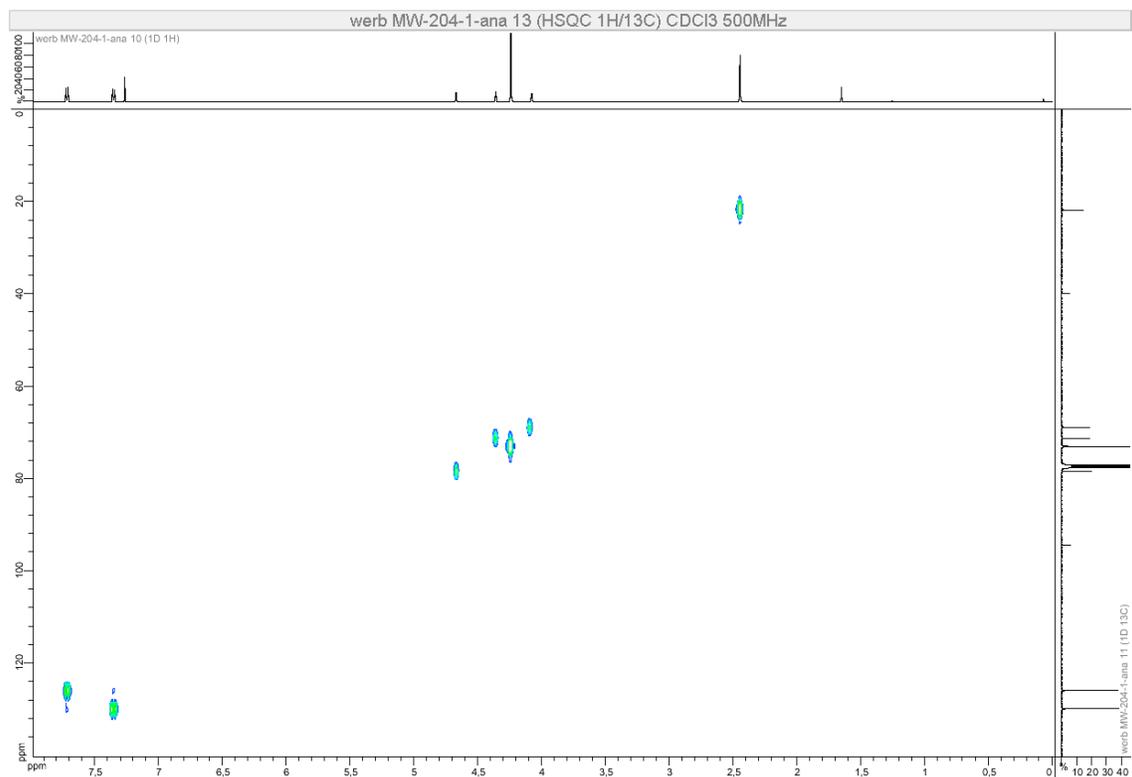
¹³C NMR (126 MHz, CDCl₃)



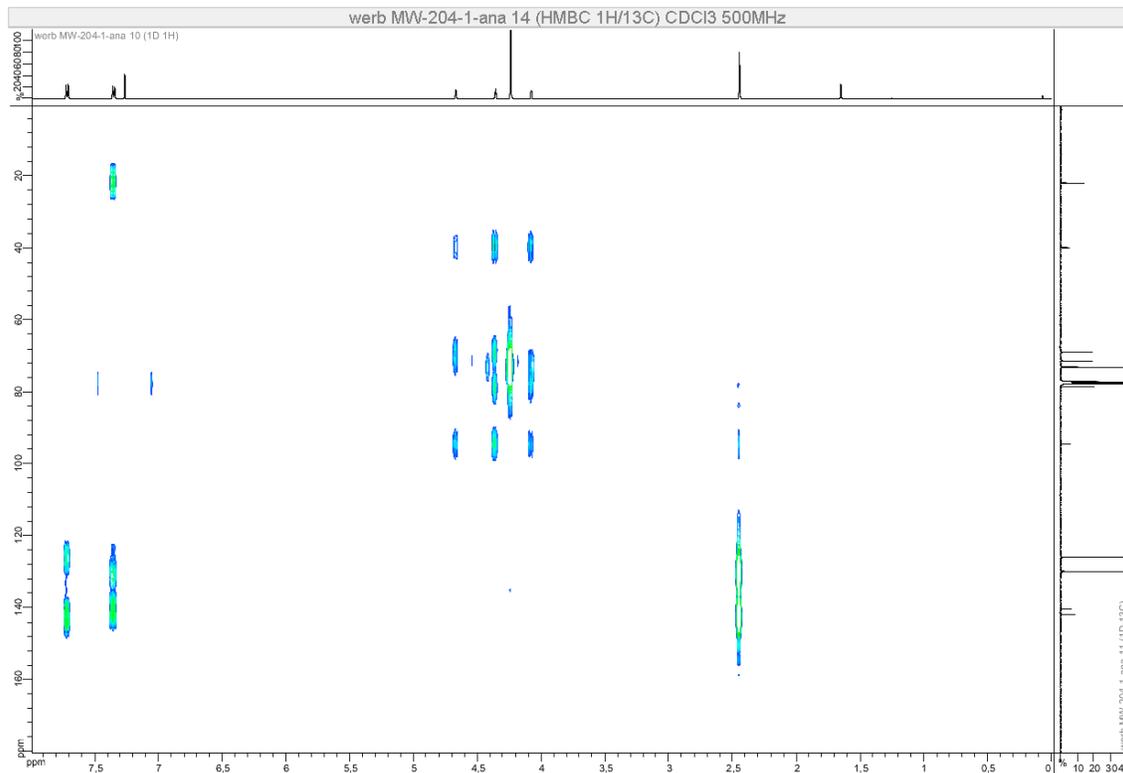
COSY (500 MHz, CDCl₃)



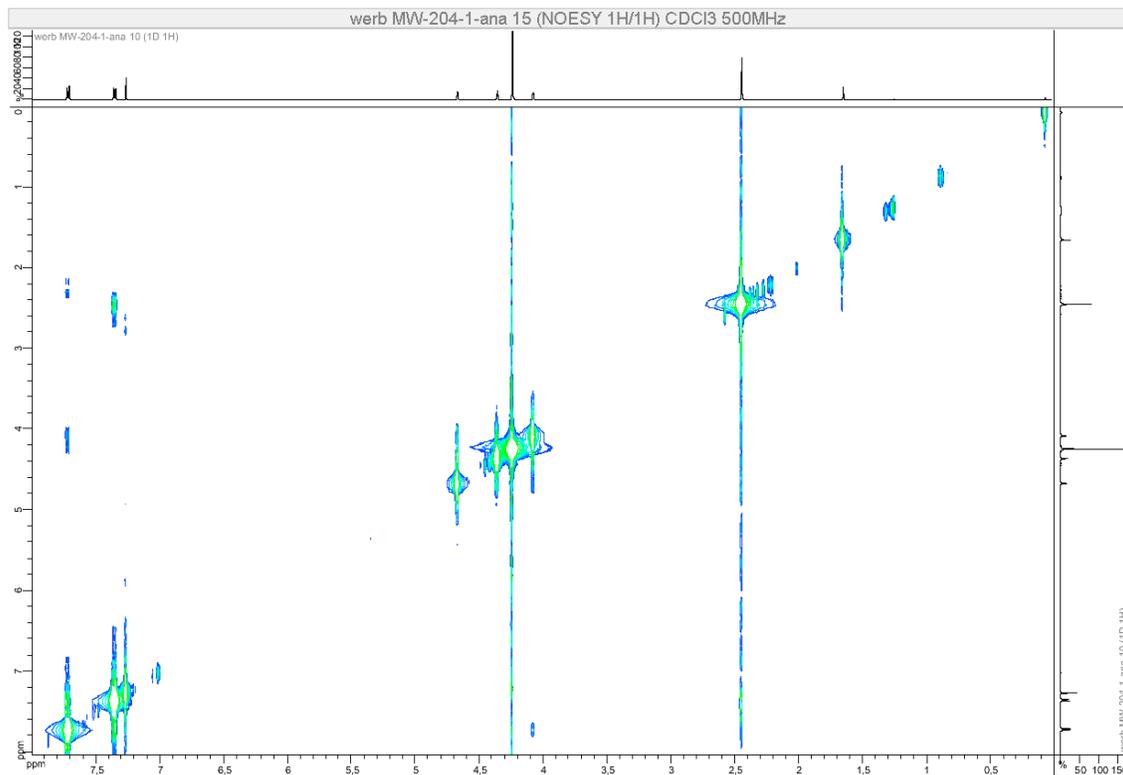
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

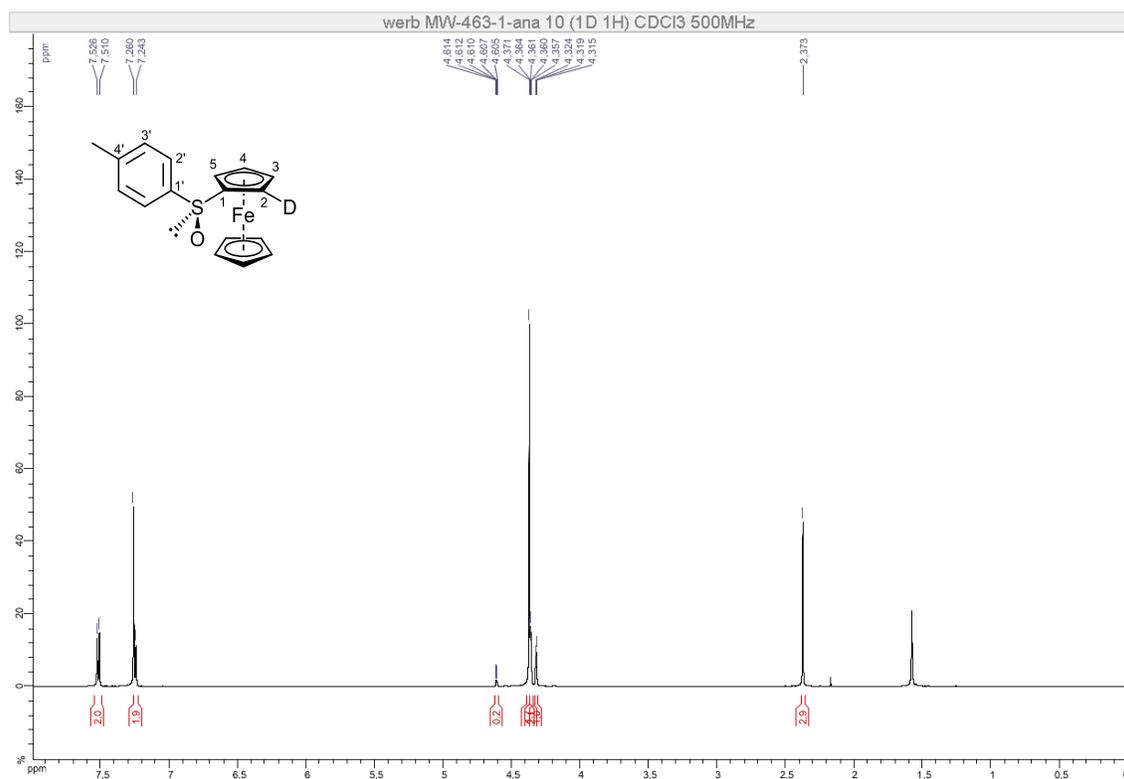


NOESY (500 MHz, CDCl₃)

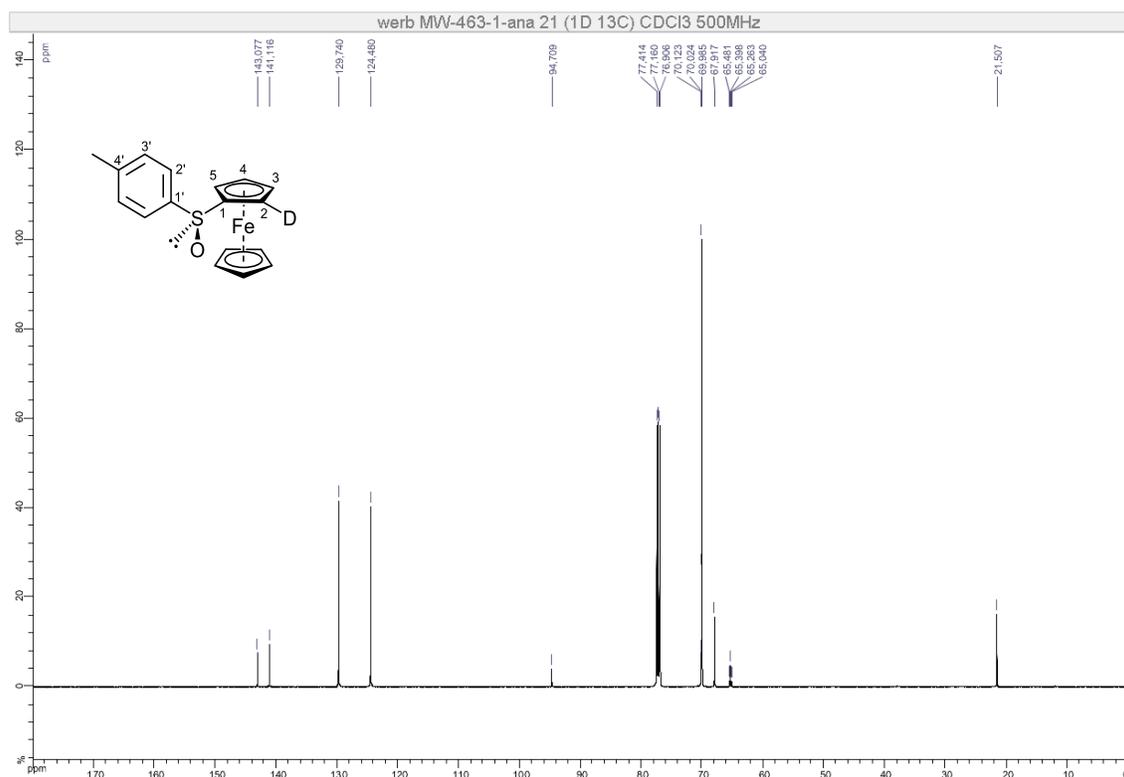


(*S,S*)-2-Deuterio-*S*-(4-*tolyl*)ferrocenesulfoxide (*S,S*)-3c

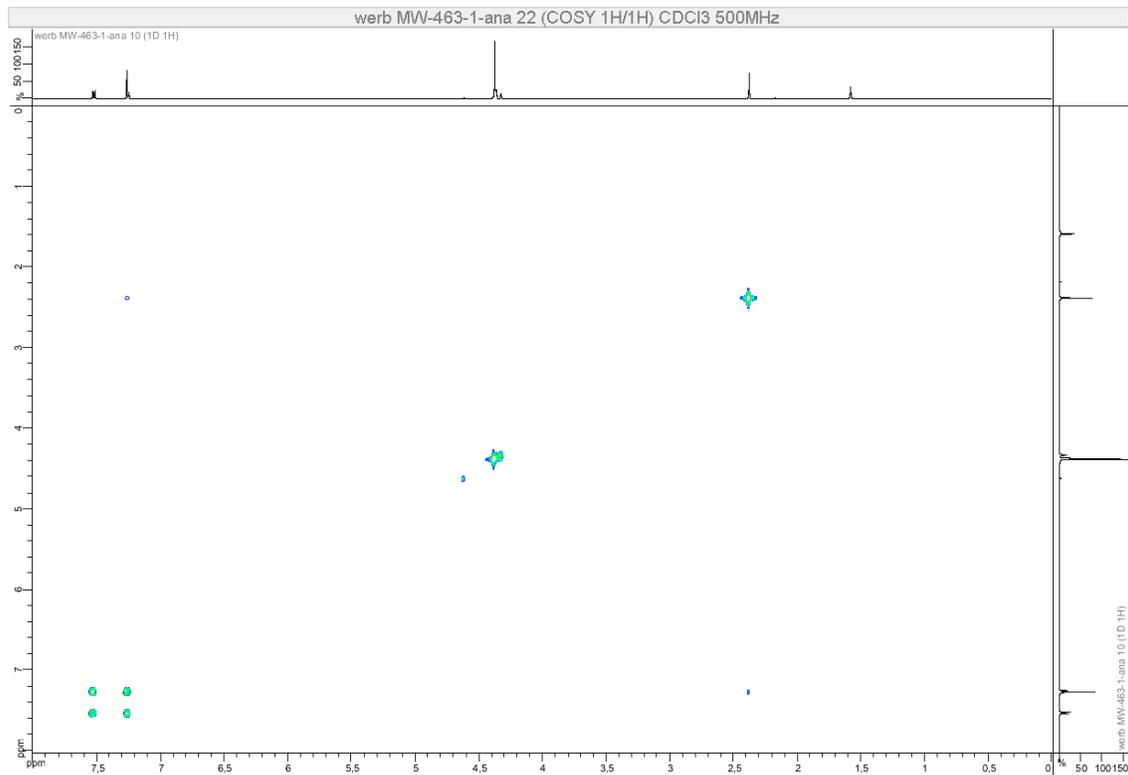
^1H NMR (500 MHz, CDCl_3)



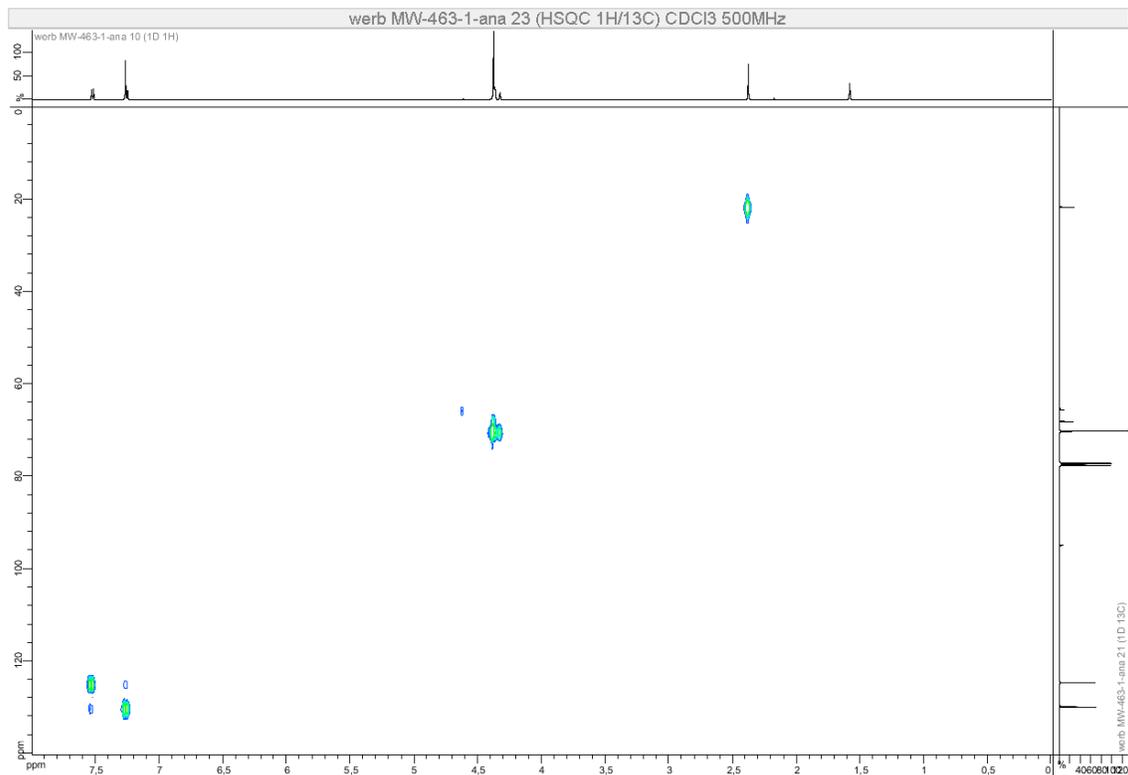
^{13}C NMR (126 MHz, CDCl_3)



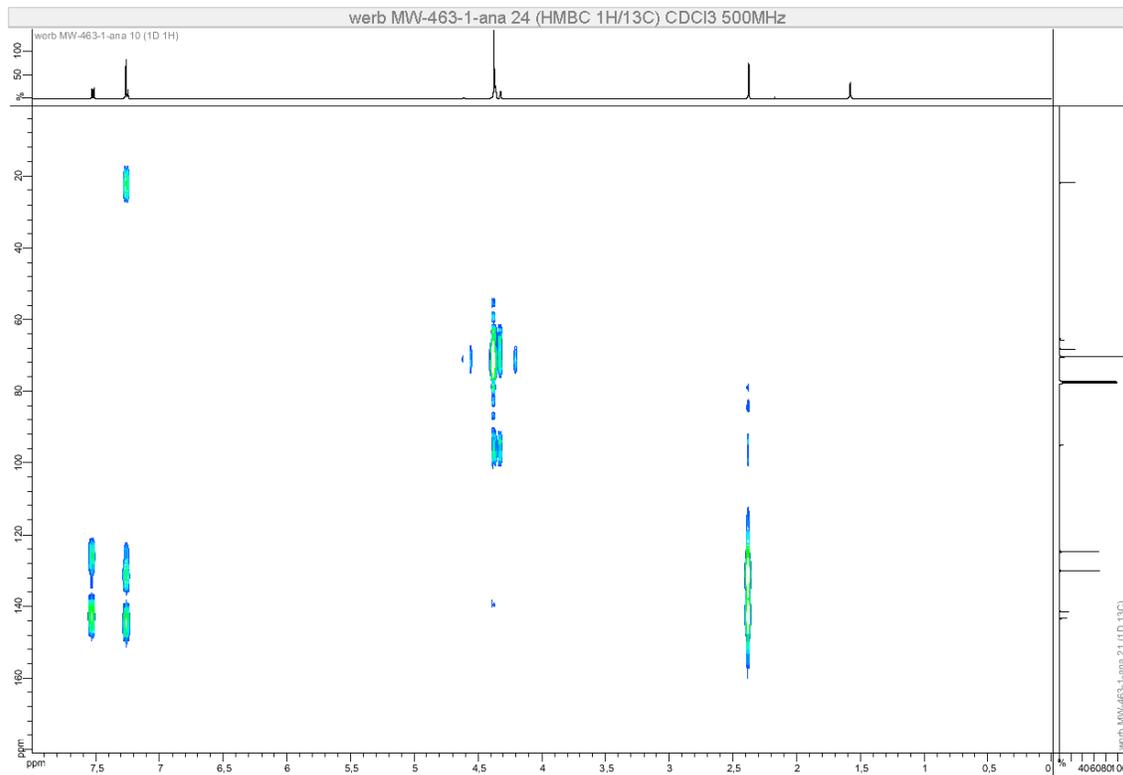
COSY (500 MHz, CDCl₃)



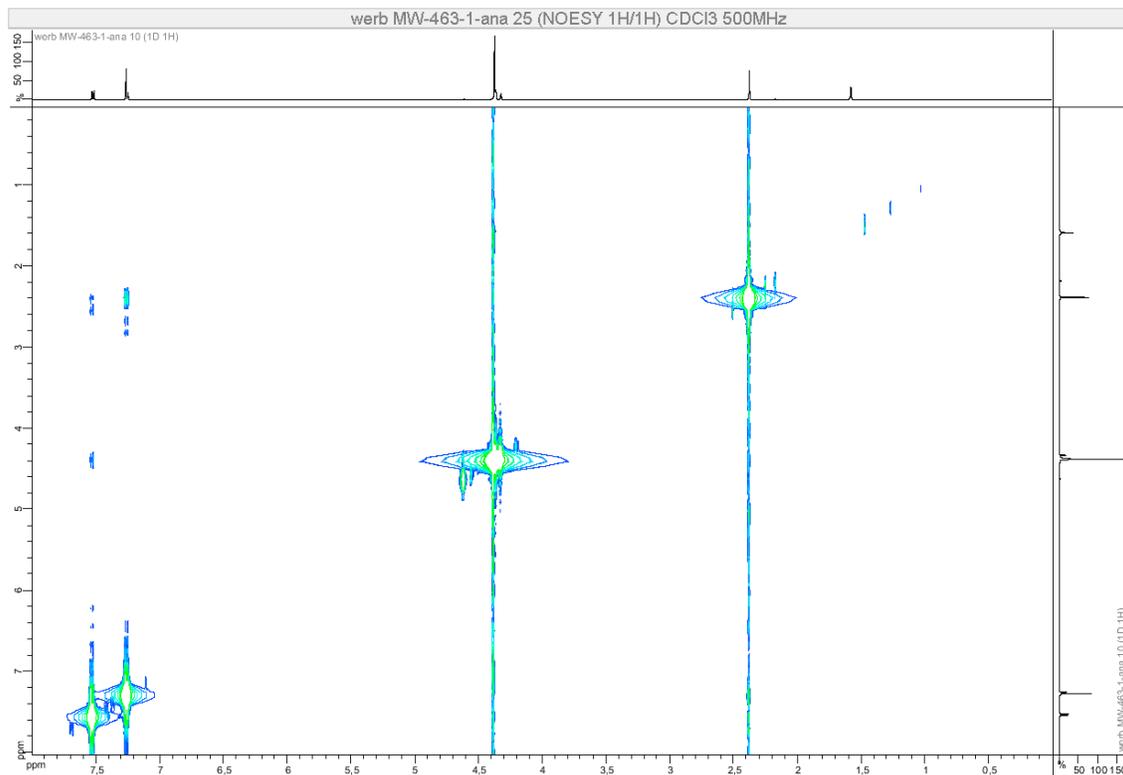
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

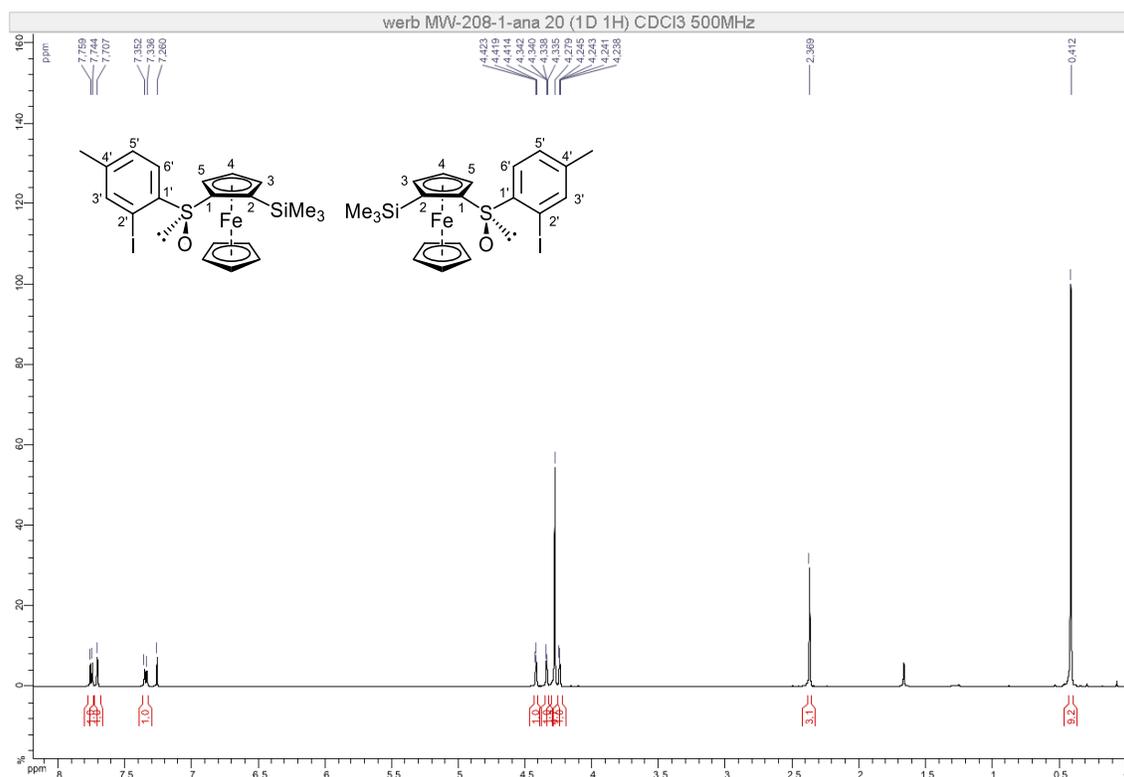


NOESY (500 MHz, CDCl₃)

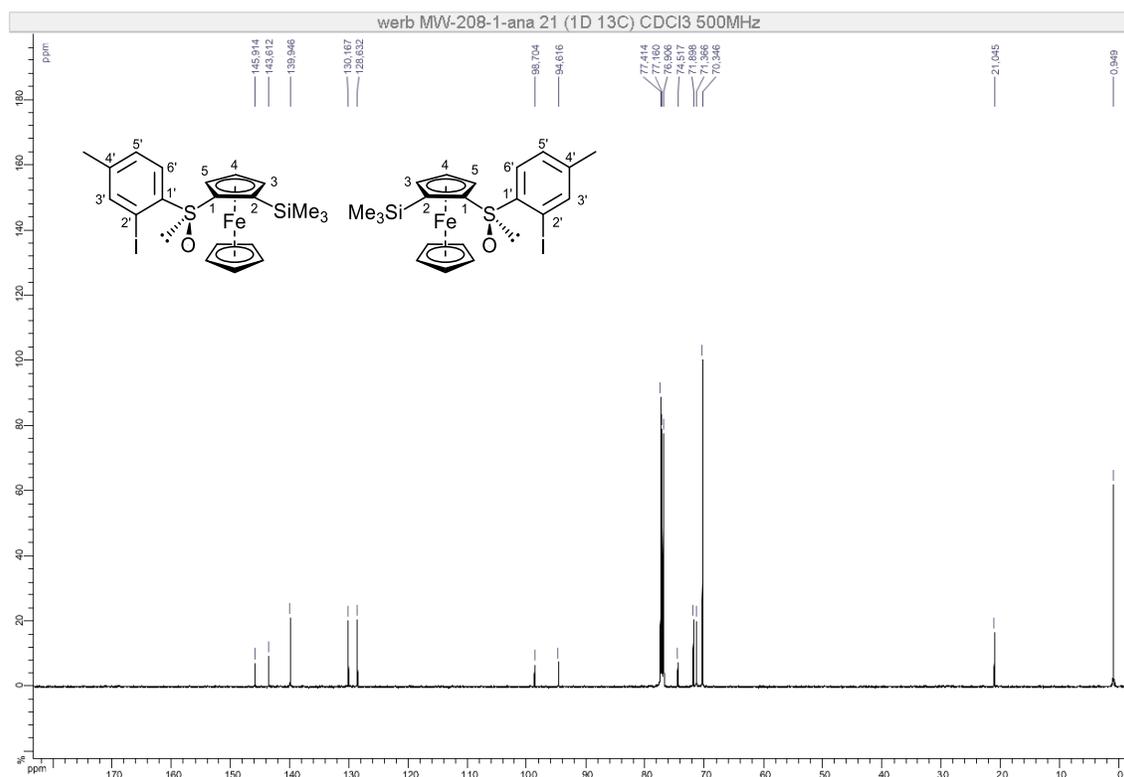


(R,R_P)- and (S,S_P)-S-(2-Iodo-4-tolyl)-2-(trimethylsilyl)ferrocenesulfoxide (R,R_P/S,S_P-4)

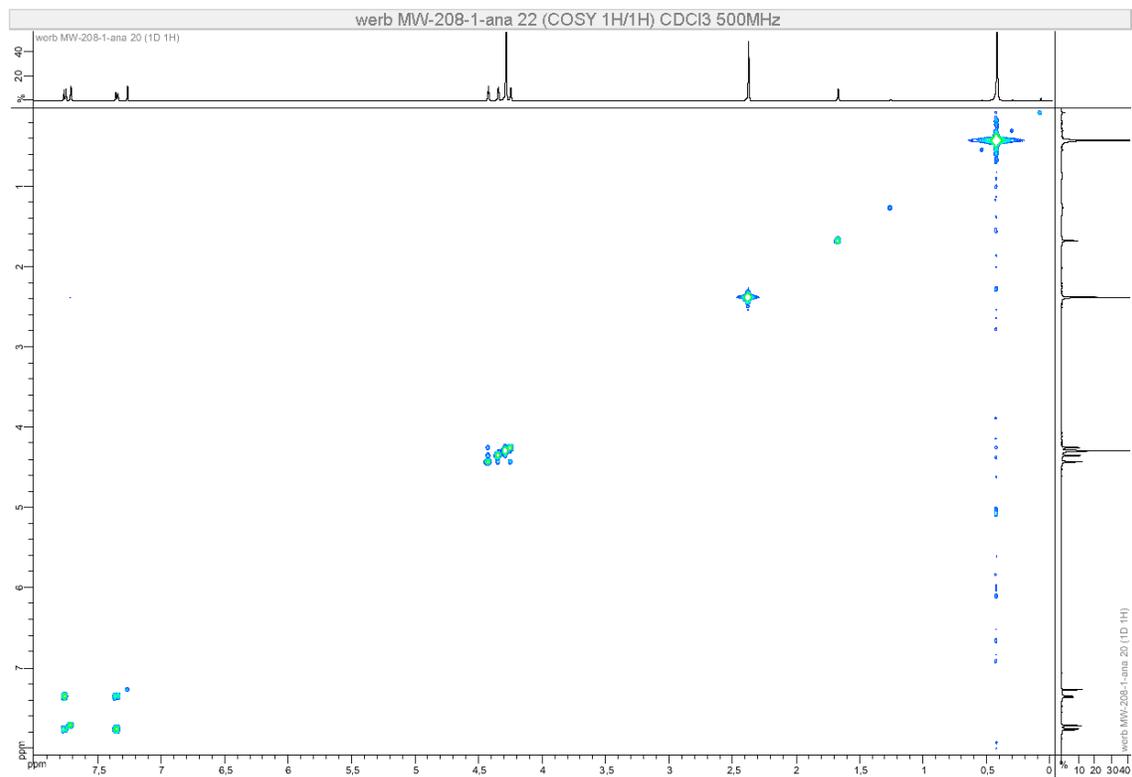
¹H NMR (500 MHz, CDCl₃)



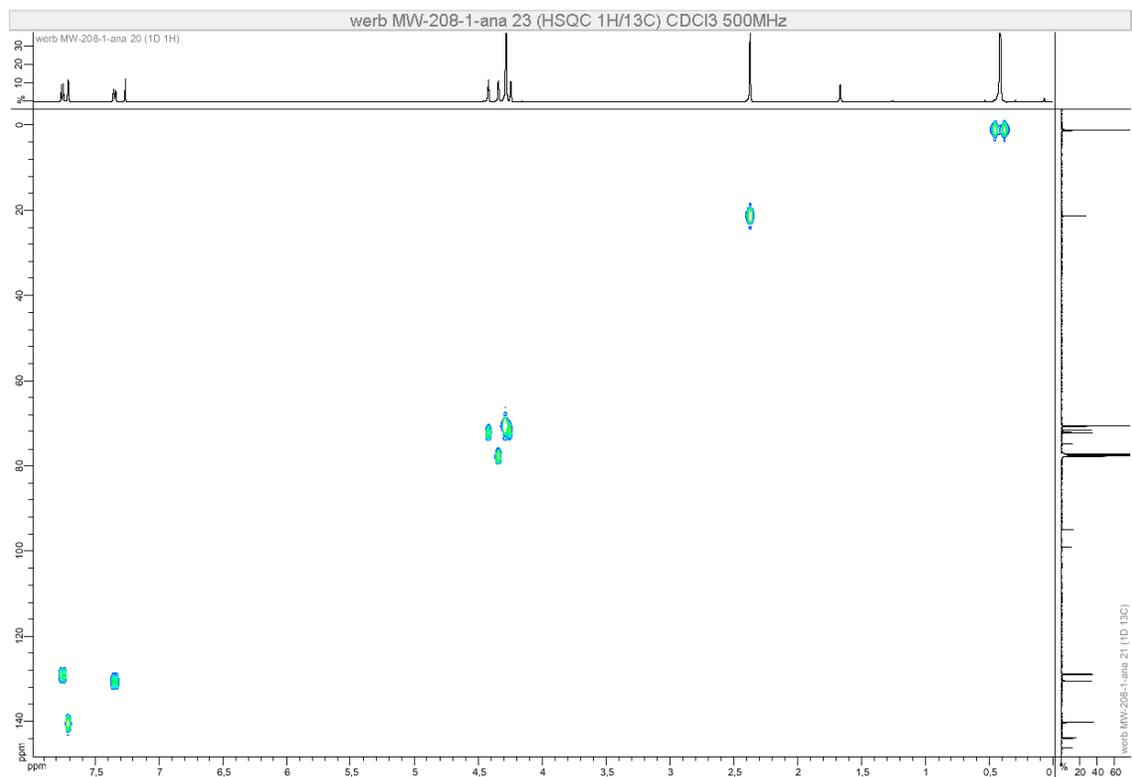
¹³C NMR (126 MHz, CDCl₃)



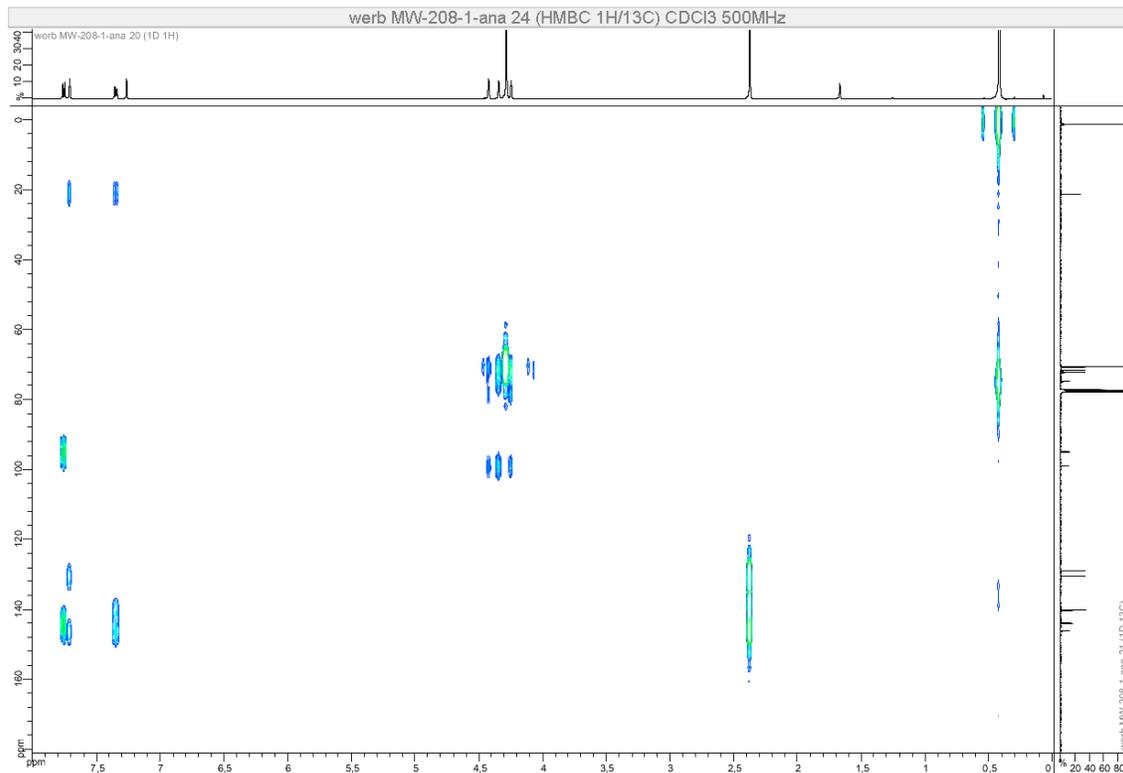
COSY (500 MHz, CDCl₃)



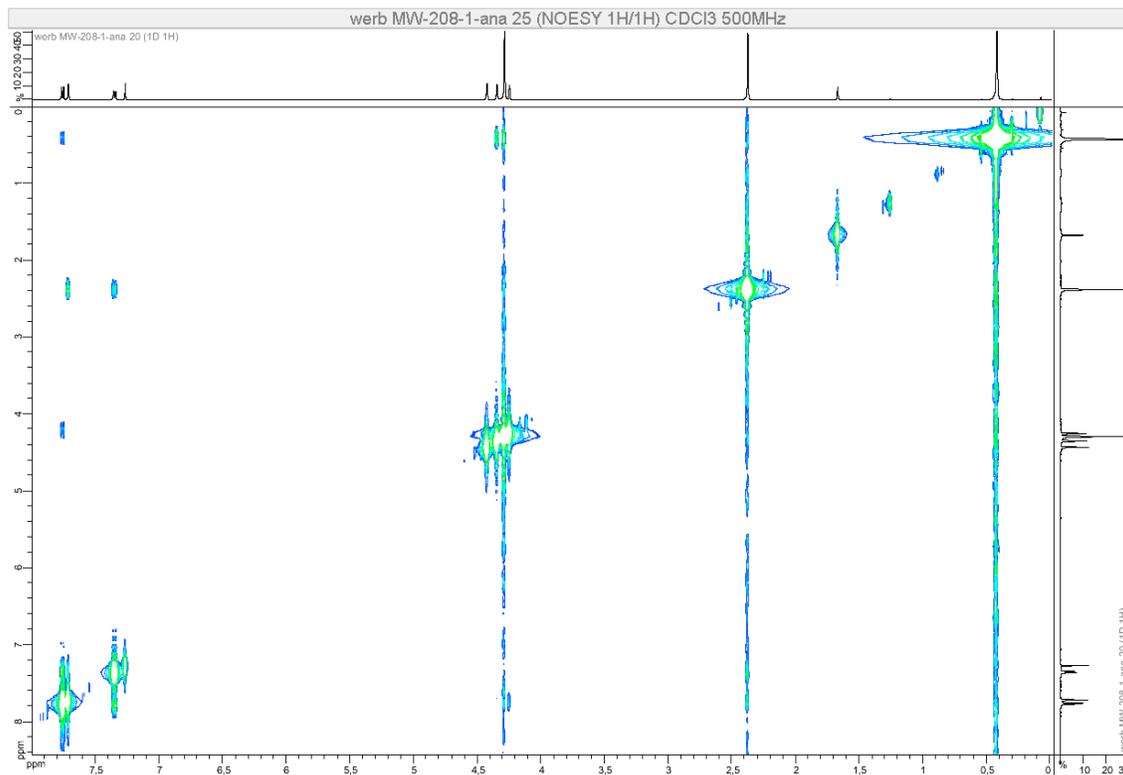
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

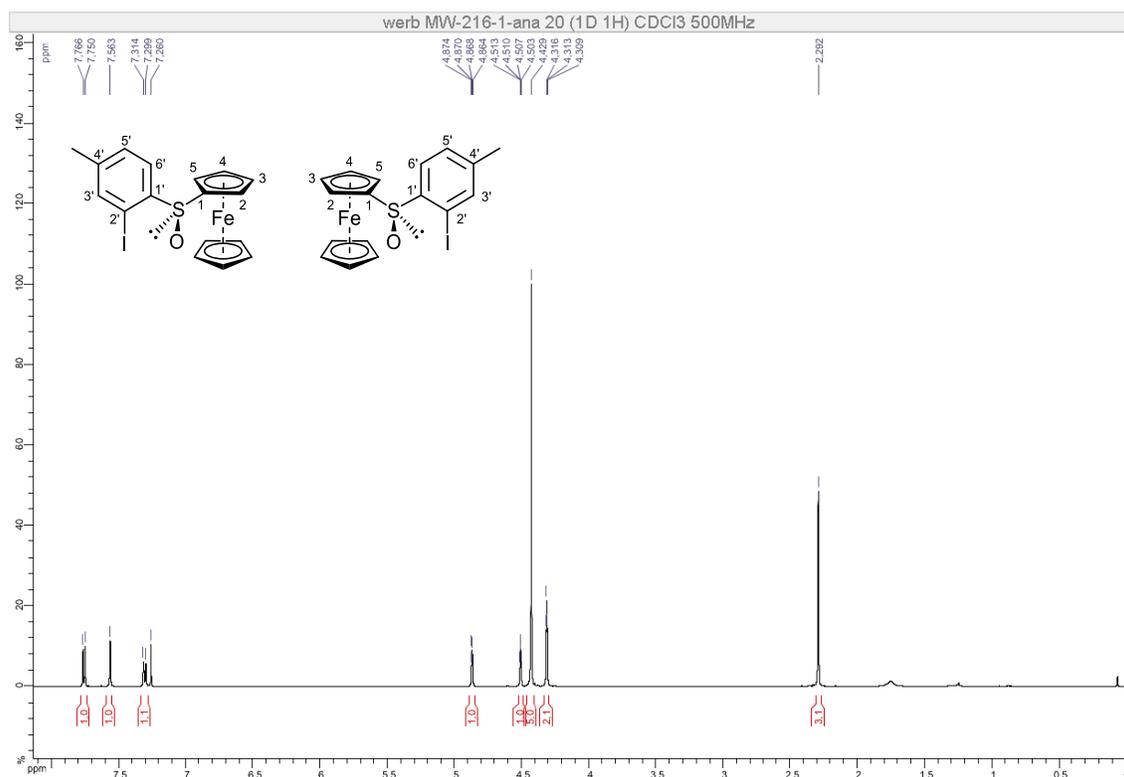


NOESY (500 MHz, CDCl₃)

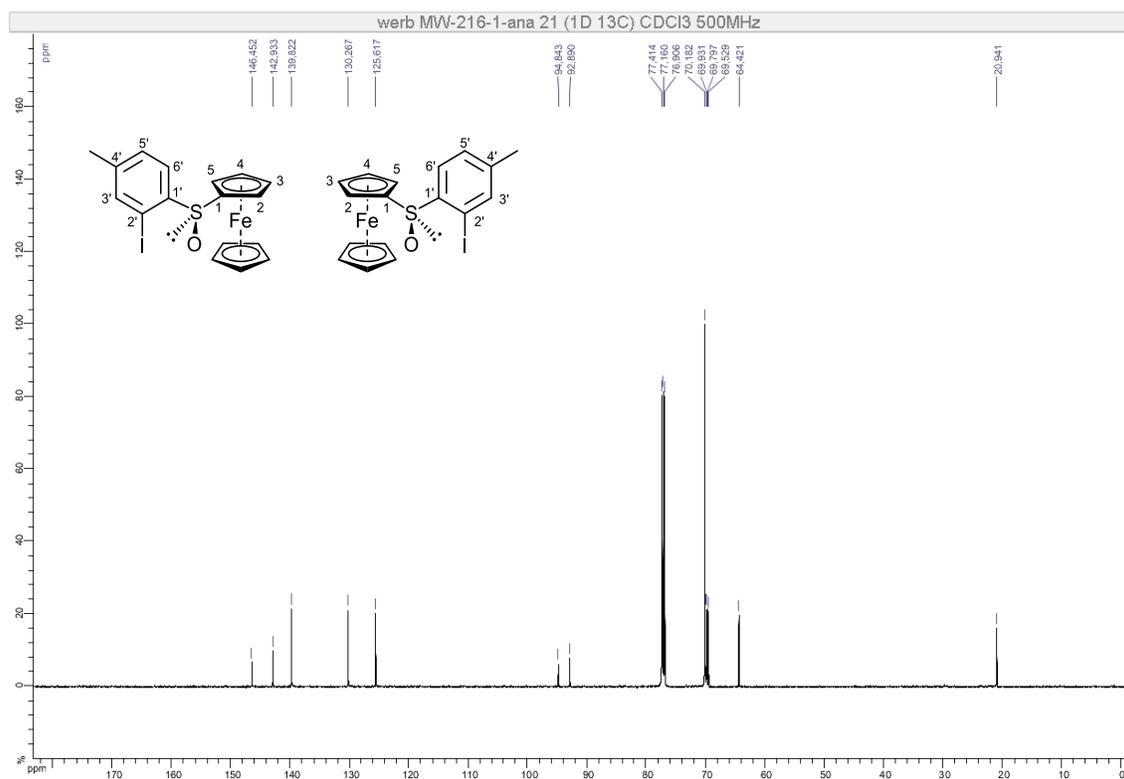


Racemic *S*-(2-Iodo-4-tolyl)ferrocenesulfoxide (*rac*-5)

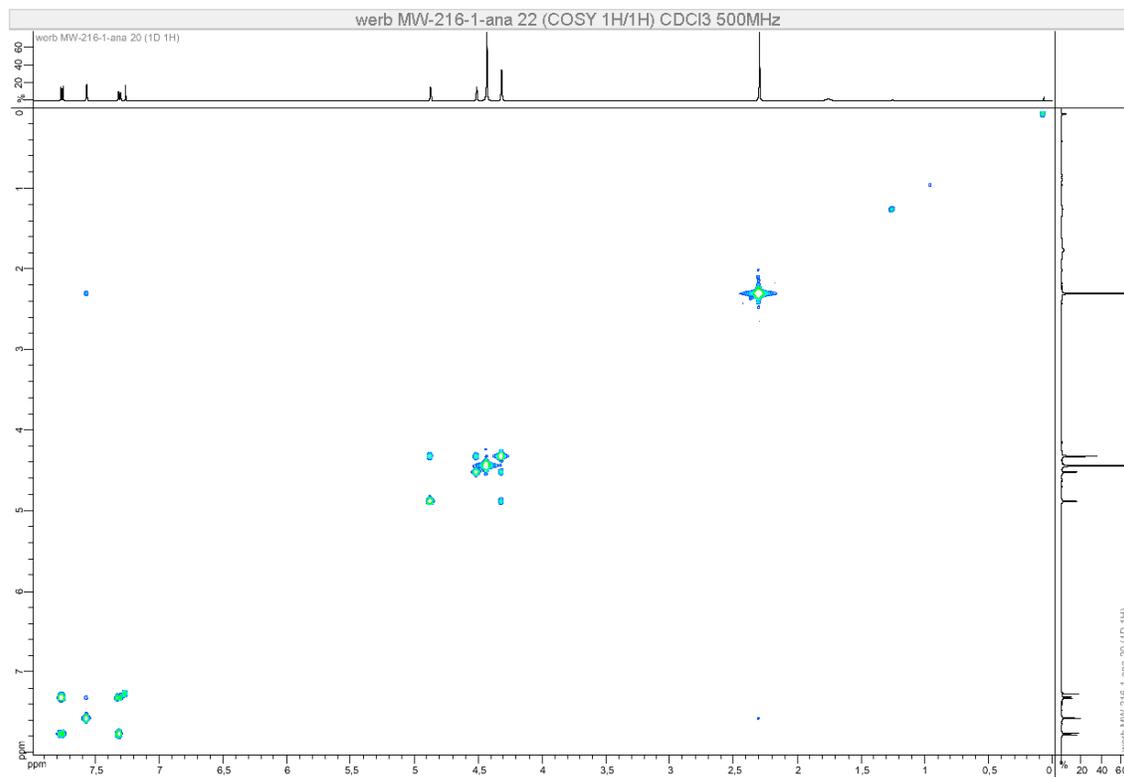
^1H NMR (500 MHz, CDCl_3)



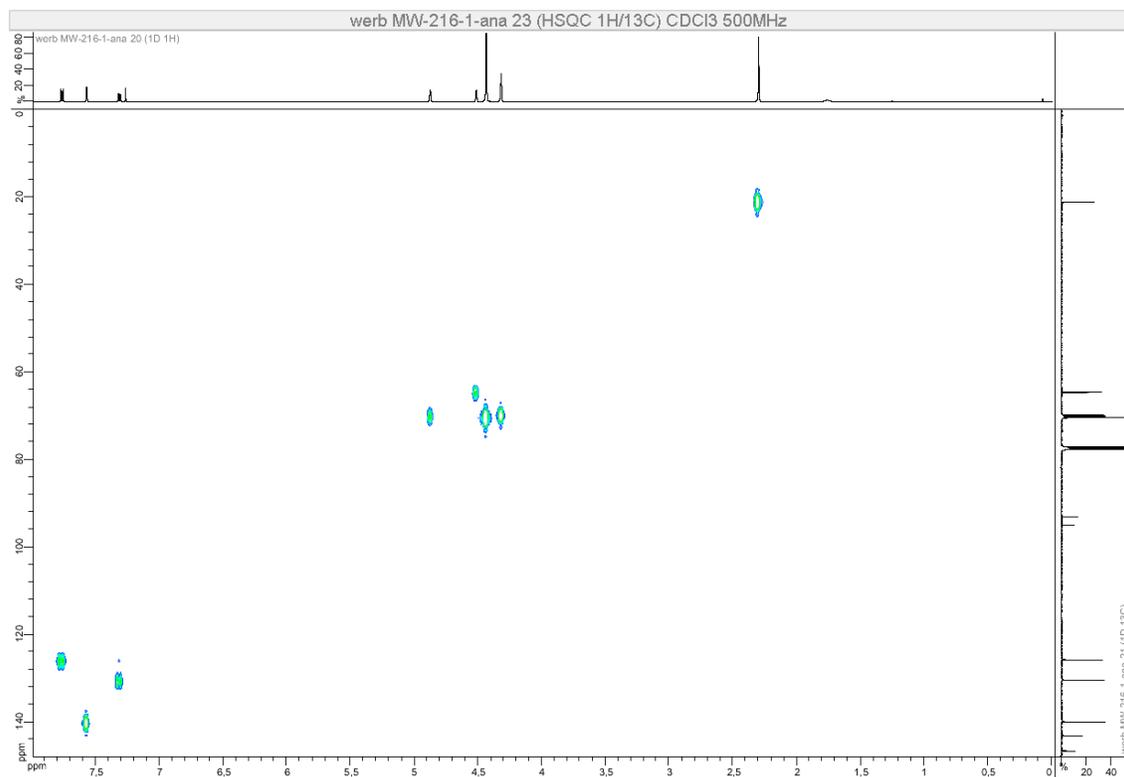
^{13}C NMR (126 MHz, CDCl_3)



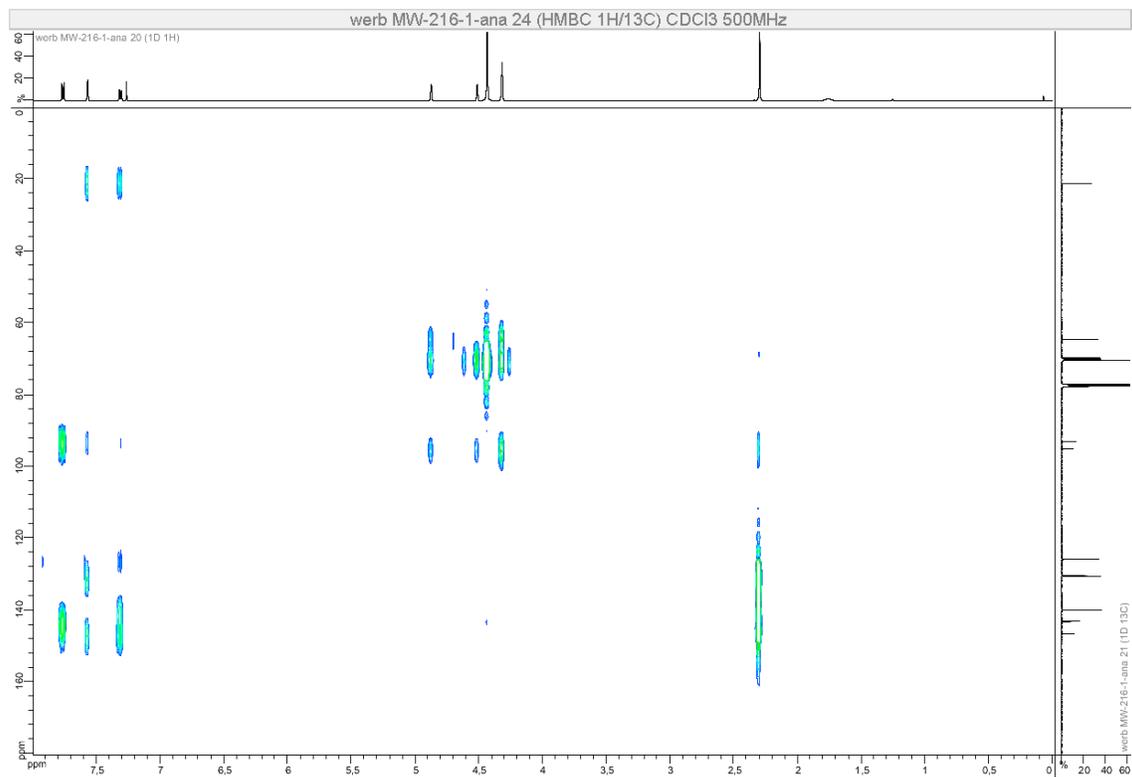
COSY (500 MHz, CDCl₃)



HSQC (500 MHz, CDCl₃)

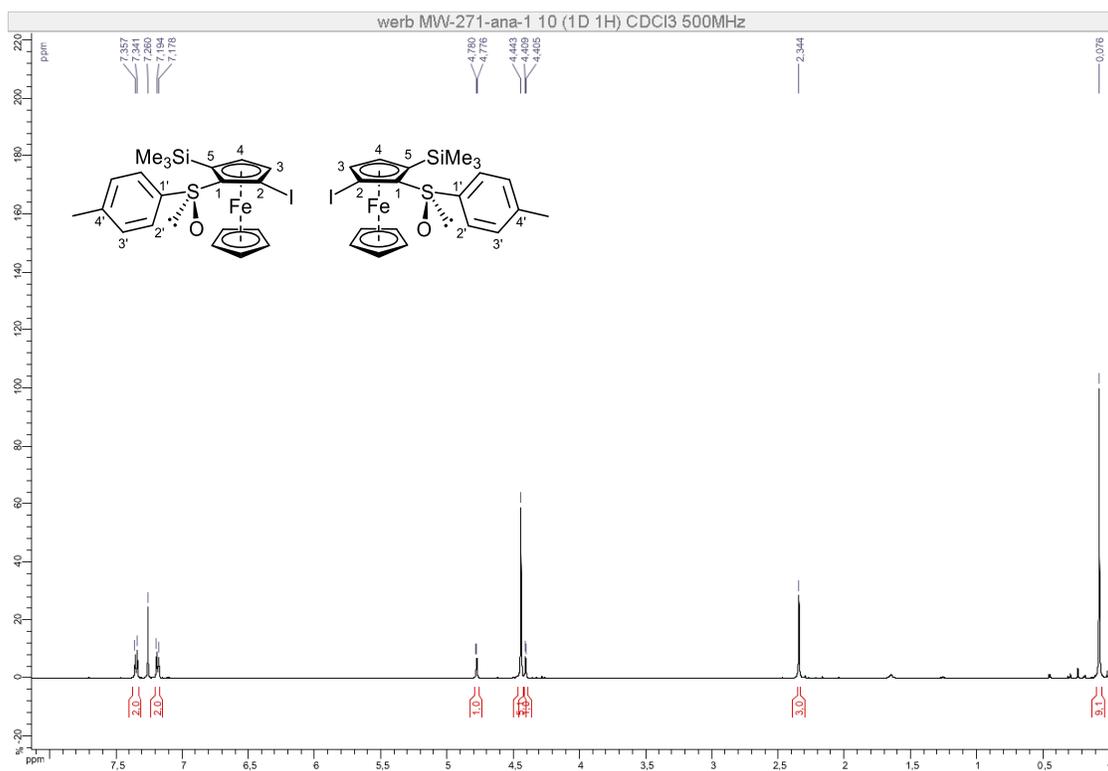


HMBC (500 MHz, CDCl₃)

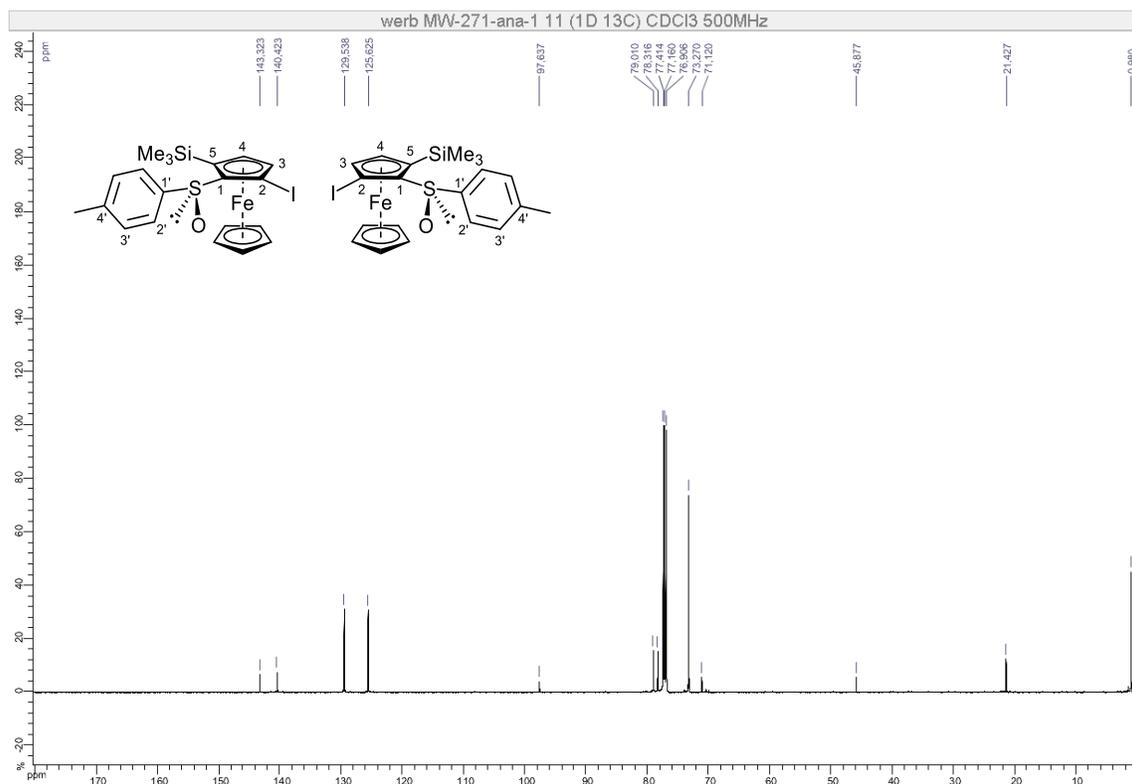


(*R,S*P)- and (*S,R*P)-2-Iodo-*S*-(4-tolyl)-5-(trimethylsilyl)ferrocenesulfoxide (*R,S*P/*S,R*P-6)

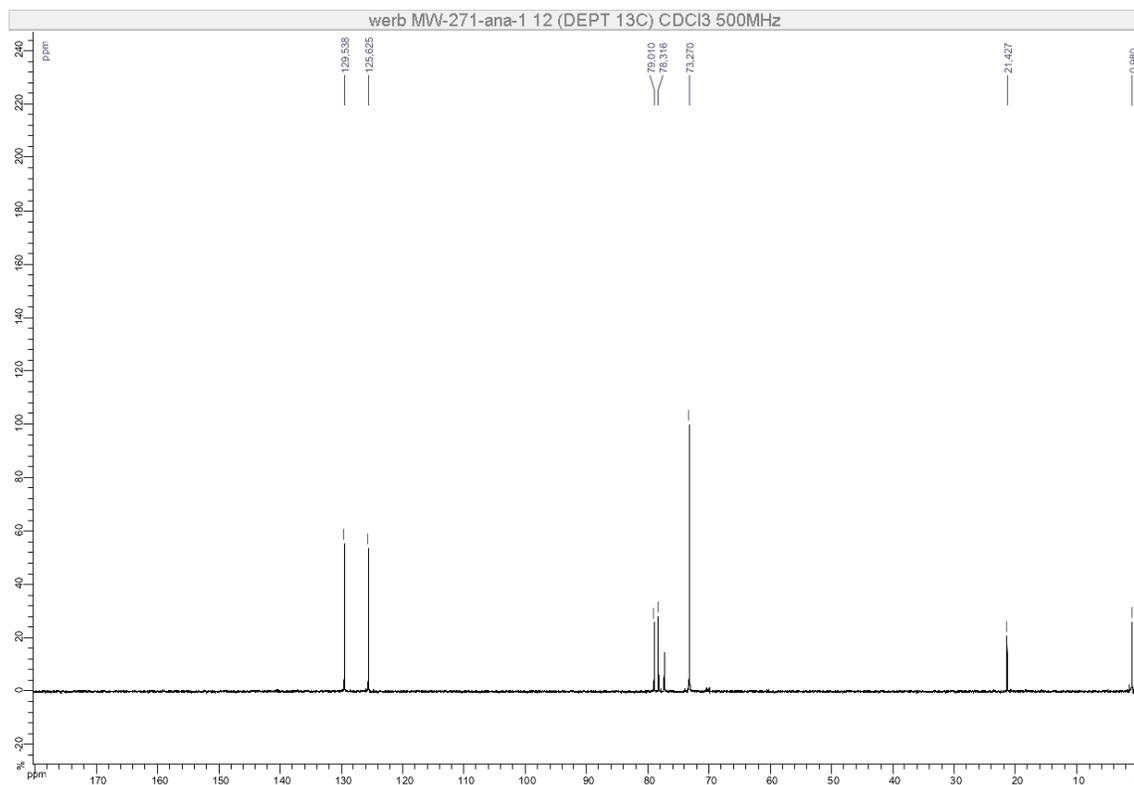
^1H NMR (500 MHz, CDCl_3)



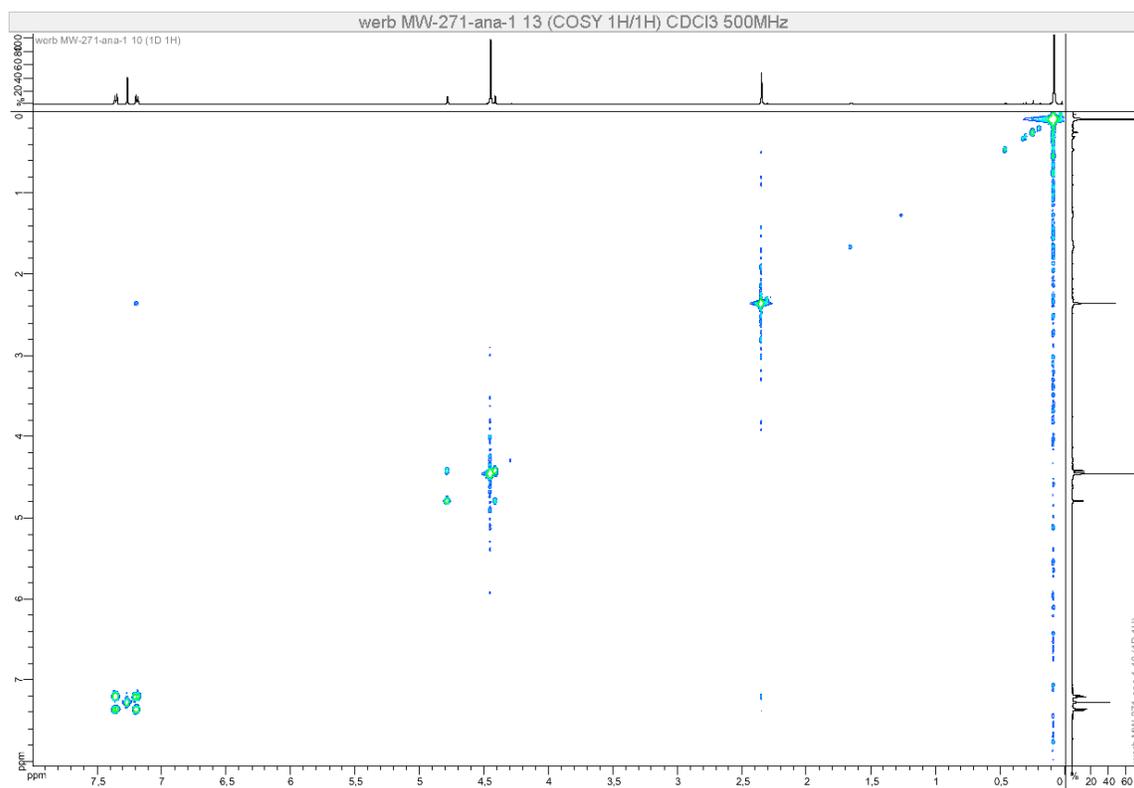
^{13}C NMR (126 MHz, CDCl_3)



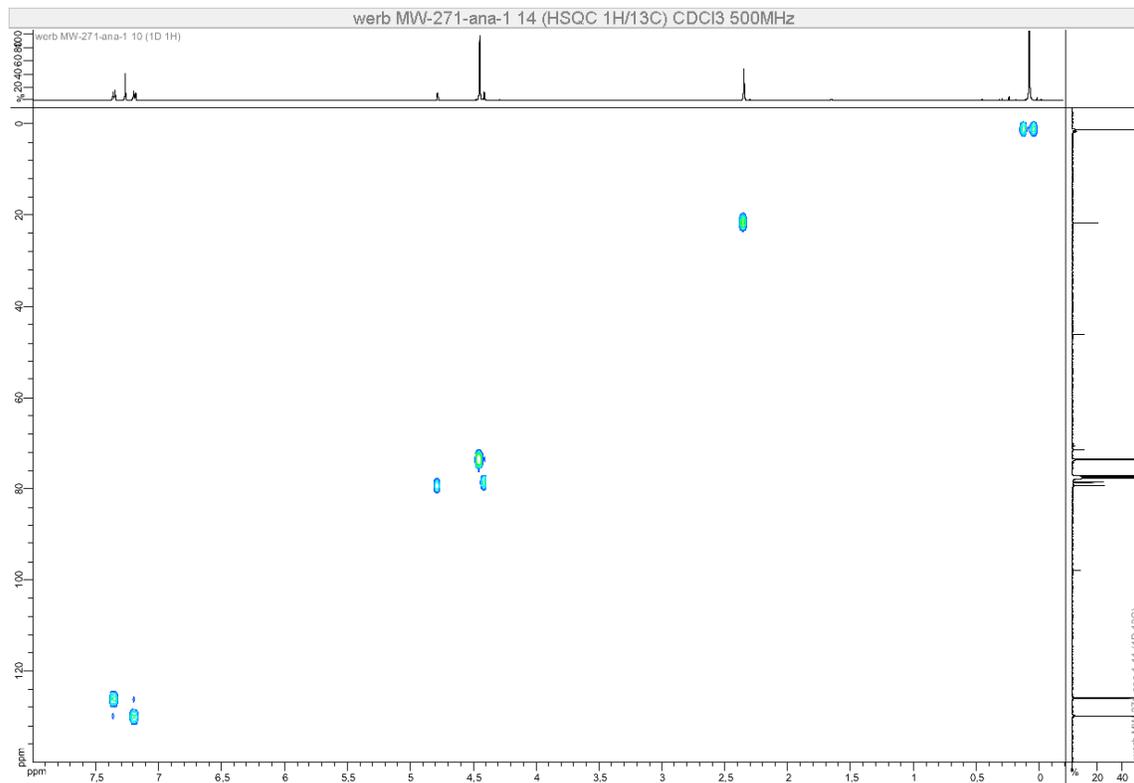
DEPT 135 (126 MHz, CDCl₃)



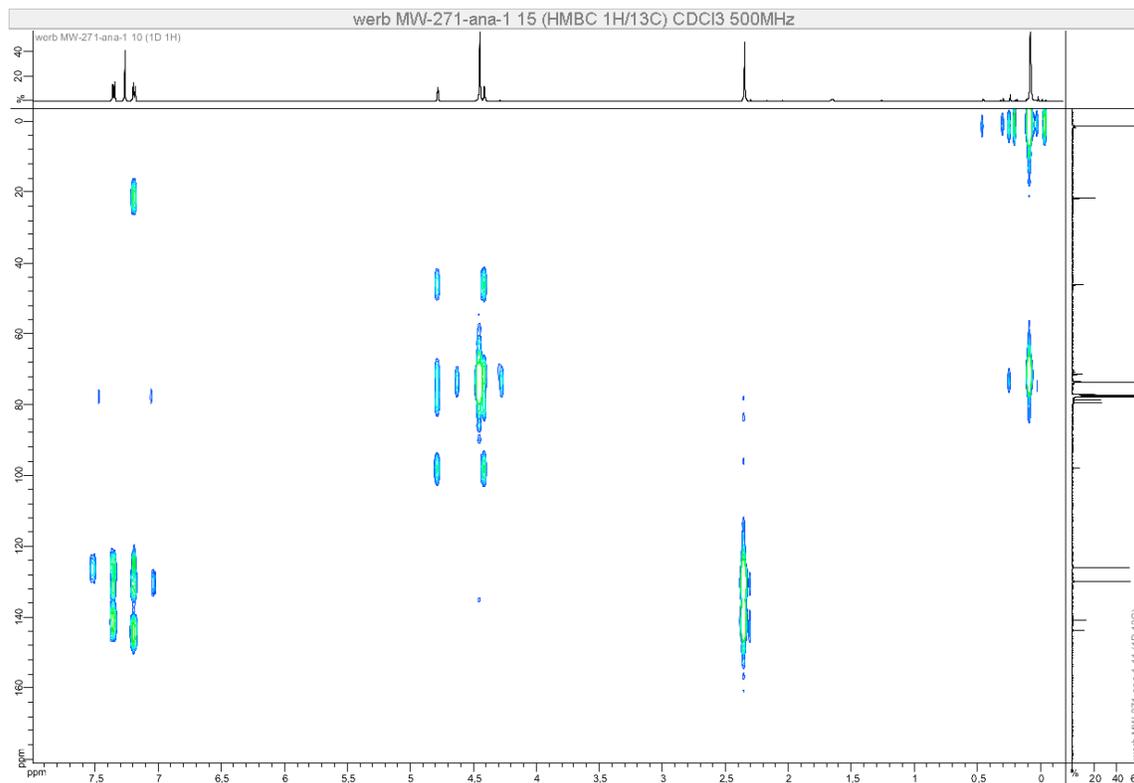
COSY (500 MHz, CDCl₃)



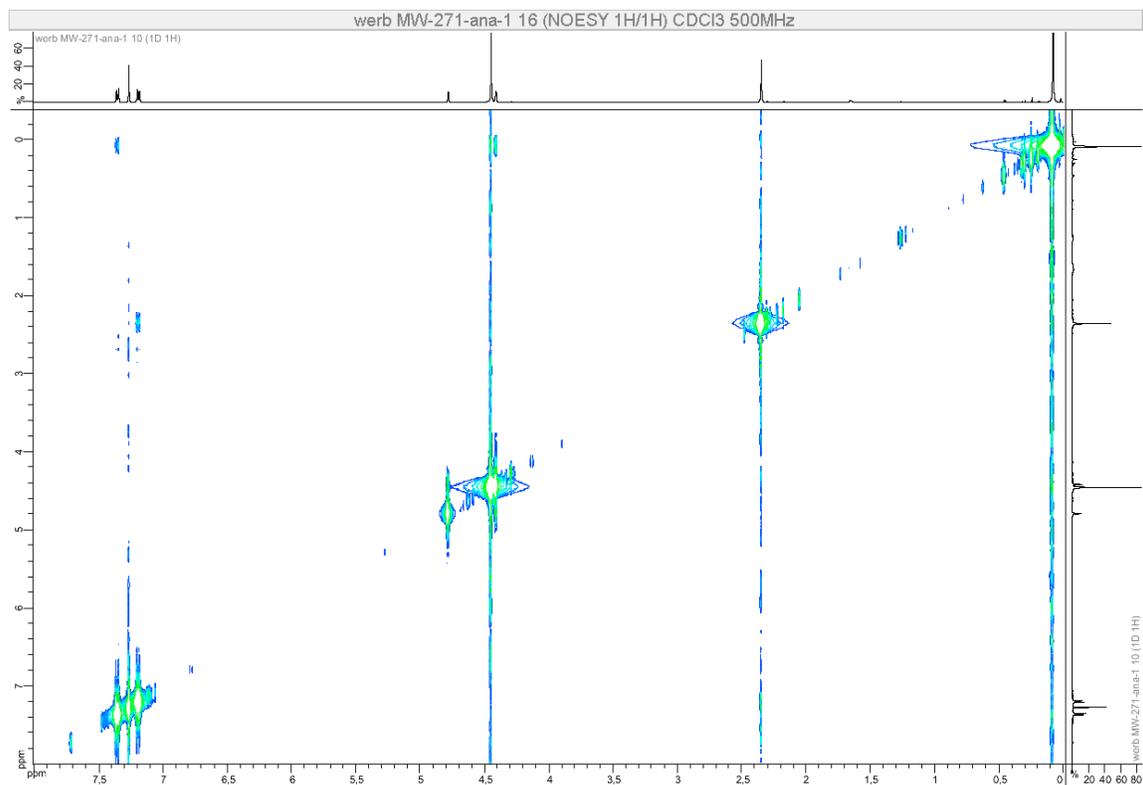
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

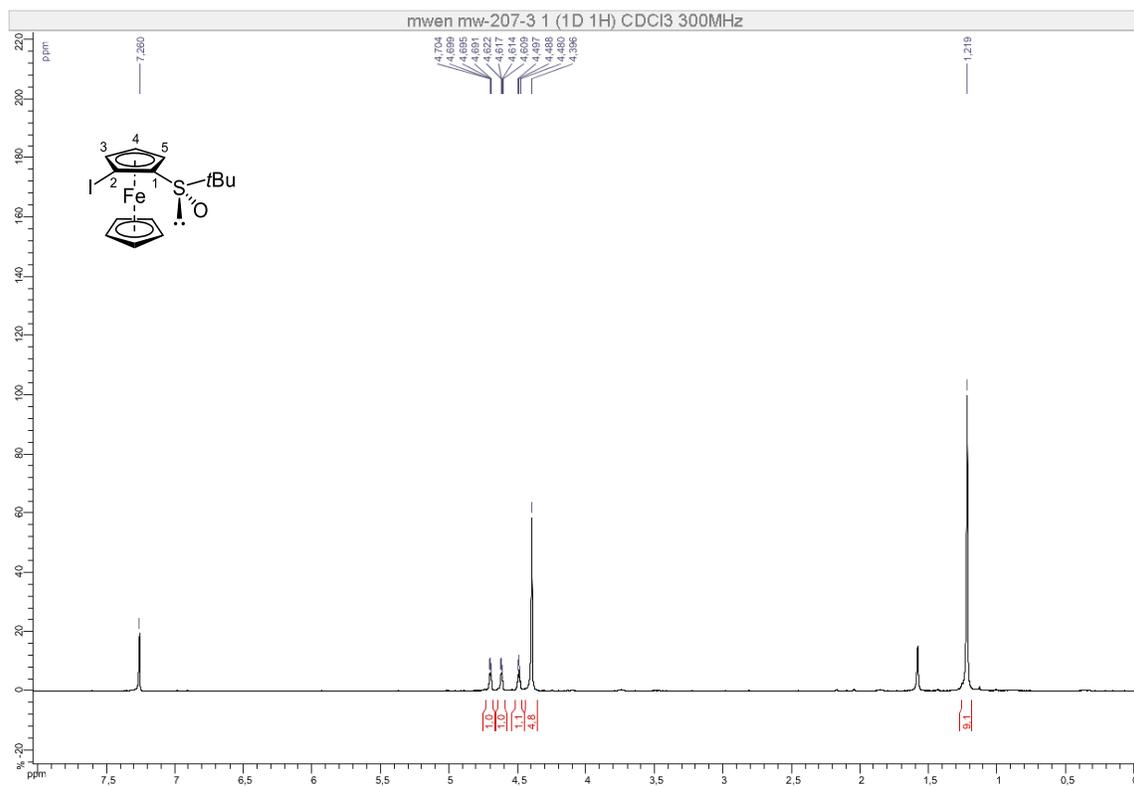


NOESY (500 MHz, CDCl₃)



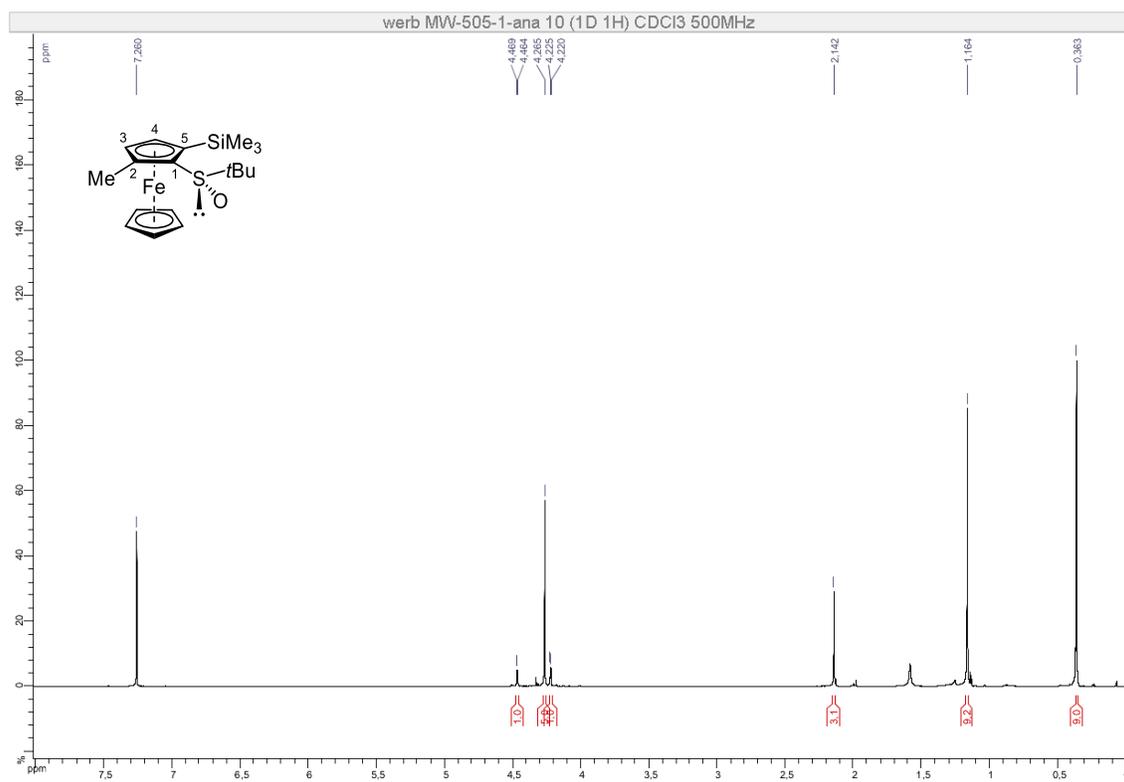
(*S,S*)-*S*-tert-Butyl-2-iodoferrocenesulfoxide (*S,S*-2ab)

¹H NMR (300 MHz, CDCl₃)

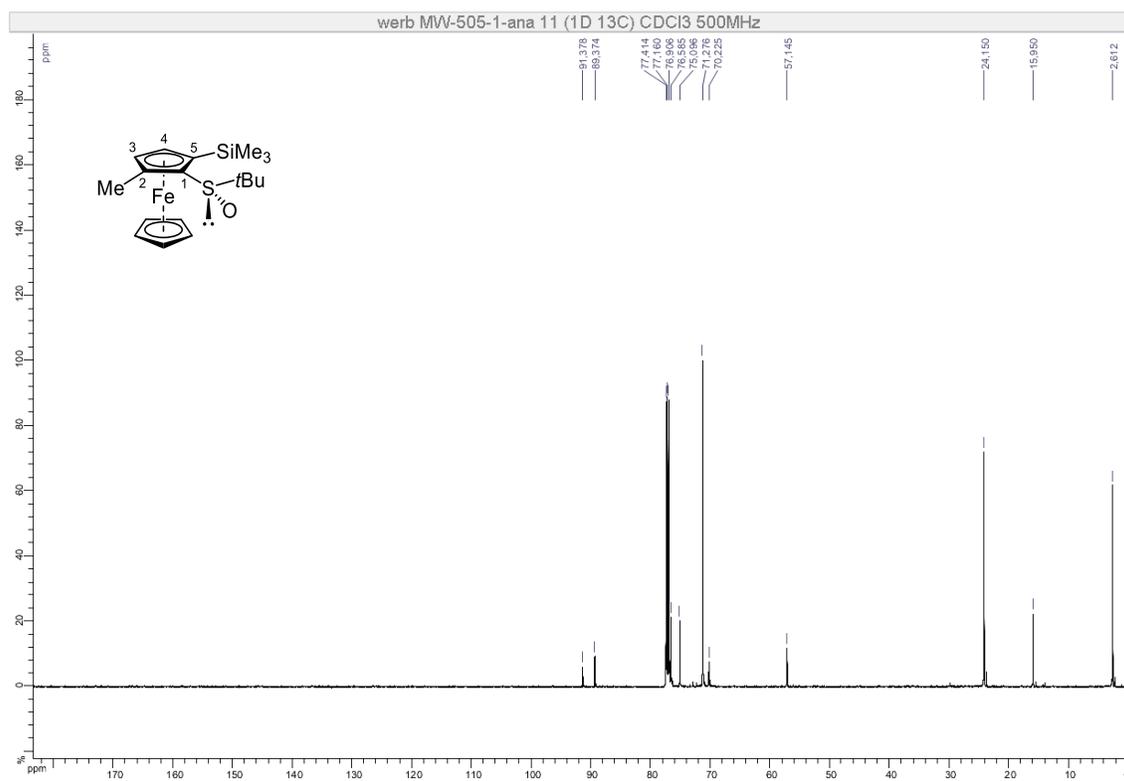


(*S,S*_P)-*S*-tert-Butyl-2-methyl-5-(trimethylsilyl)ferrocenesulfoxide (*S,S*_P-2ad)

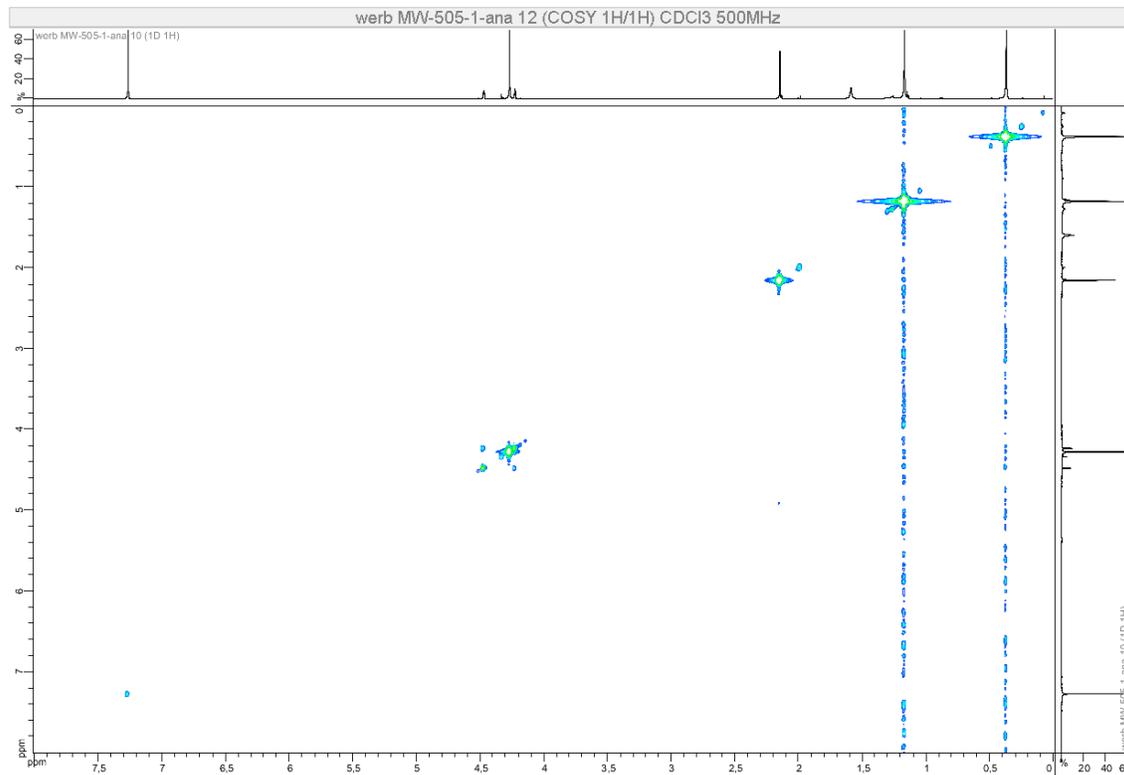
¹H NMR (500 MHz, CDCl₃)



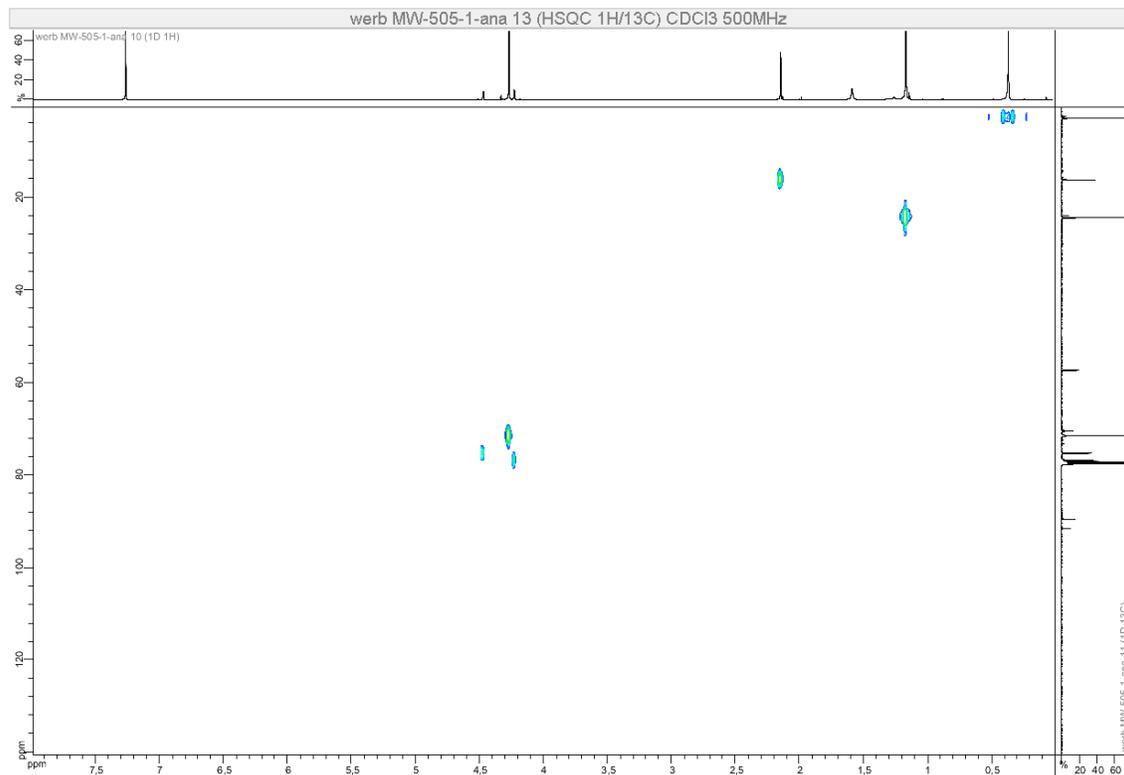
¹³C NMR (126 MHz, CDCl₃)



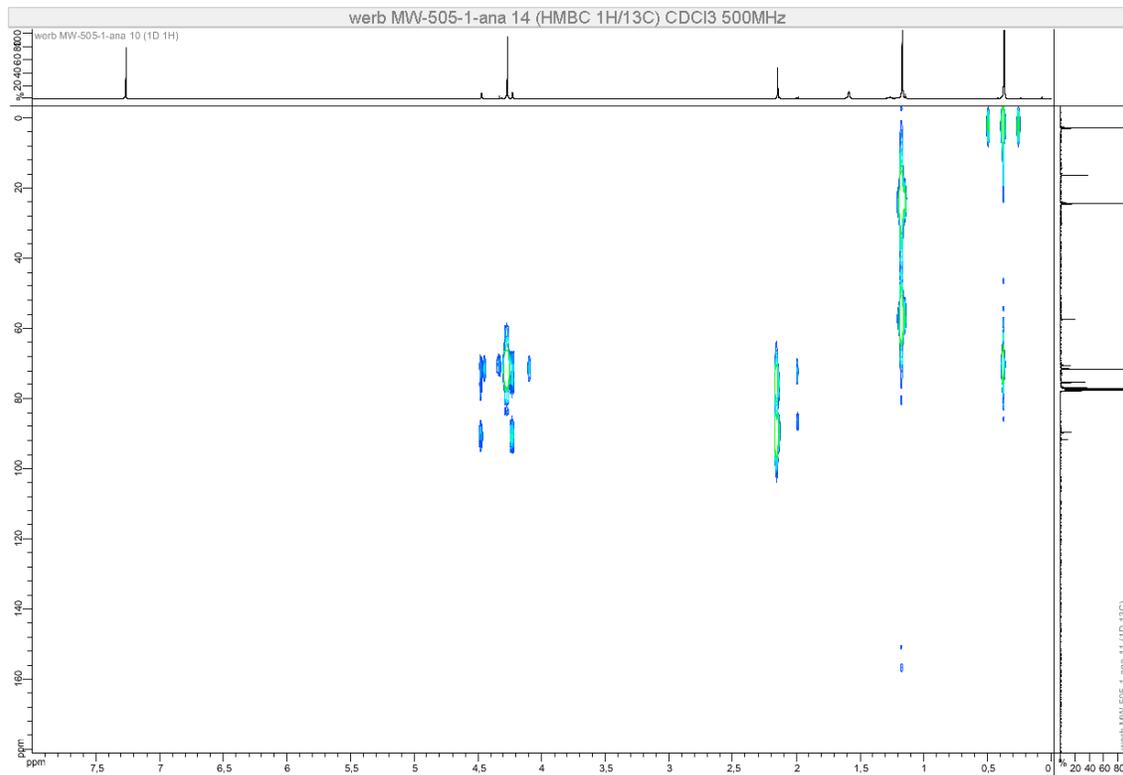
COSY (500 MHz, CDCl₃)



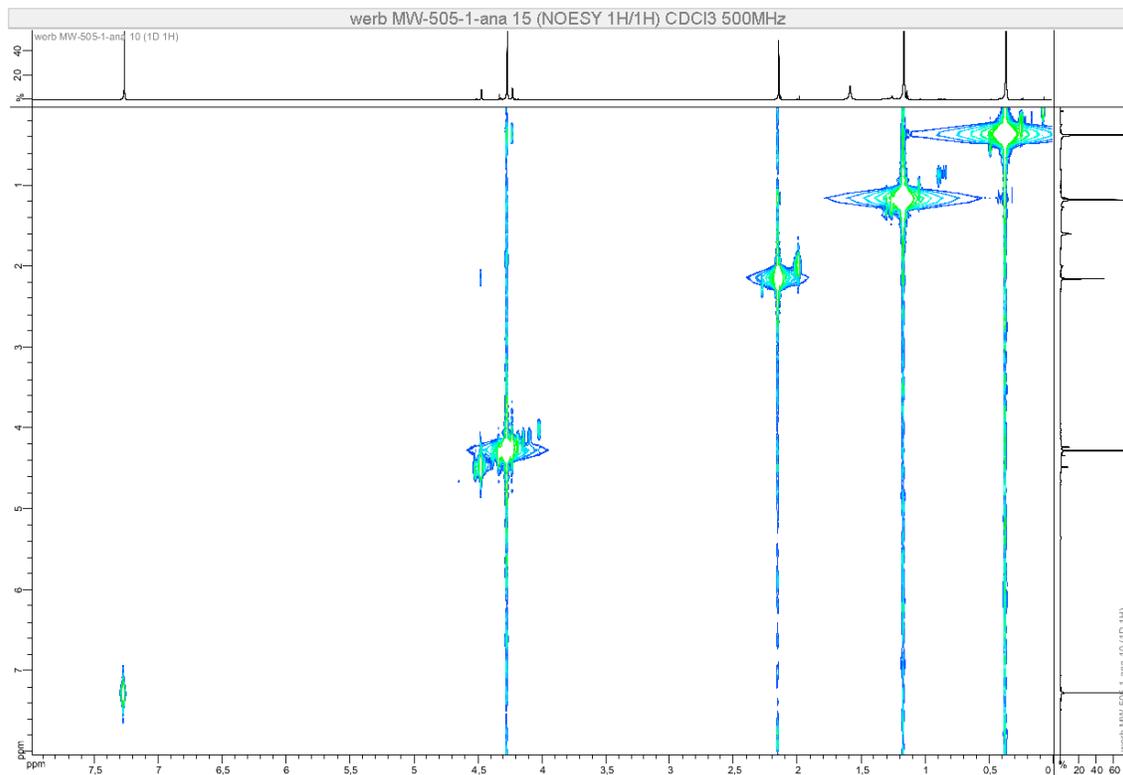
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

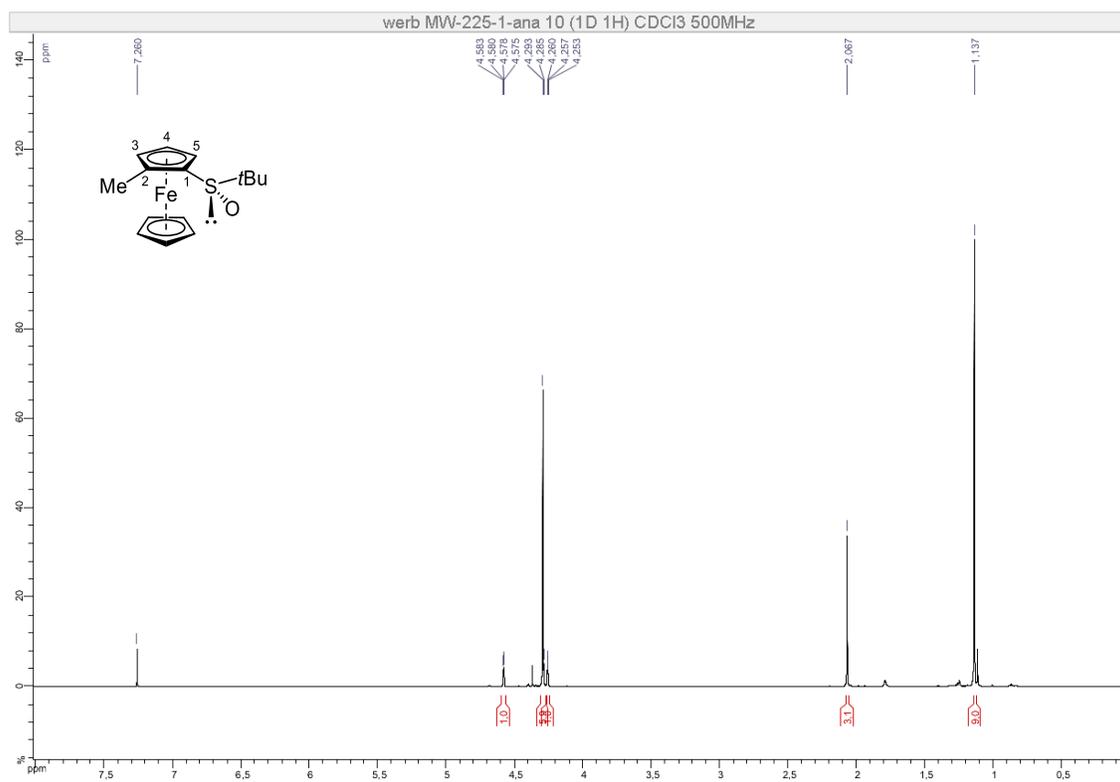


NOESY (500 MHz, CDCl₃)

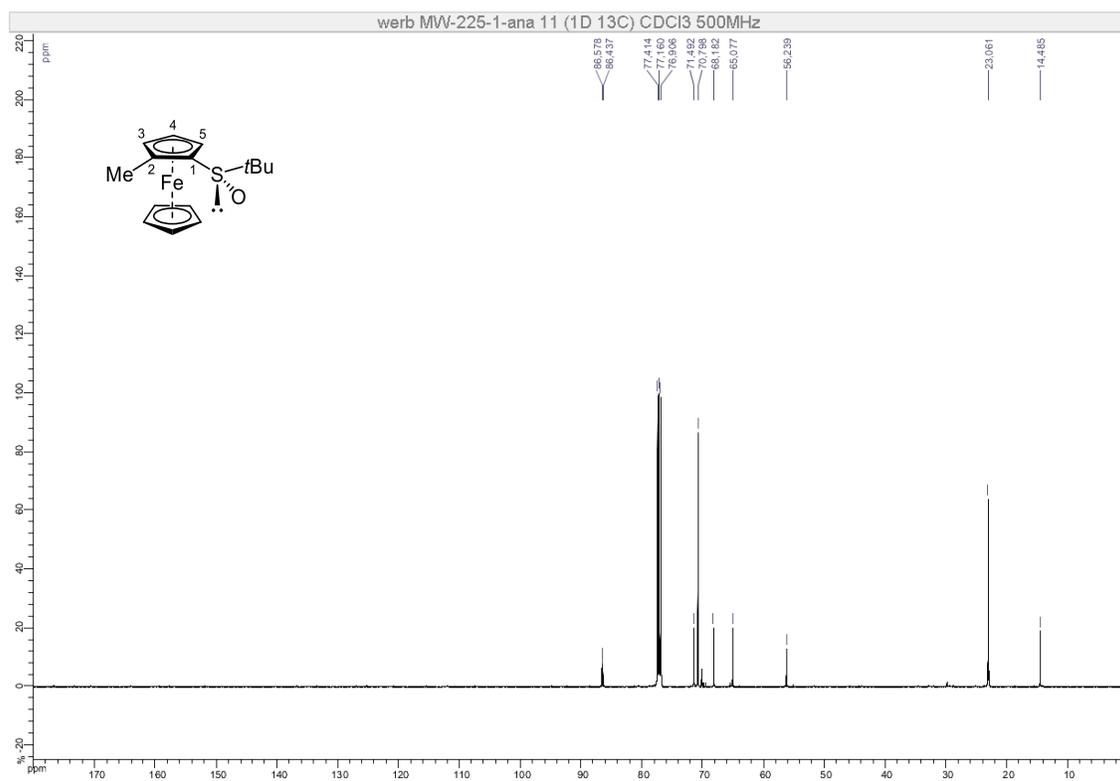


(S,R_P)-S-tert-Butyl-2-methylferrocenesulfoxide (S,R_P-1d)

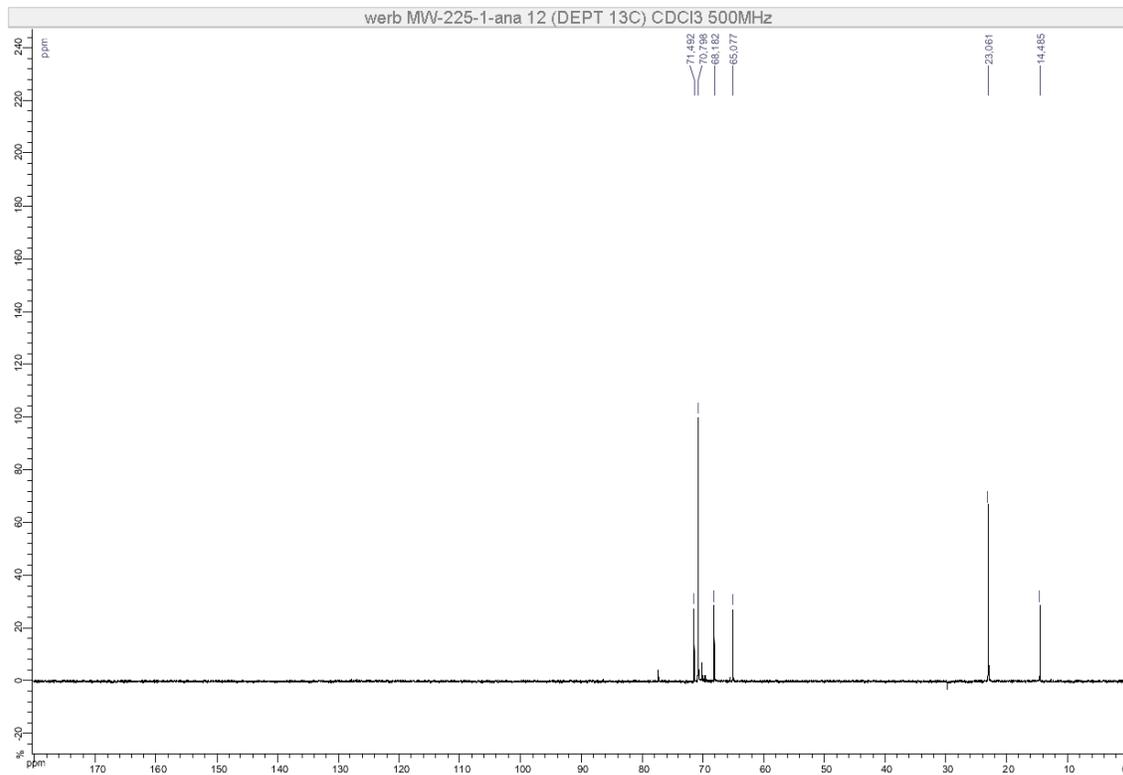
¹H NMR (500 MHz, CDCl₃)



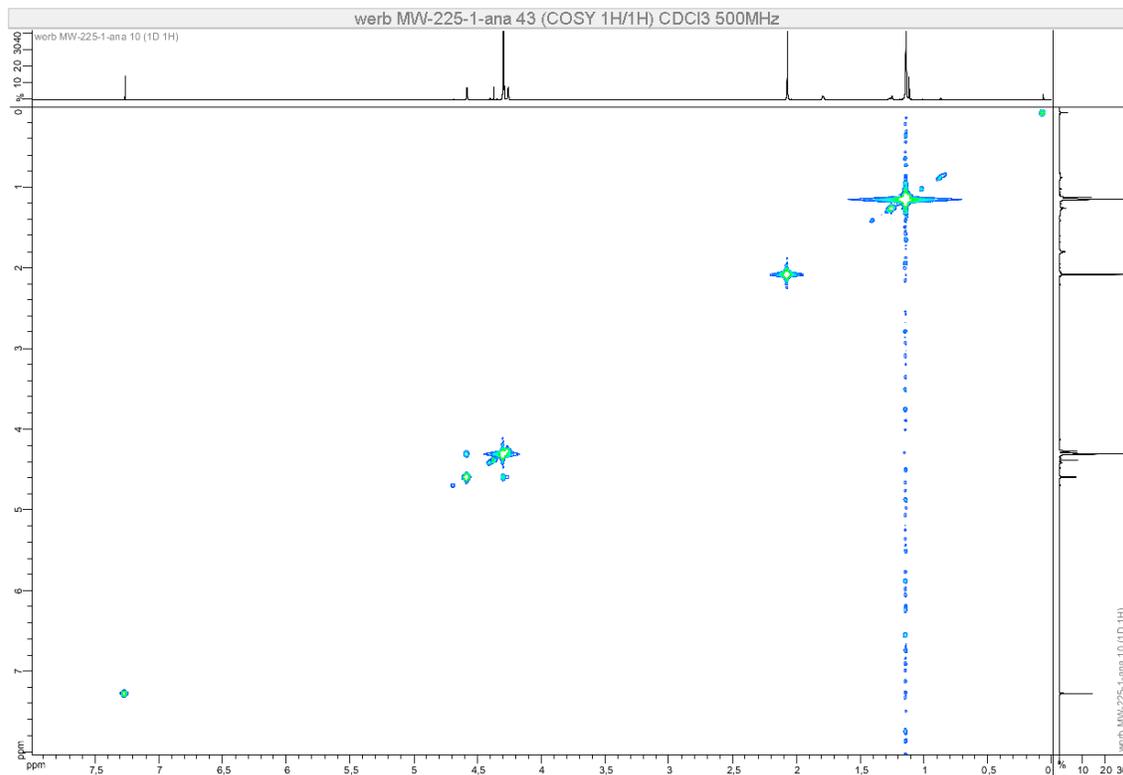
¹³C NMR (126 MHz, CDCl₃)



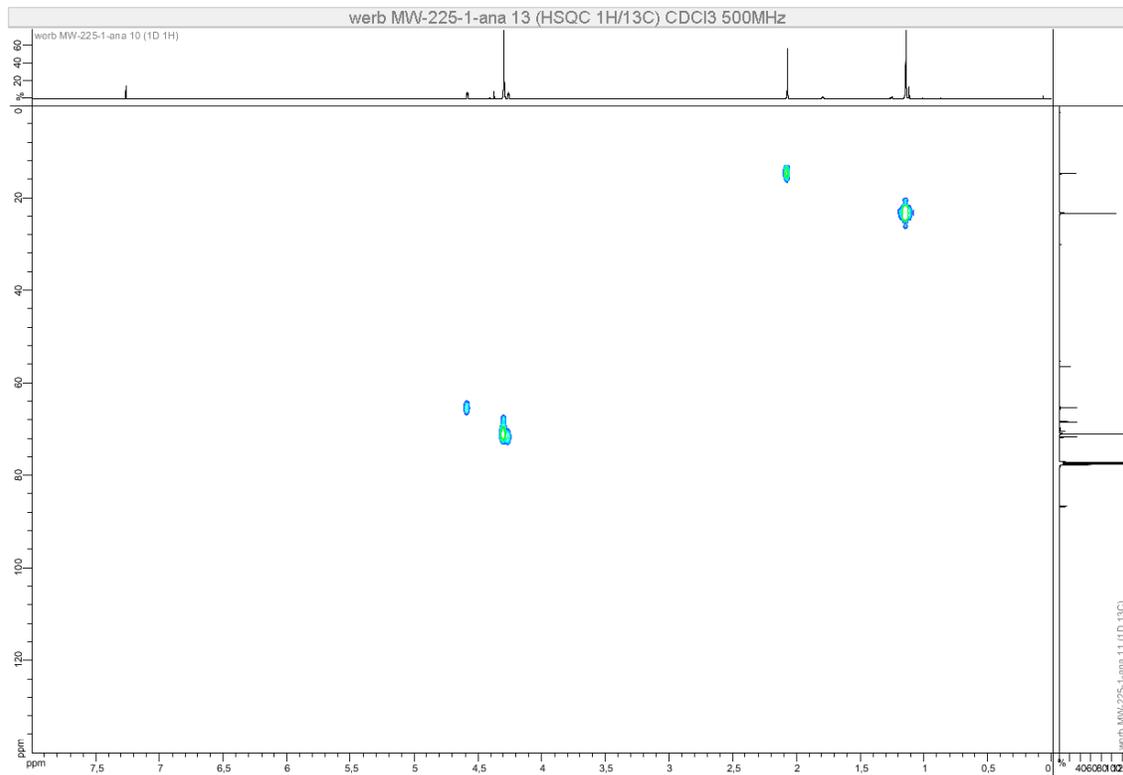
DEPT 135 (126 MHz, CDCl₃)



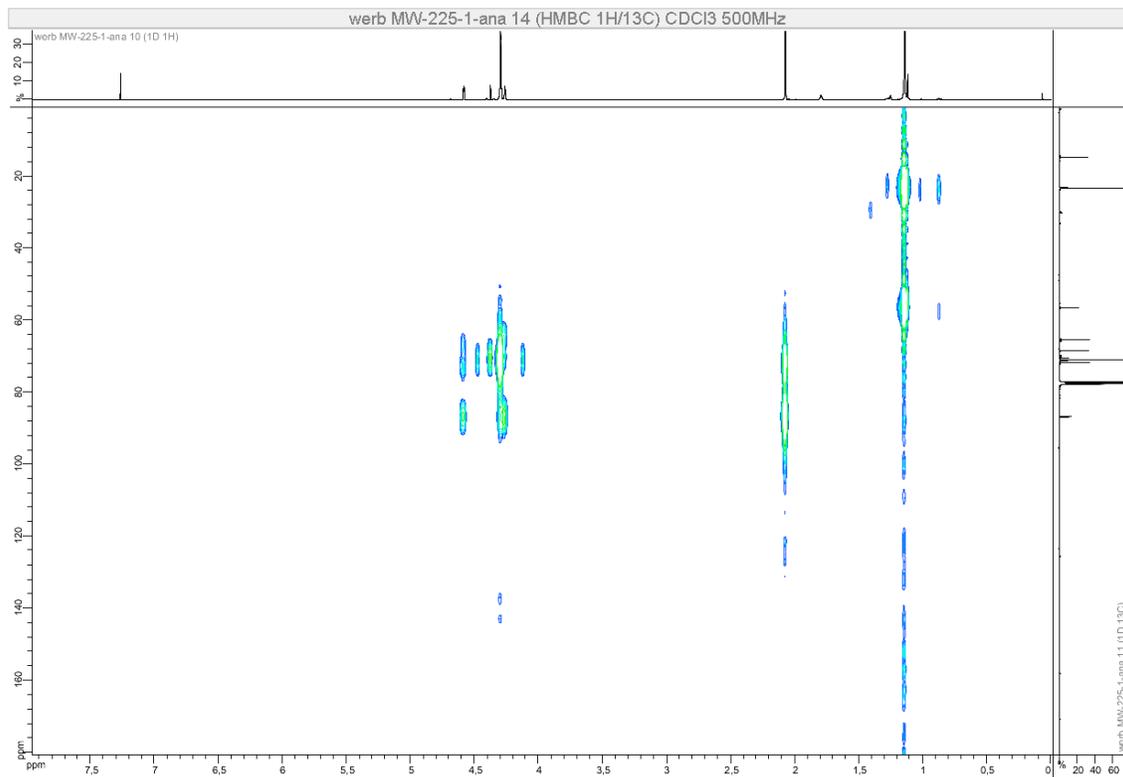
COSY (500 MHz, CDCl₃)



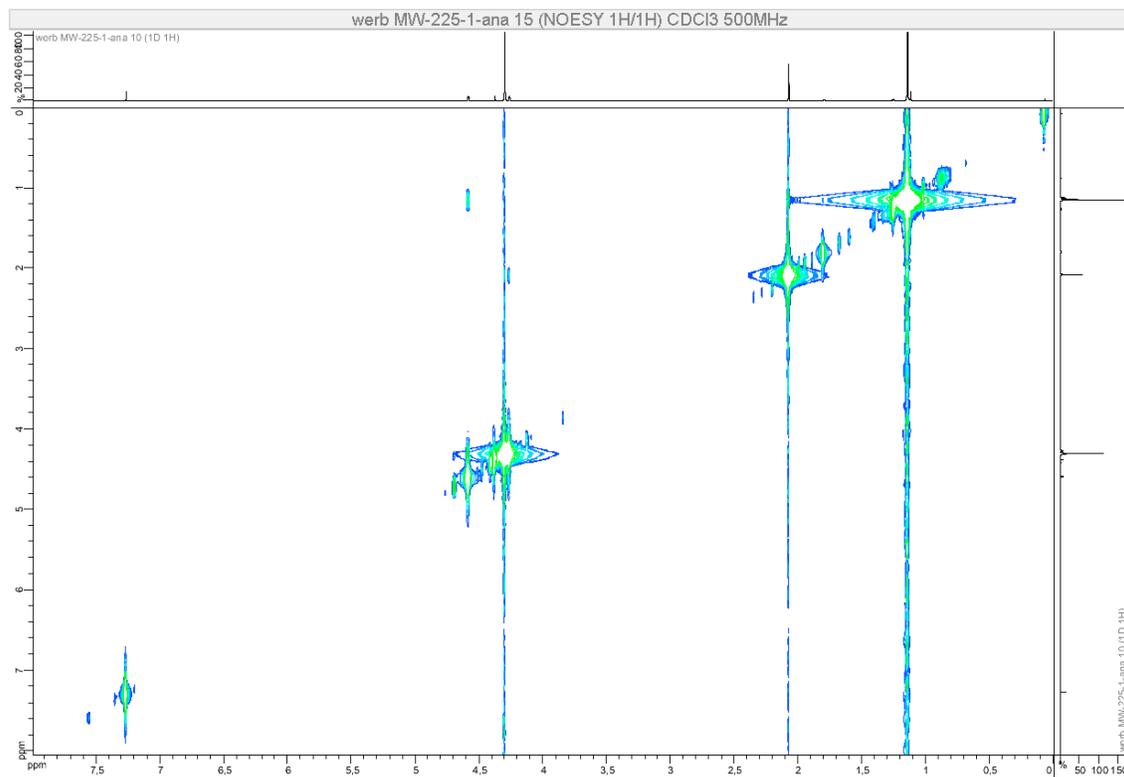
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

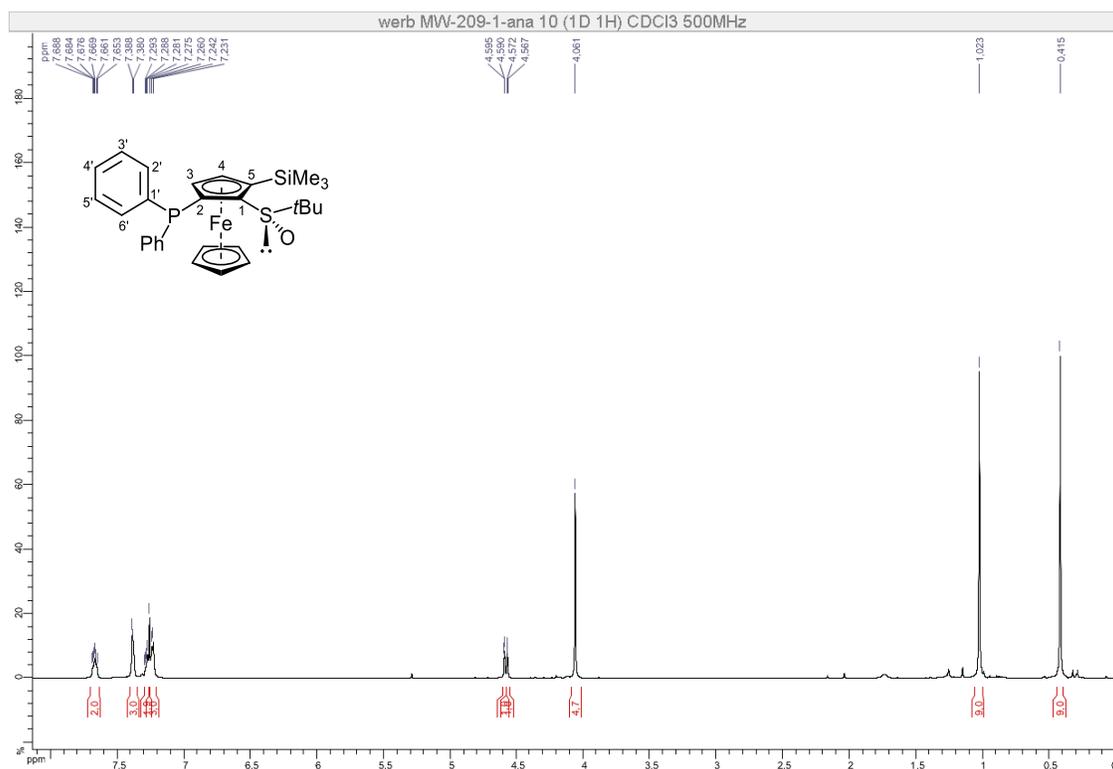


NOESY (500 MHz, CDCl₃)

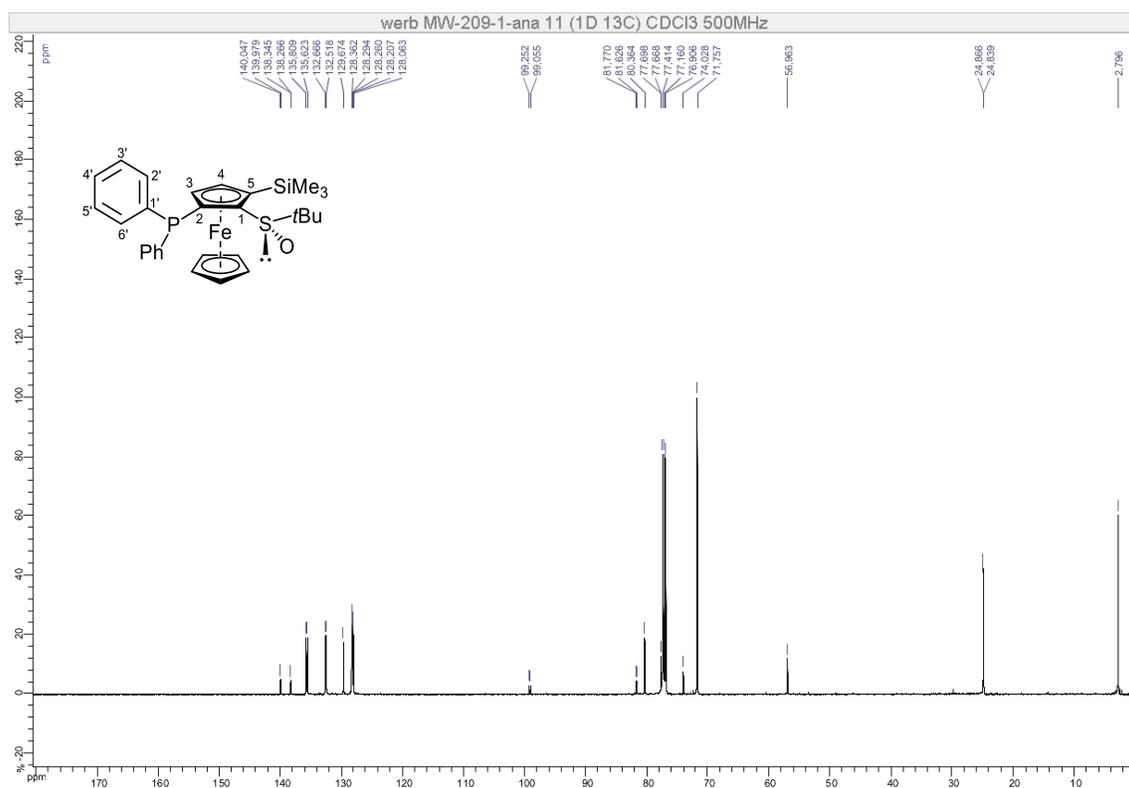


(*S,R*_P)-*S*-tert-Butyl-2-(diphenylphosphino)-5-(trimethylsilyl)ferrocenesulfoxide (*S,R*_P-2ae)

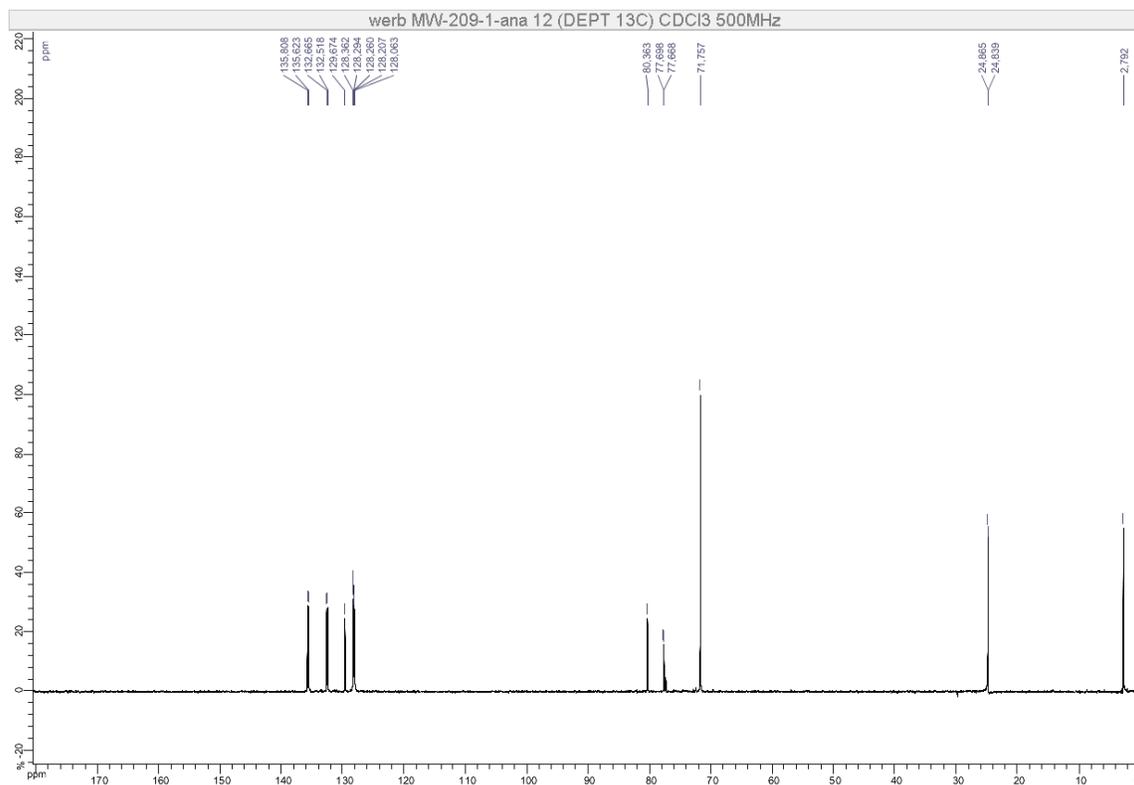
¹H NMR (500 MHz, CDCl₃)



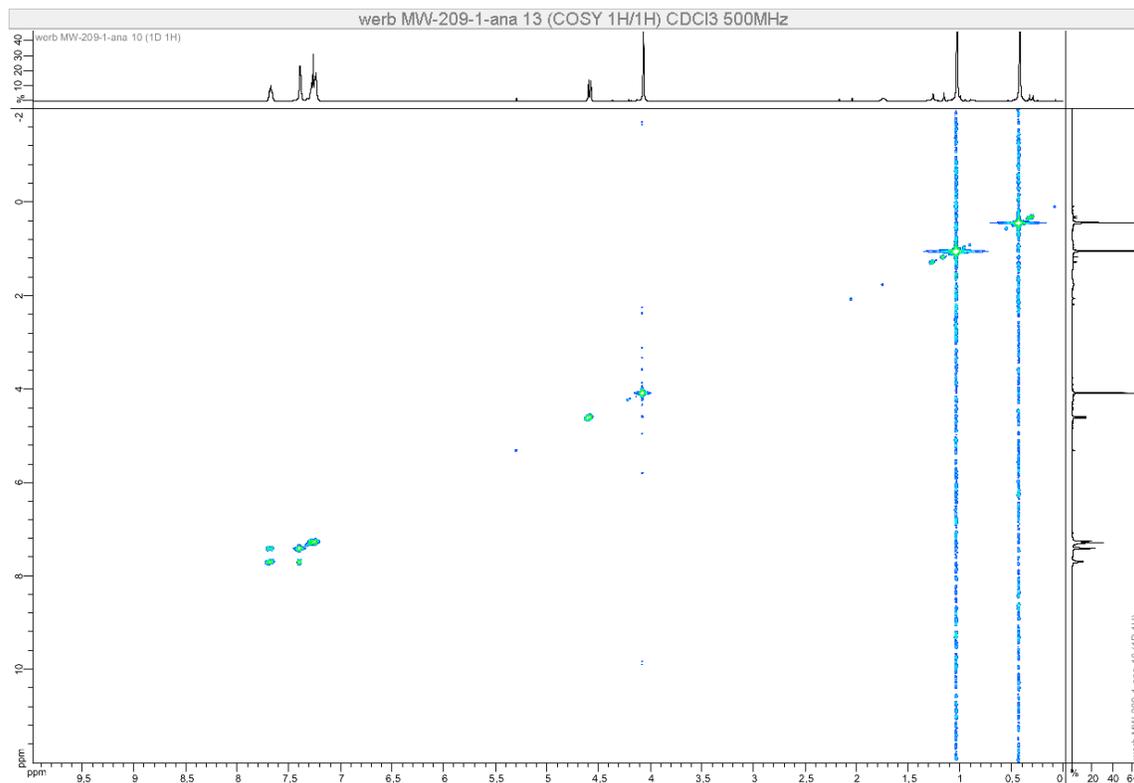
¹³C NMR (126 MHz, CDCl₃)



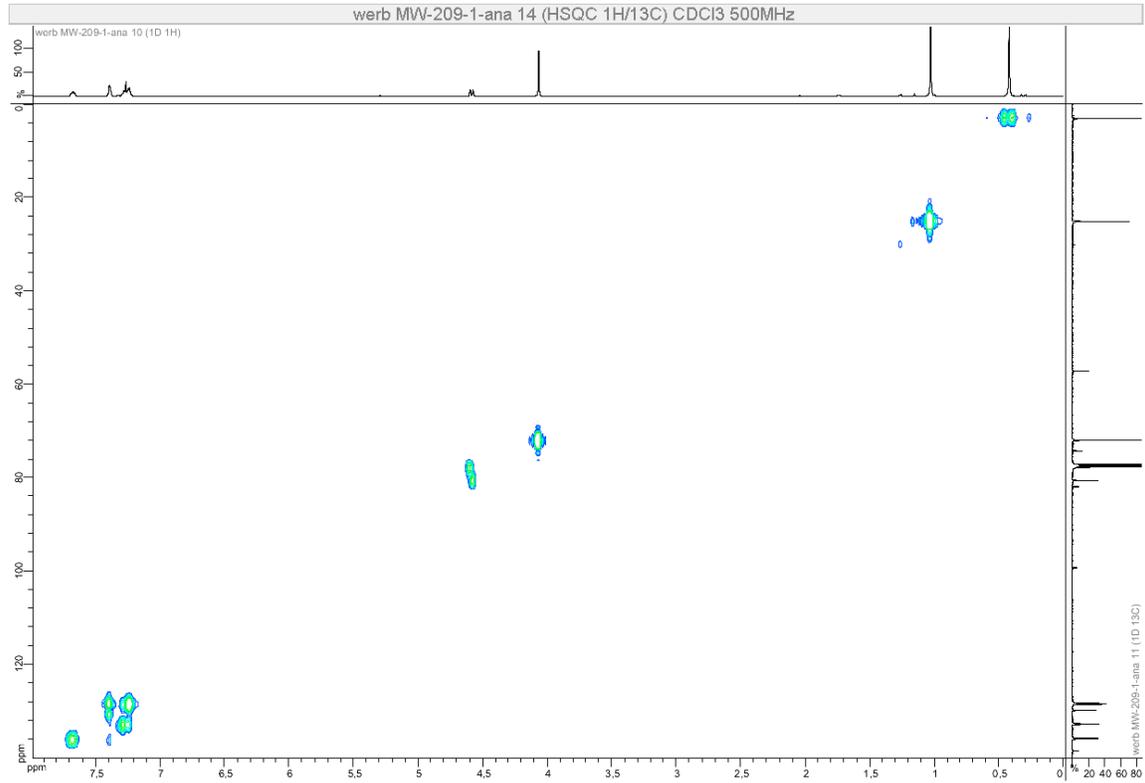
DEPT 135 (126 MHz, CDCl₃)



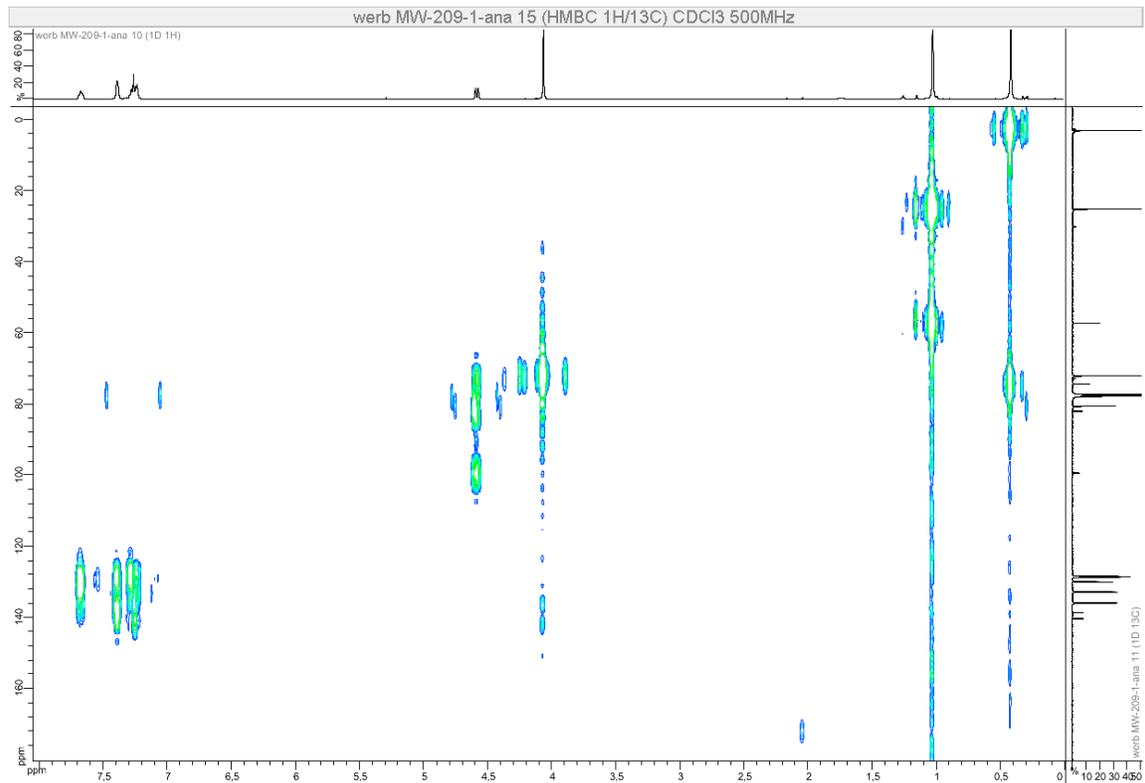
COSY (500 MHz, CDCl₃)



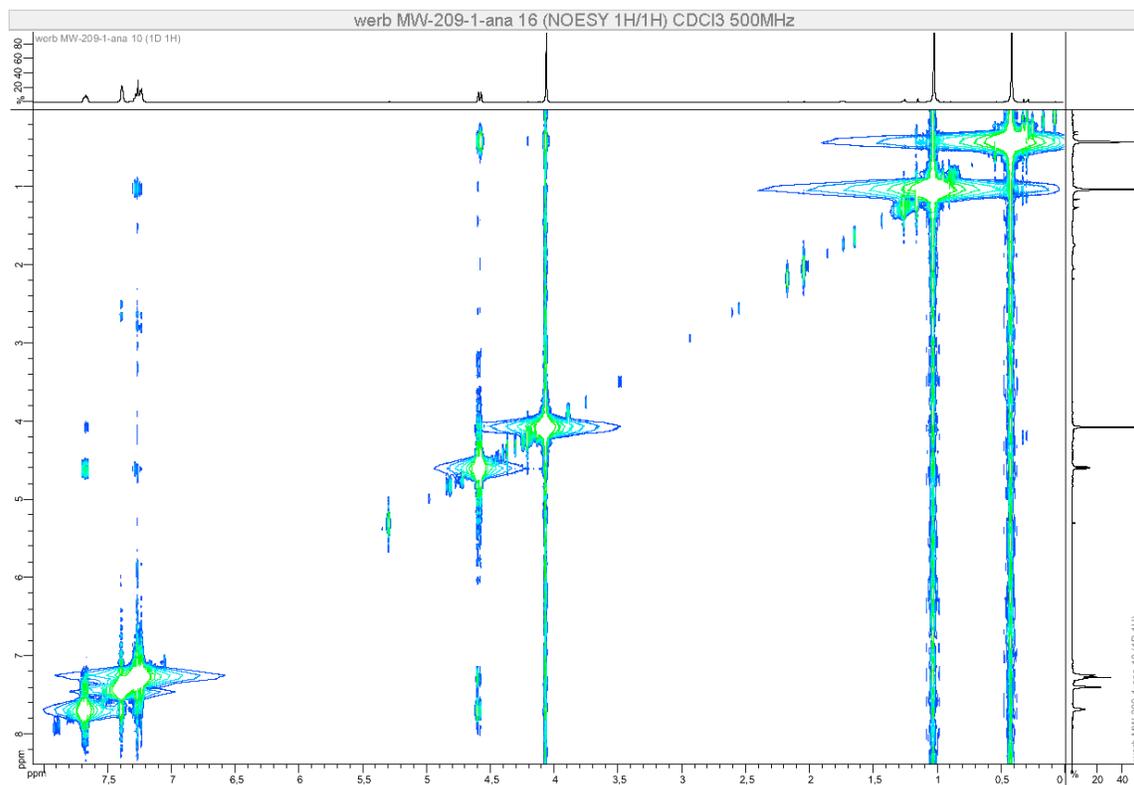
HSQC (500 MHz, CDCl₃)



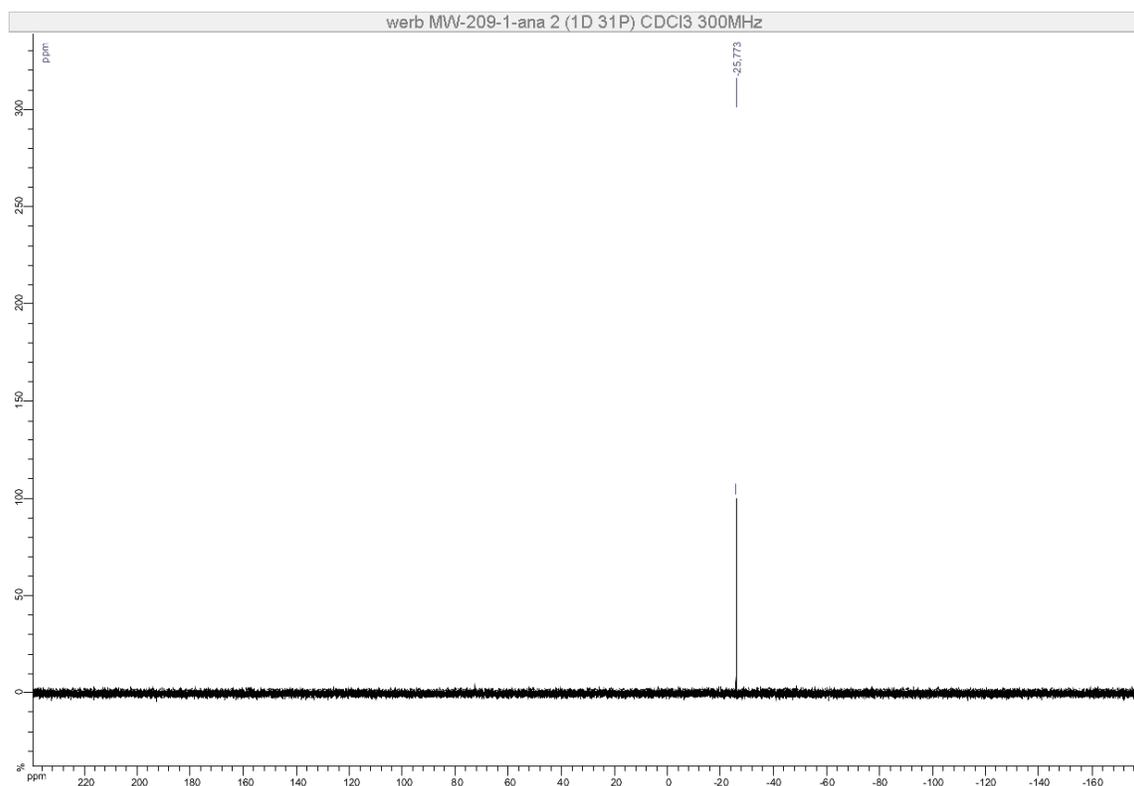
HMBC (500 MHz, CDCl₃)



NOESY (500 MHz, CDCl₃)

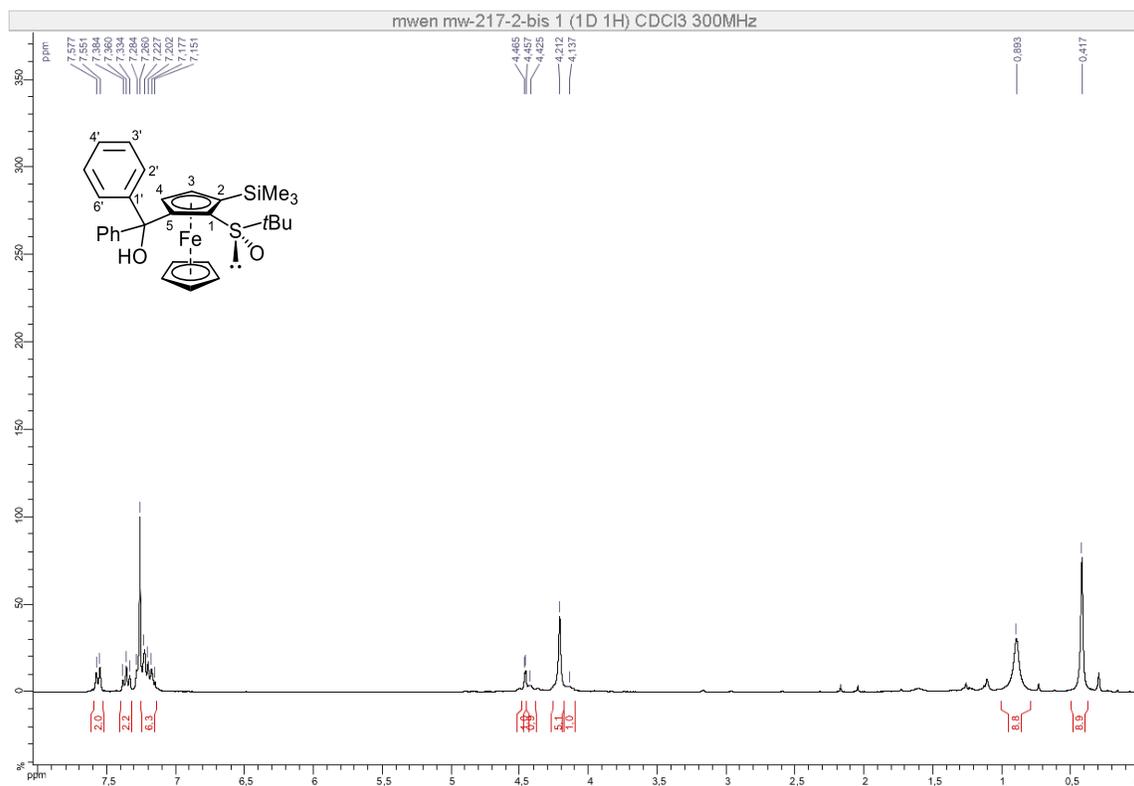


³¹P NMR (121 MHz, CDCl₃)



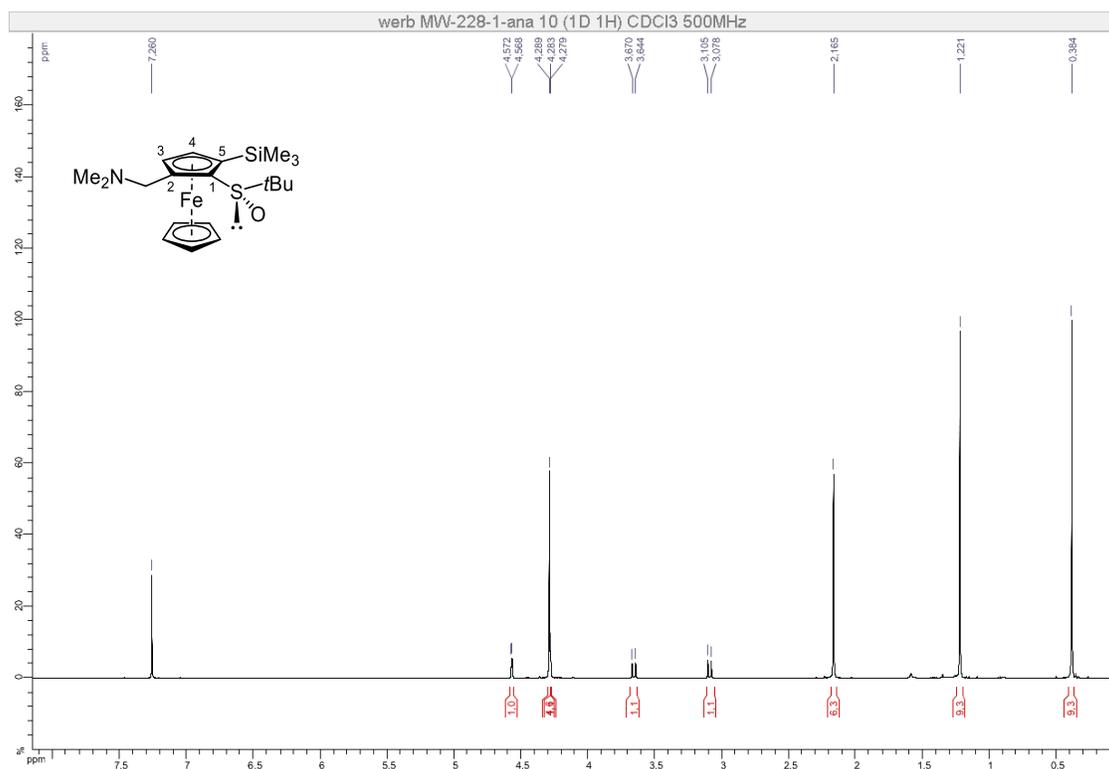
(*S,S*)-*S*-tert-Butyl-2-[(α,α -diphenyl)hydroxymethyl]-5-(trimethylsilyl)ferrocenesulfoxide (*S,S*P-2ag)

^1H NMR (300 MHz, CDCl_3)

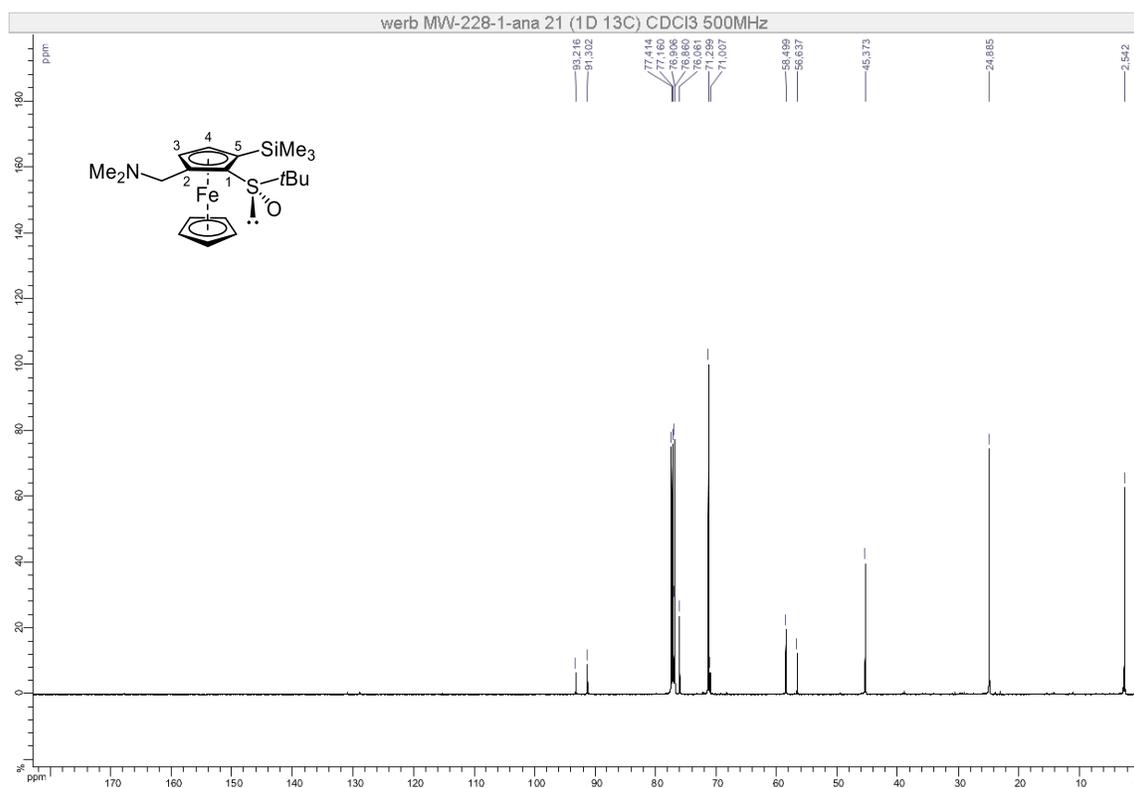


(*S,S*_P)-*S*-tert-Butyl-2-(dimethylaminomethyl)-5-(trimethylsilyl)ferrocenesulfoxide (*S,S*_P-2ah)

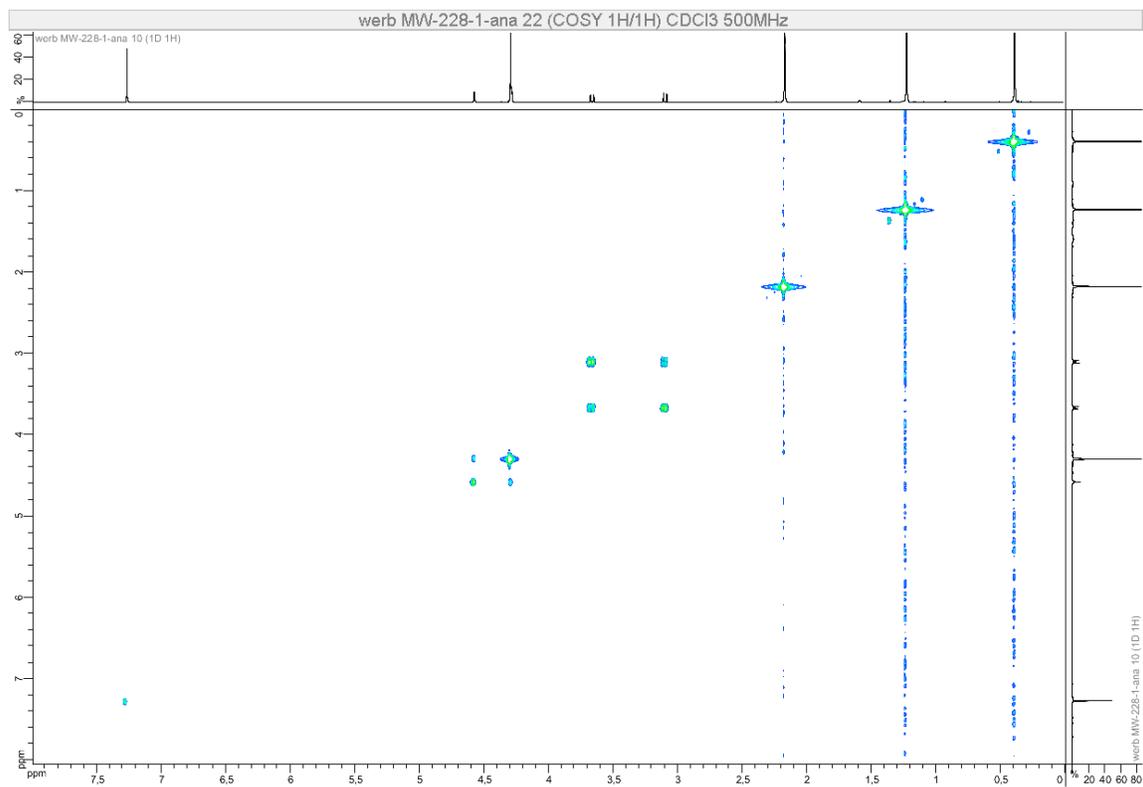
¹H NMR (500 MHz, CDCl₃)



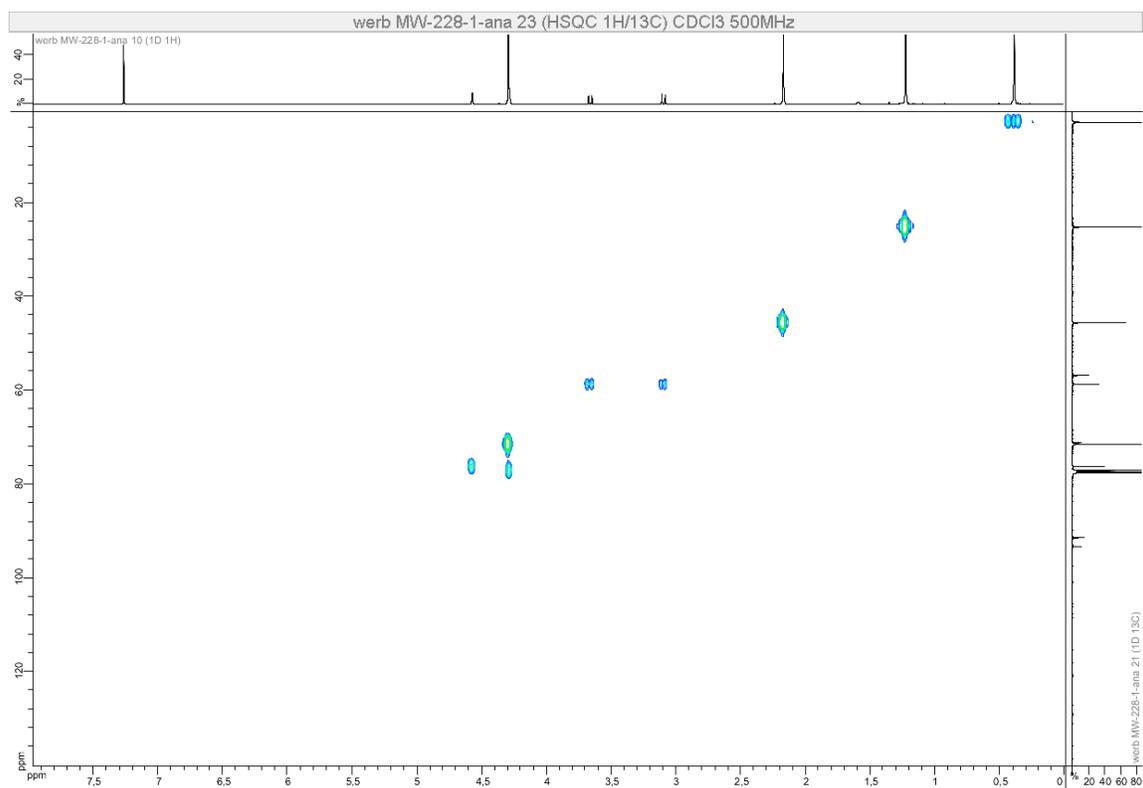
¹³C NMR (126 MHz, CDCl₃)



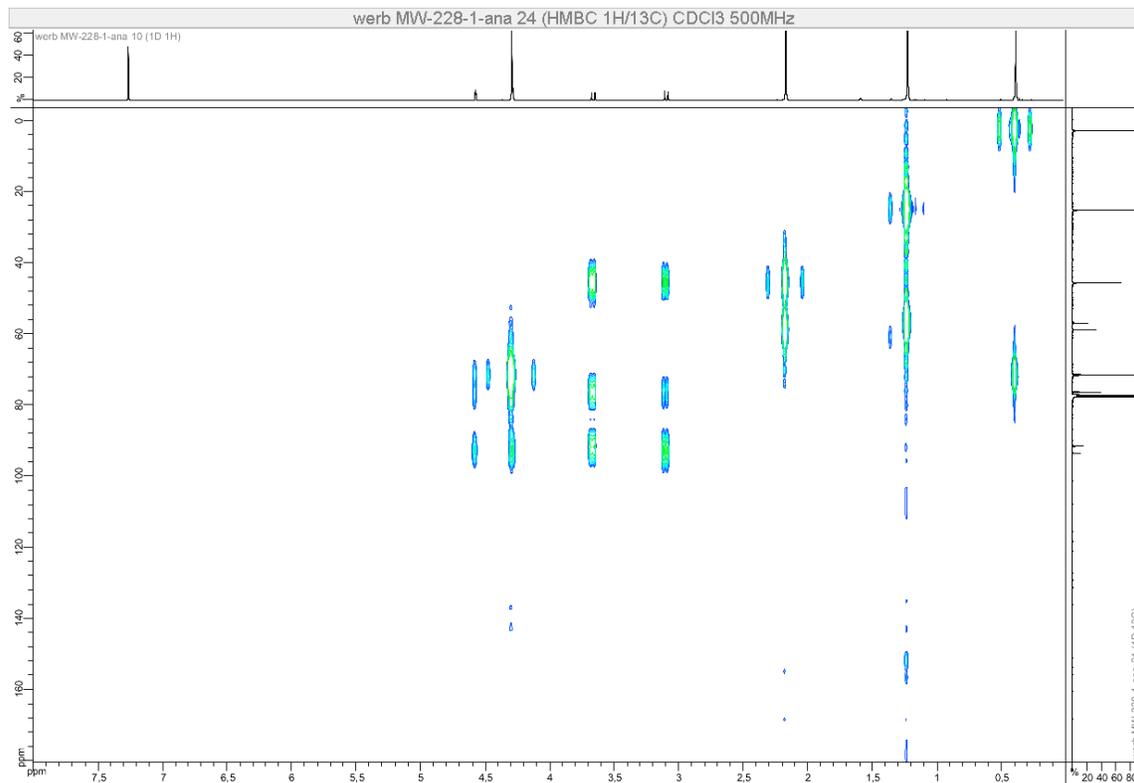
COSY (500 MHz, CDCl₃)



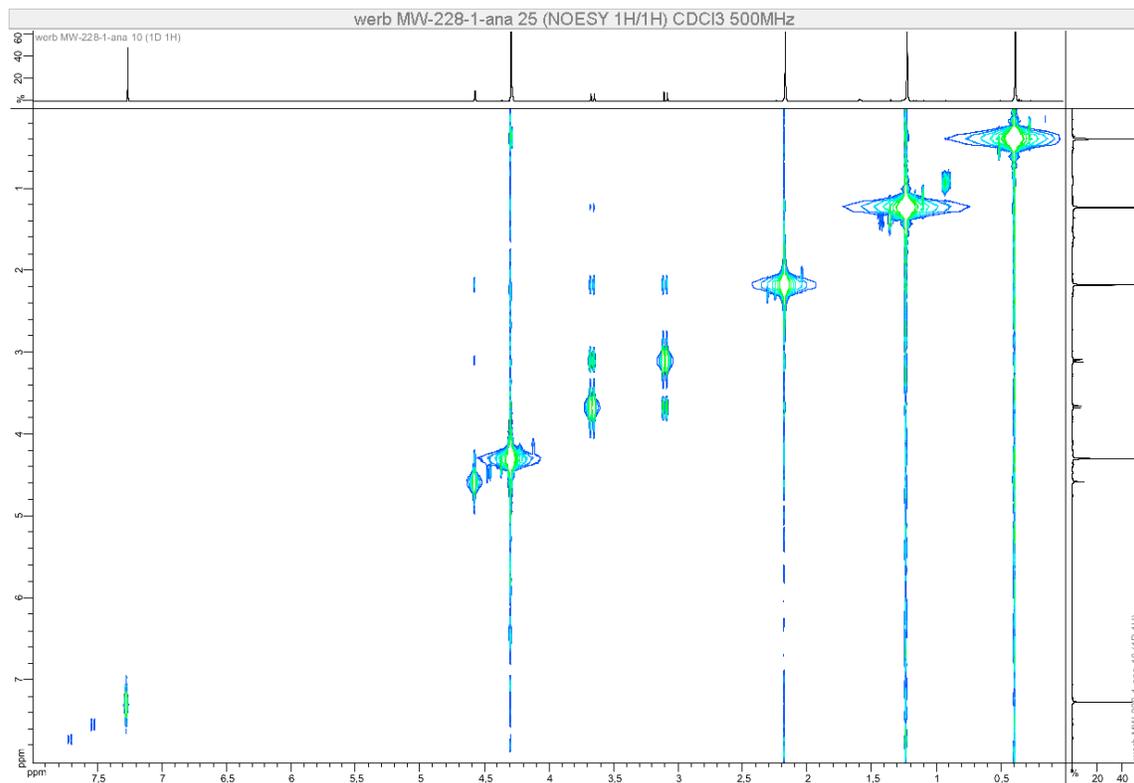
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

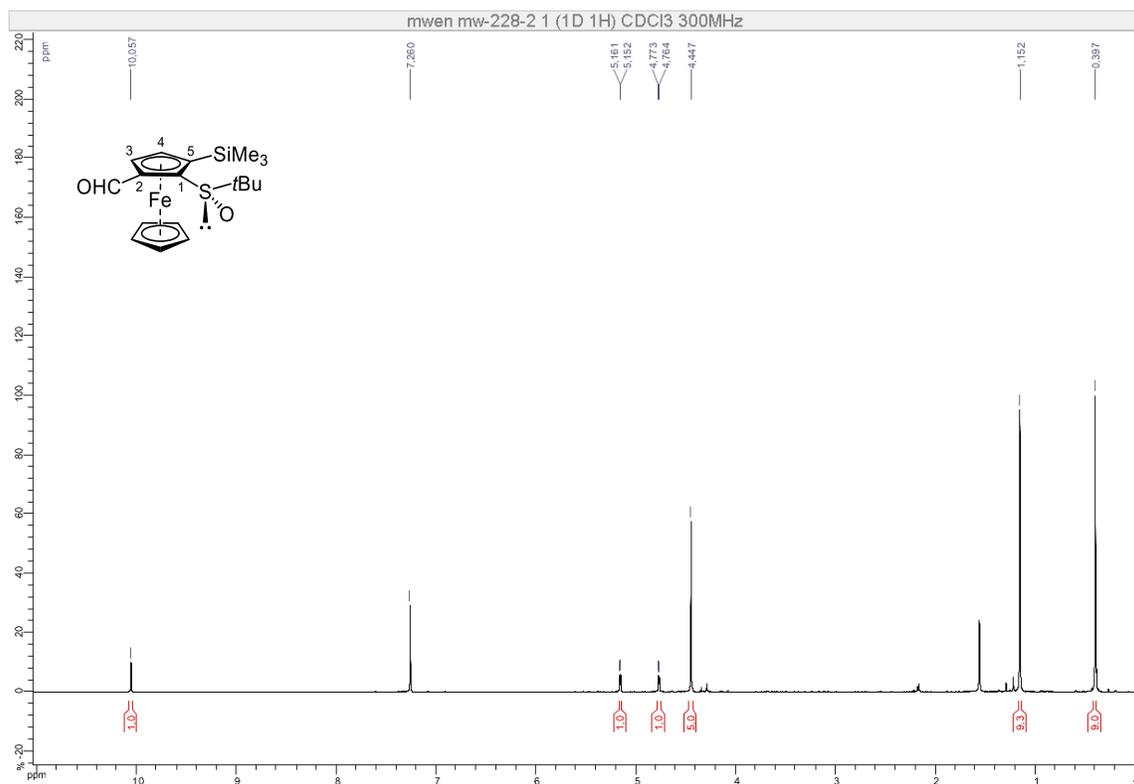


NOESY (500 MHz, CDCl₃)



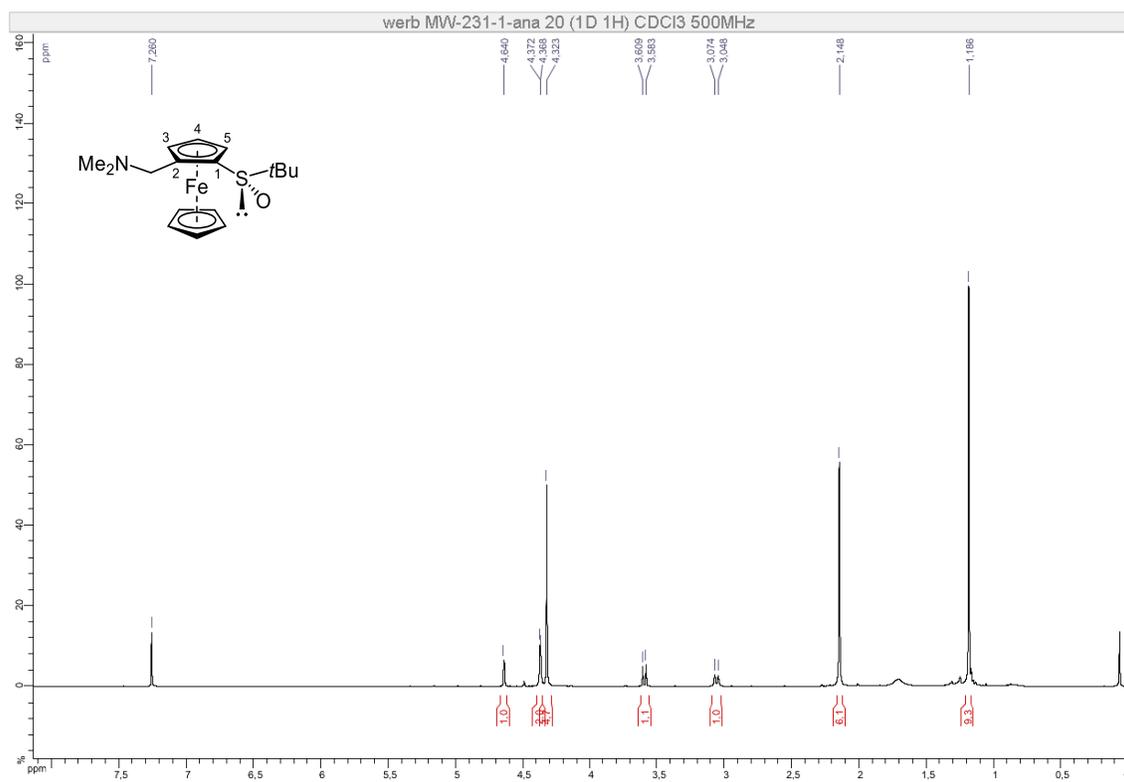
(*S,S*)-*S*-tert-Butyl-2-formyl-5-(trimethylsilyl)ferrocenesulfoxide (*S,S*-2ah')

¹H NMR (300 MHz, CDCl₃)

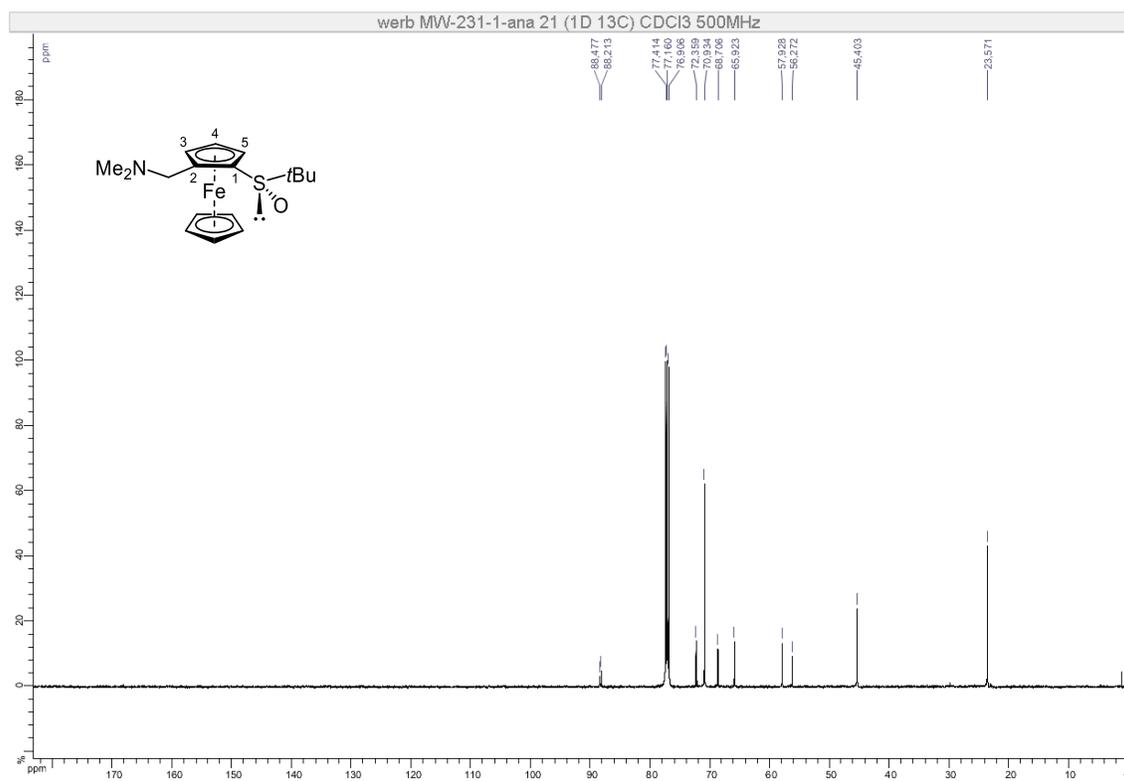


(*S,R*_P)-*S*-tert-Butyl-2-(dimethylaminomethyl)ferrocenesulfoxide (*S,R*_P-1h)

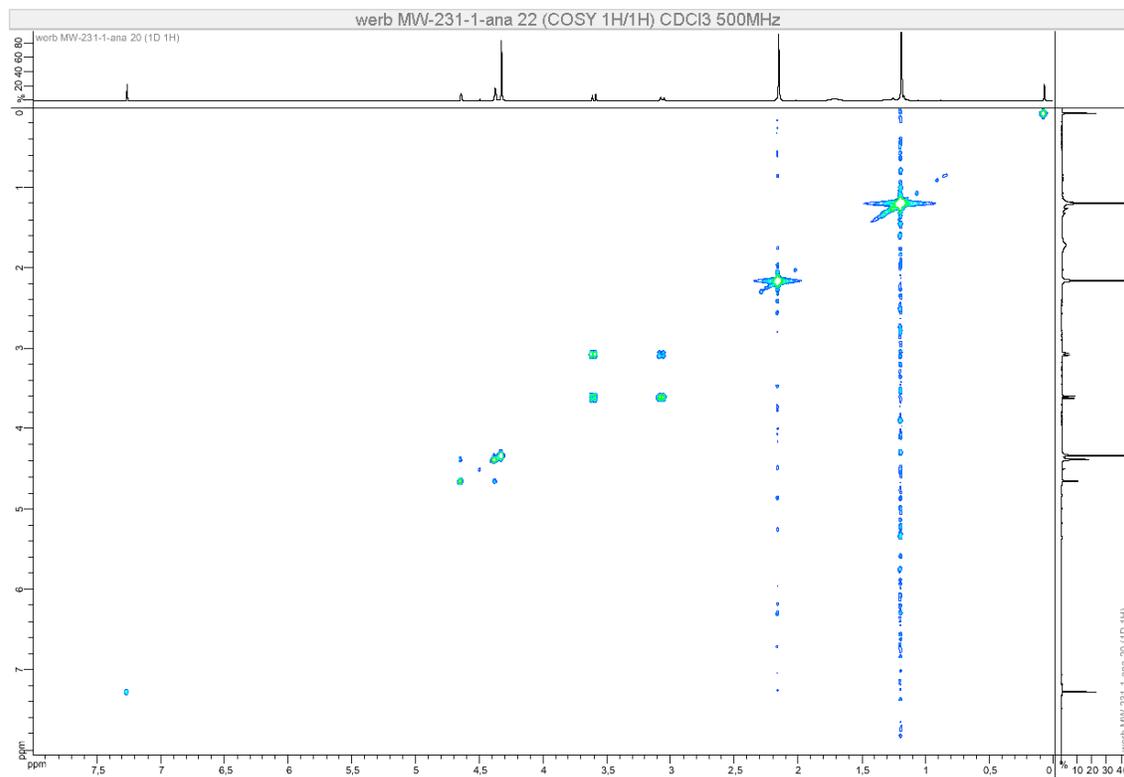
¹H NMR (500 MHz, CDCl₃)



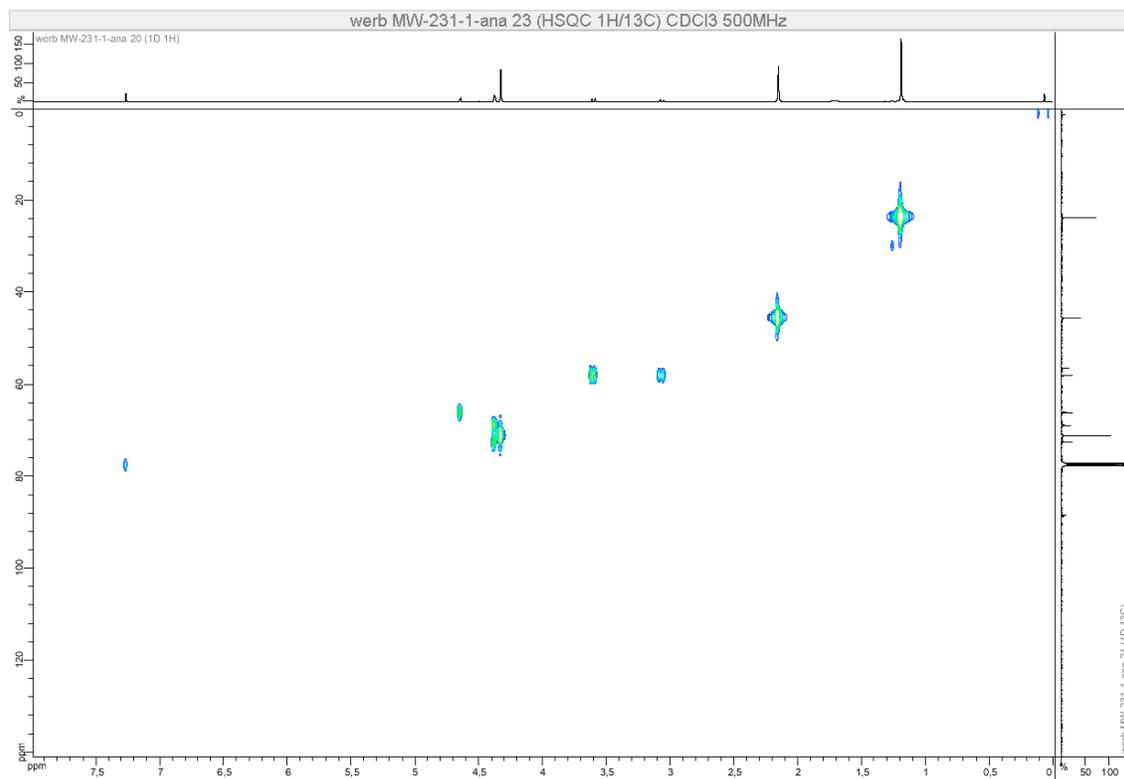
¹³C NMR (126 MHz, CDCl₃)



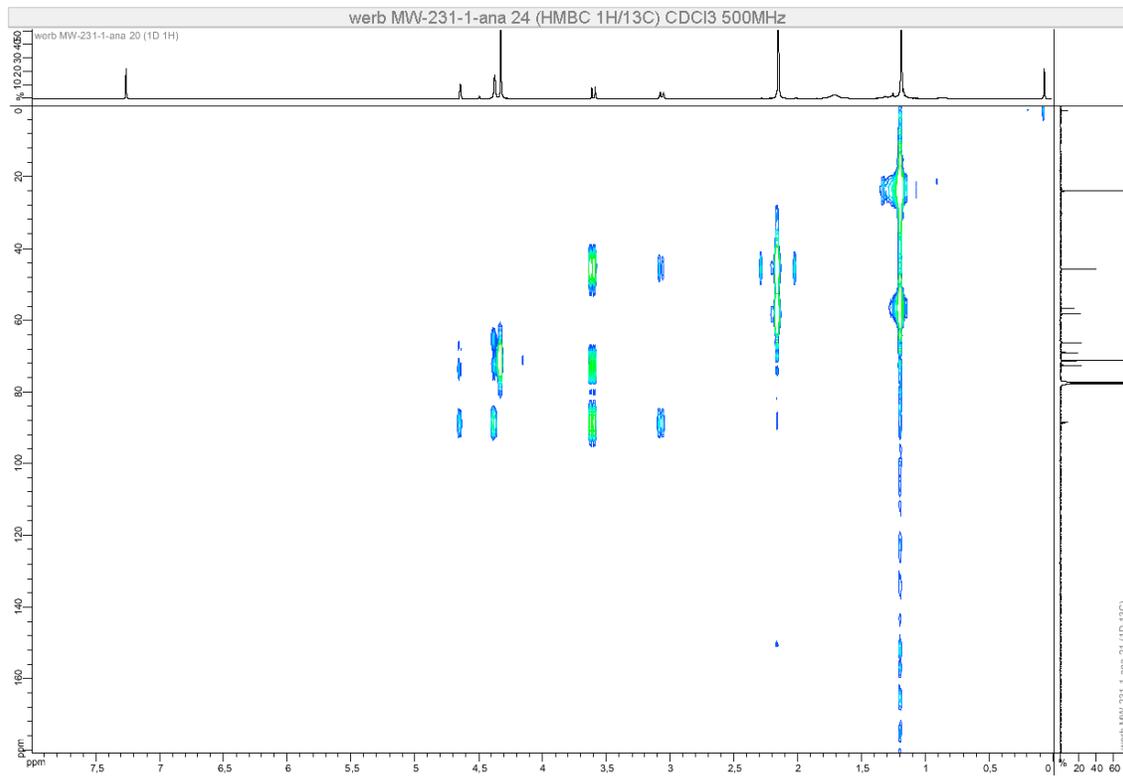
COSY (500 MHz, CDCl₃)



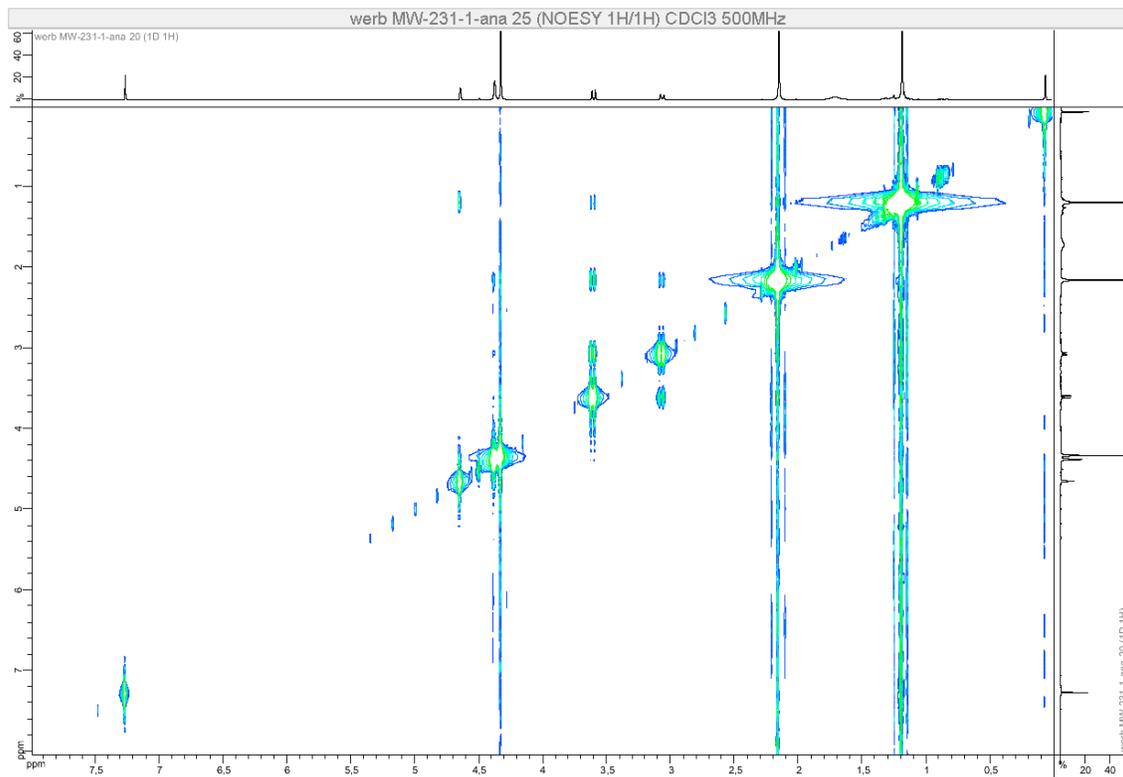
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

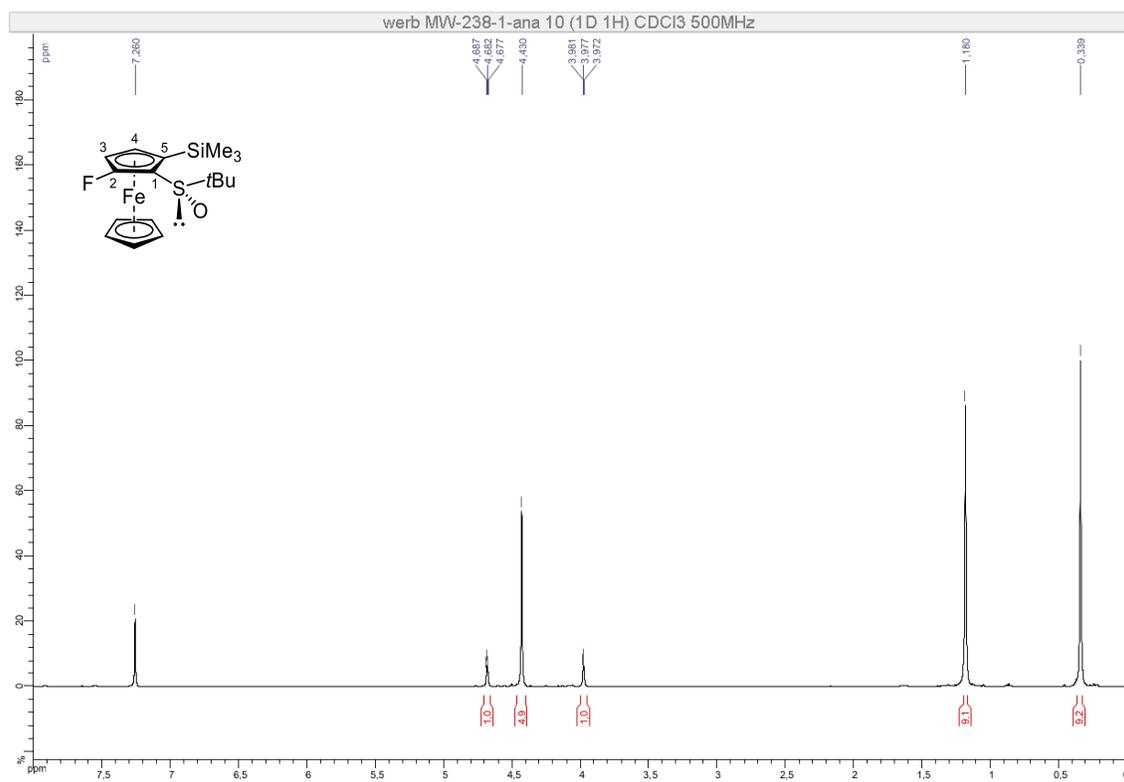


NOESY (500 MHz, CDCl₃)

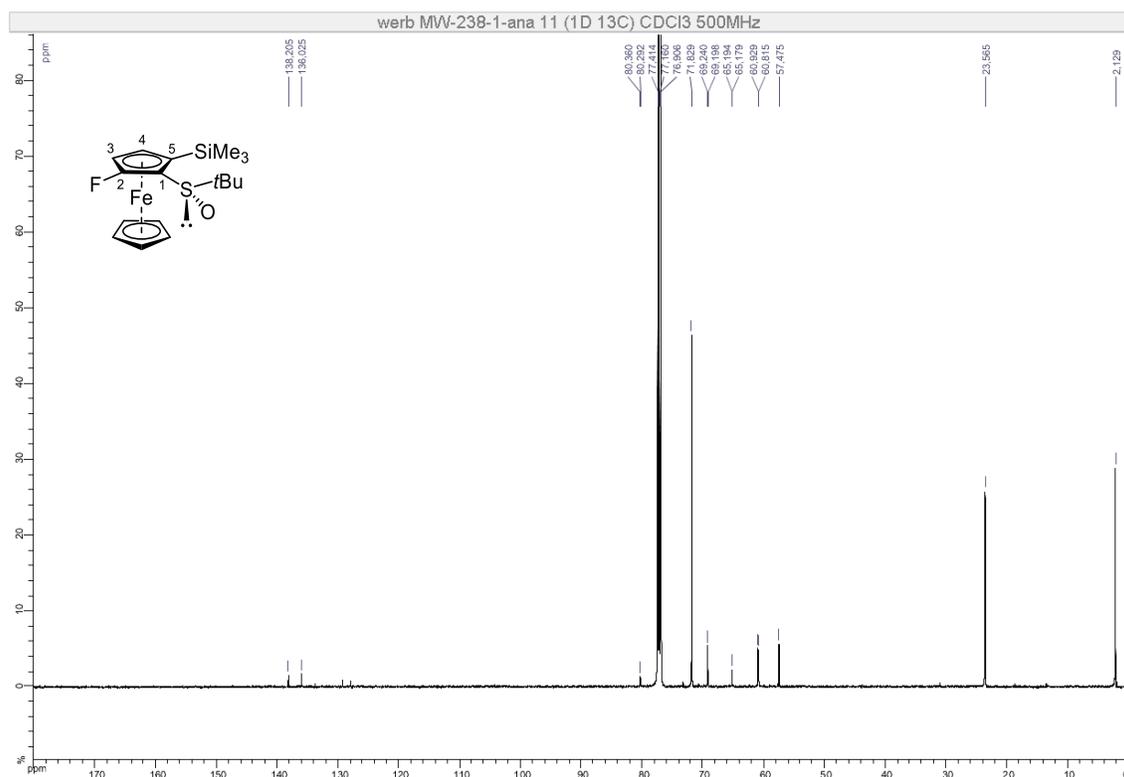


(*S,S*_P)-*S*-tert-Butyl-2-fluoro-5-(trimethylsilyl)ferrocenesulfoxide (*S,S*_P-2ai)

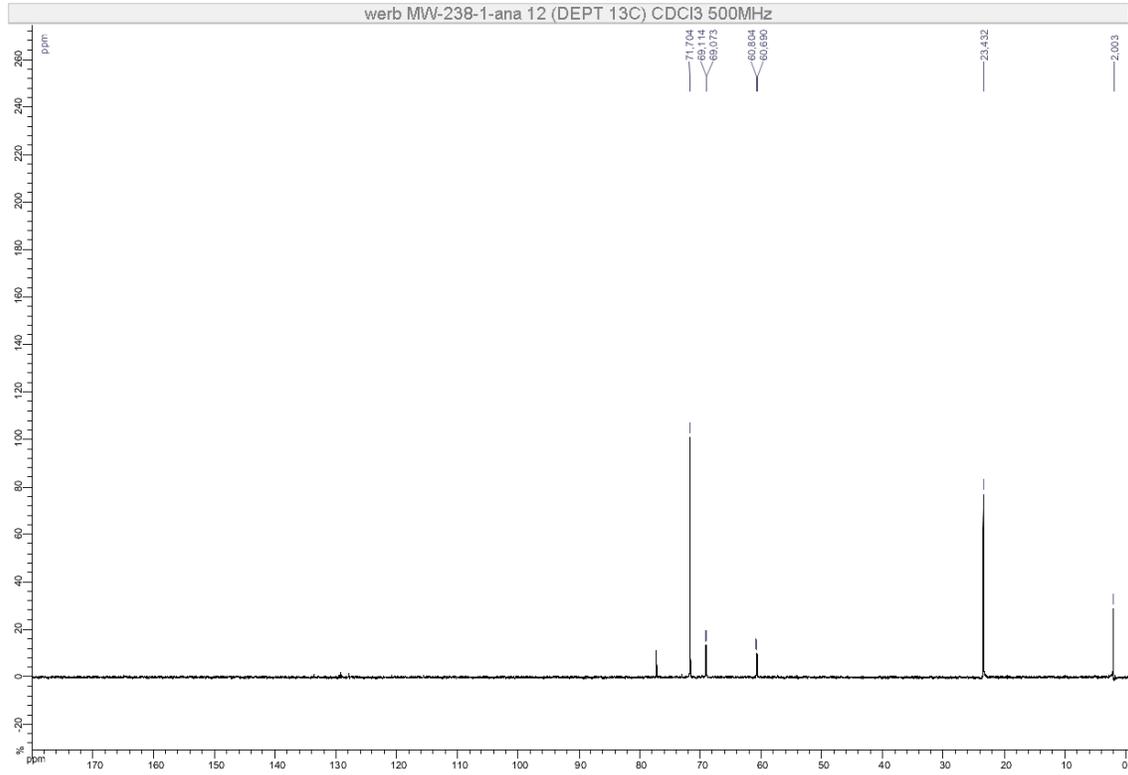
¹H NMR (500 MHz, CDCl₃)



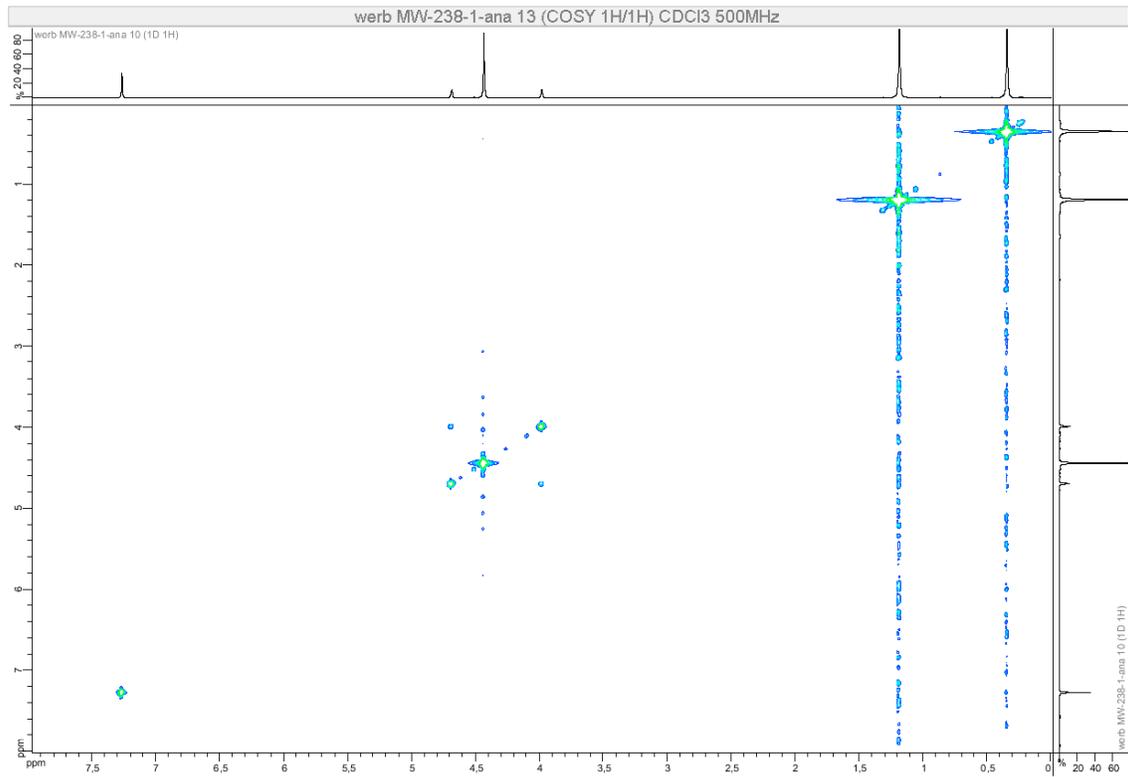
¹³C NMR (126 MHz, CDCl₃)



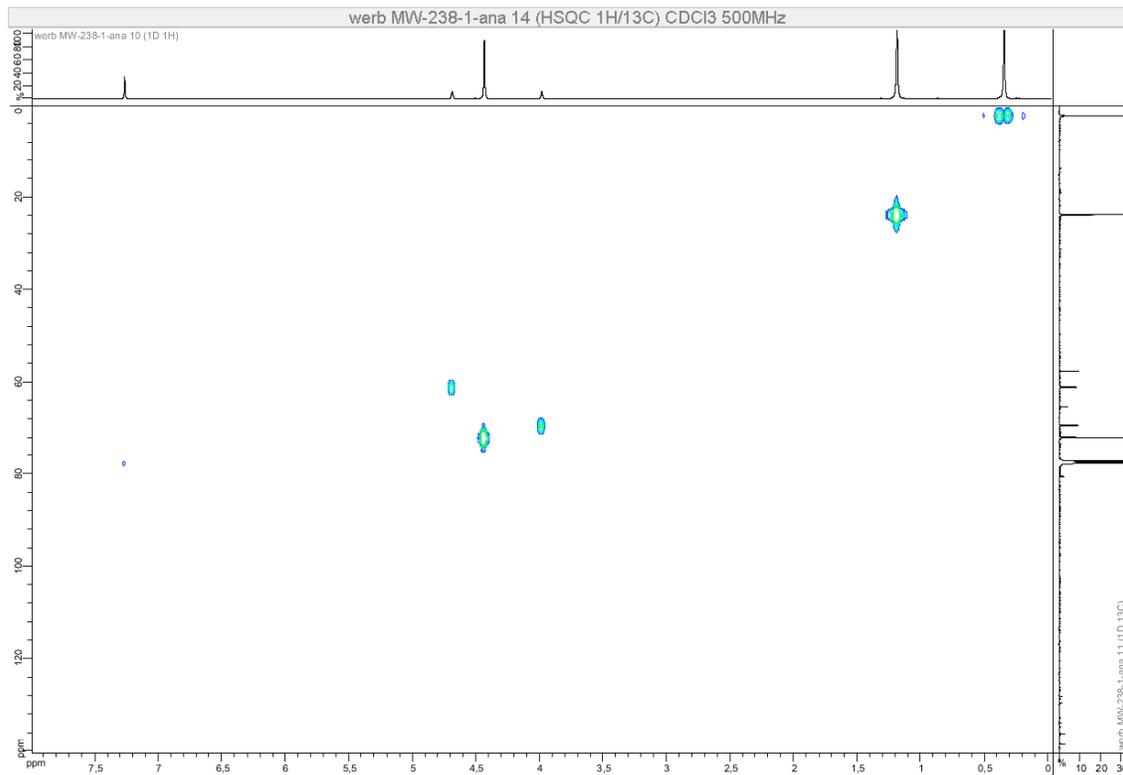
DEPT 135 (126 MHz, CDCl₃)



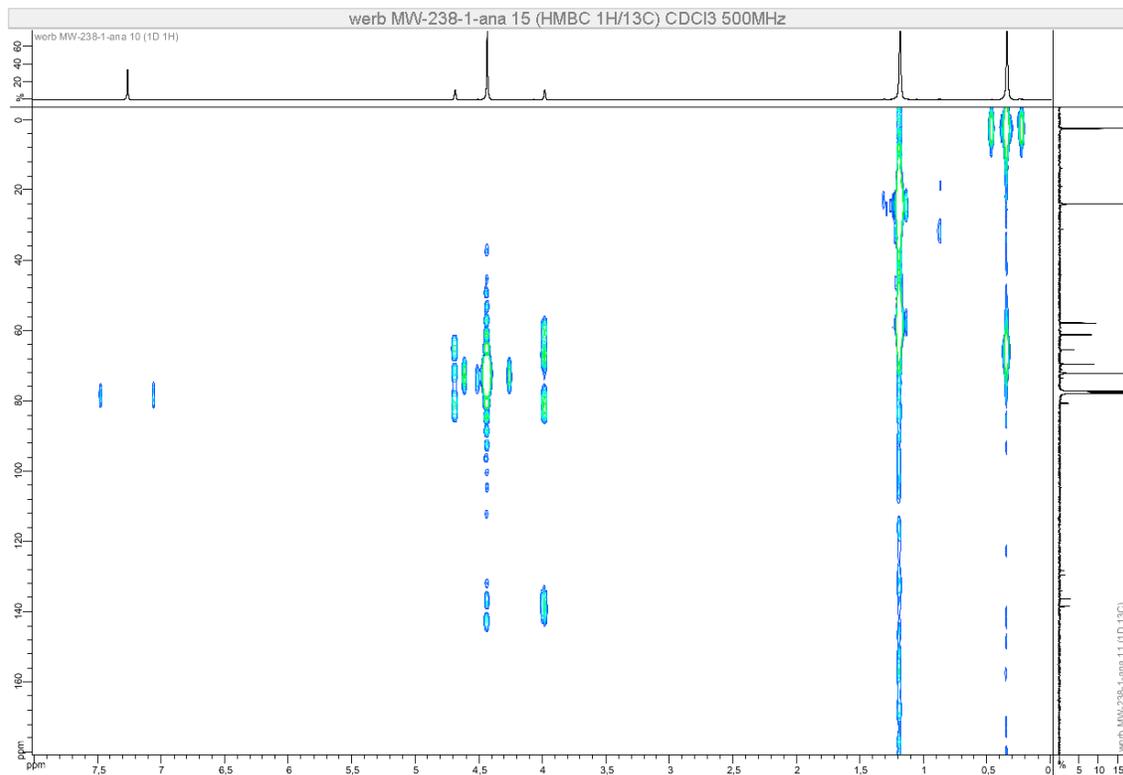
COSY (500 MHz, CDCl₃)



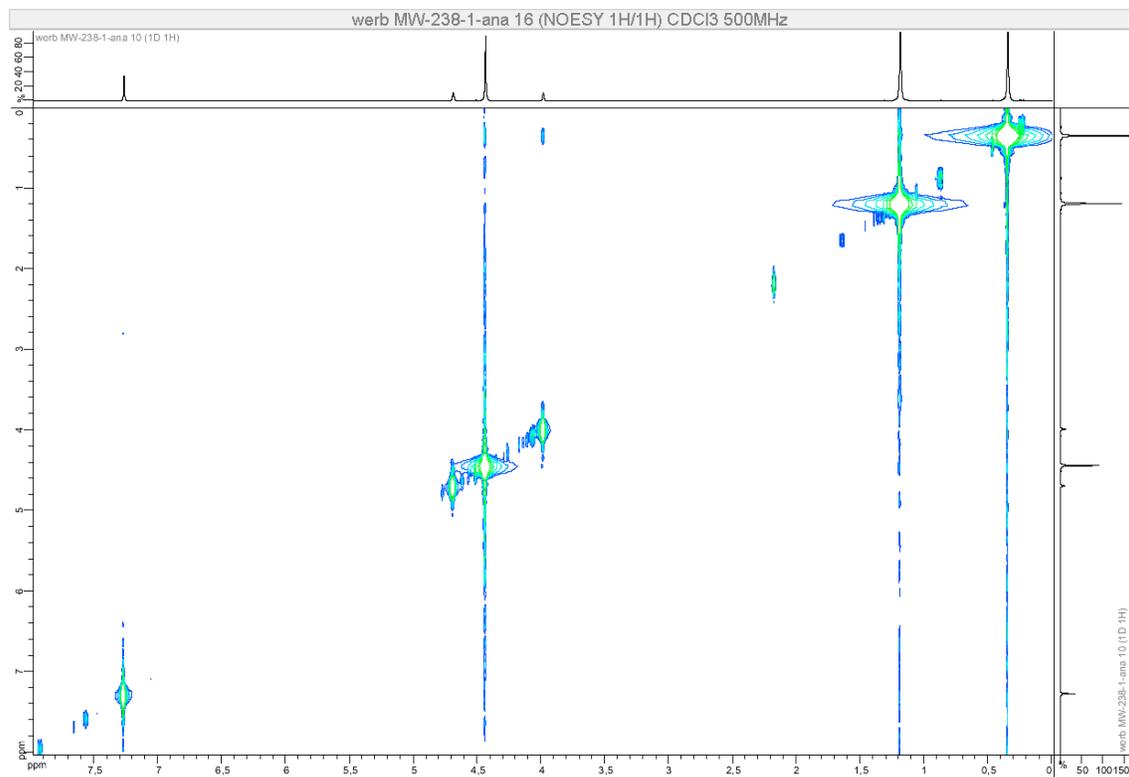
HSQC (500 MHz, CDCl₃)



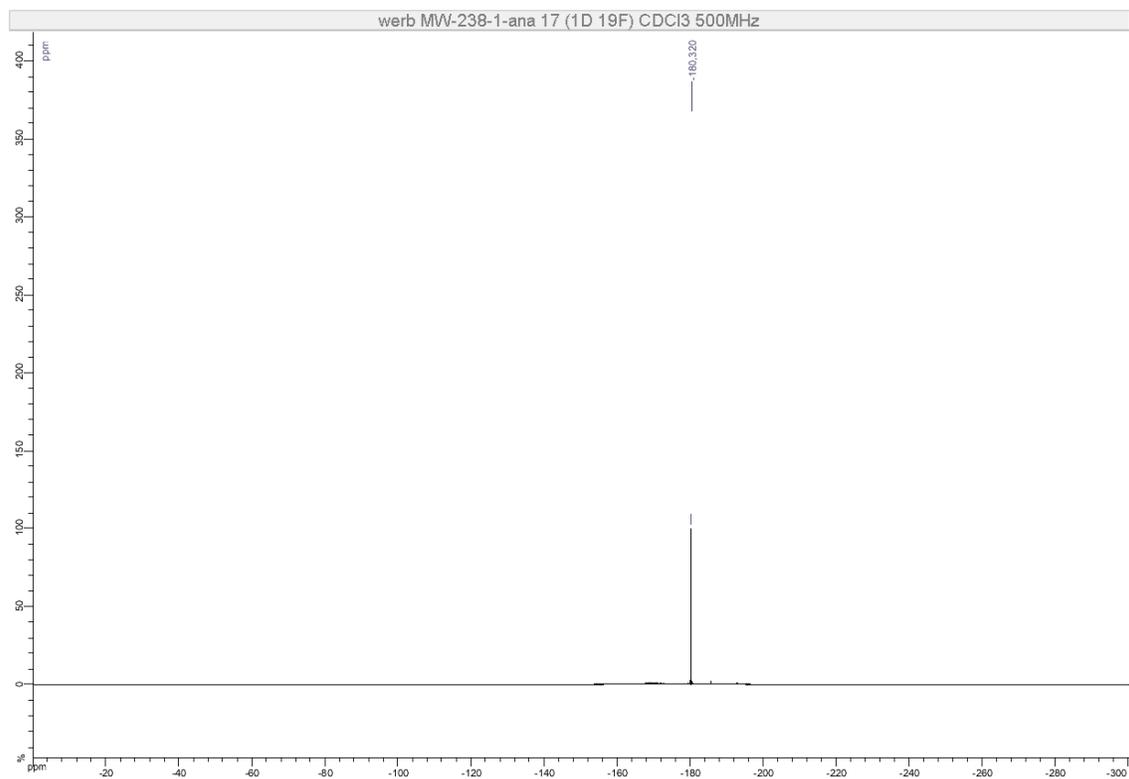
HMBC (500 MHz, CDCl₃)



NOESY (500 MHz, CDCl₃)

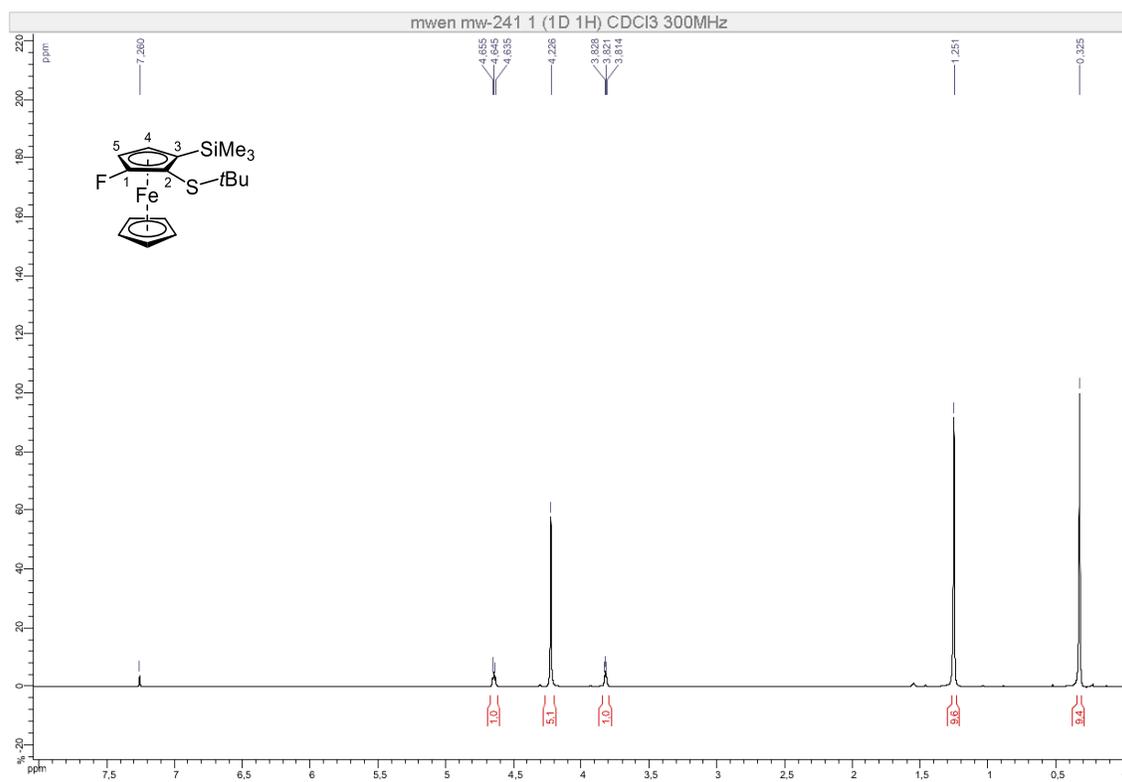


¹⁹F NMR (471 MHz, CDCl₃)



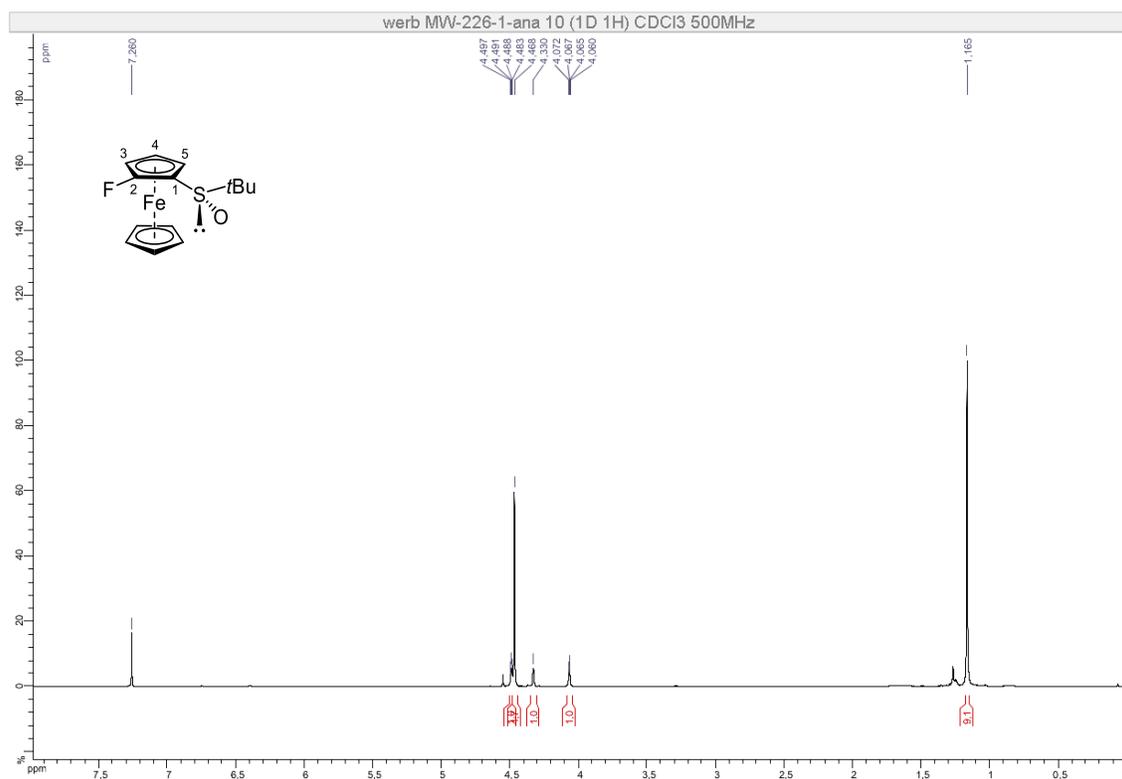
(*S_P*)-2-(*tert*-Butylthio)-1-fluoro-3-(trimethylsilyl)ferrocene (*S_P*-8ai)

¹H NMR (300 MHz, CDCl₃)

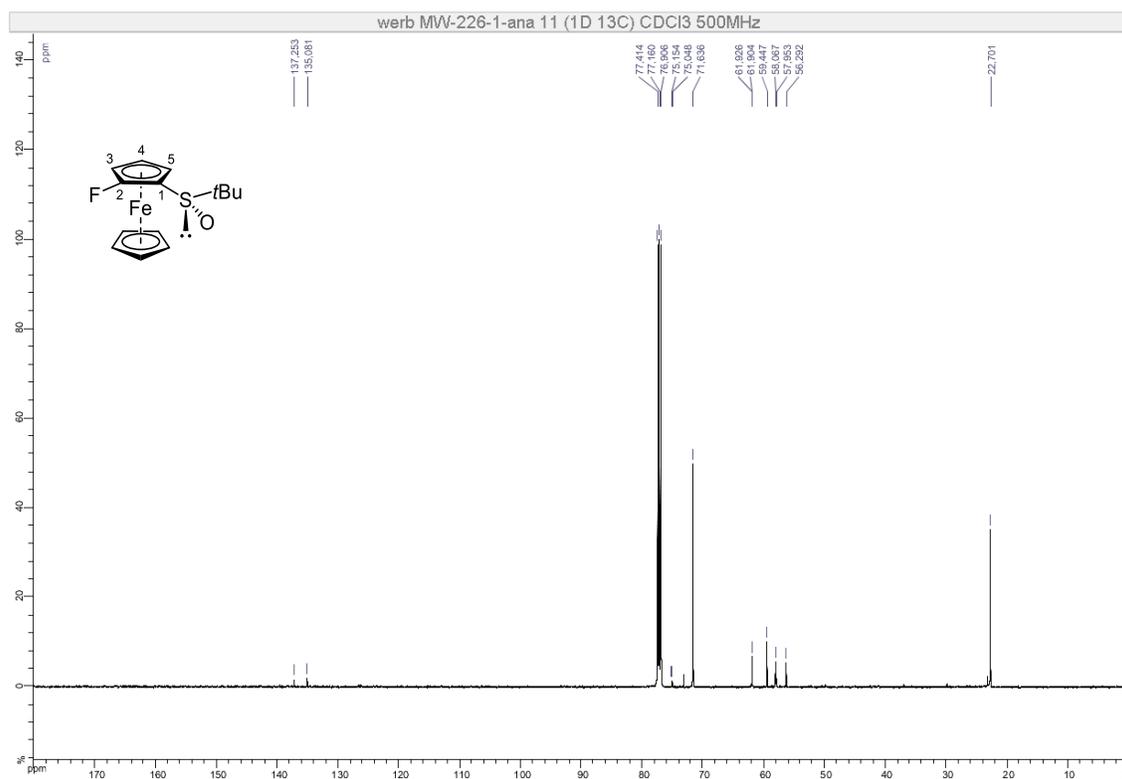


(*S,R_P*)-*S-tert*-Butyl-2-fluoroferrrocenesulfoxide (*S,R_P*-1i)

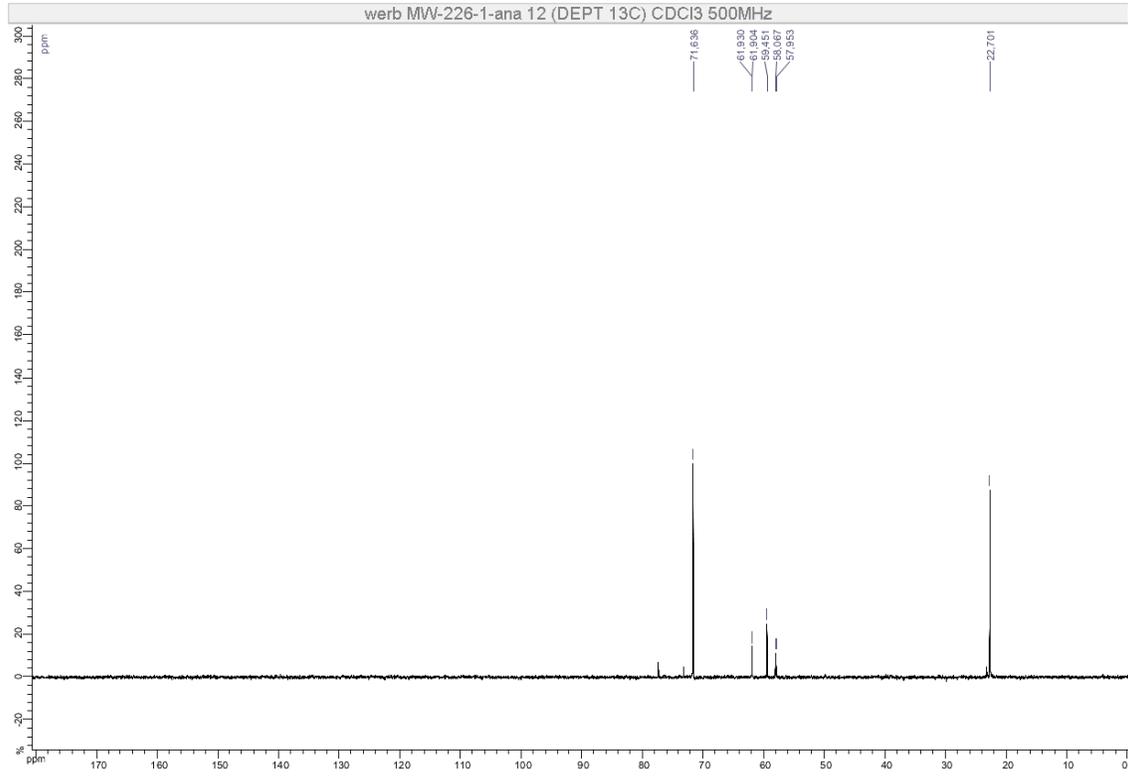
^1H NMR (500 MHz, CDCl_3)



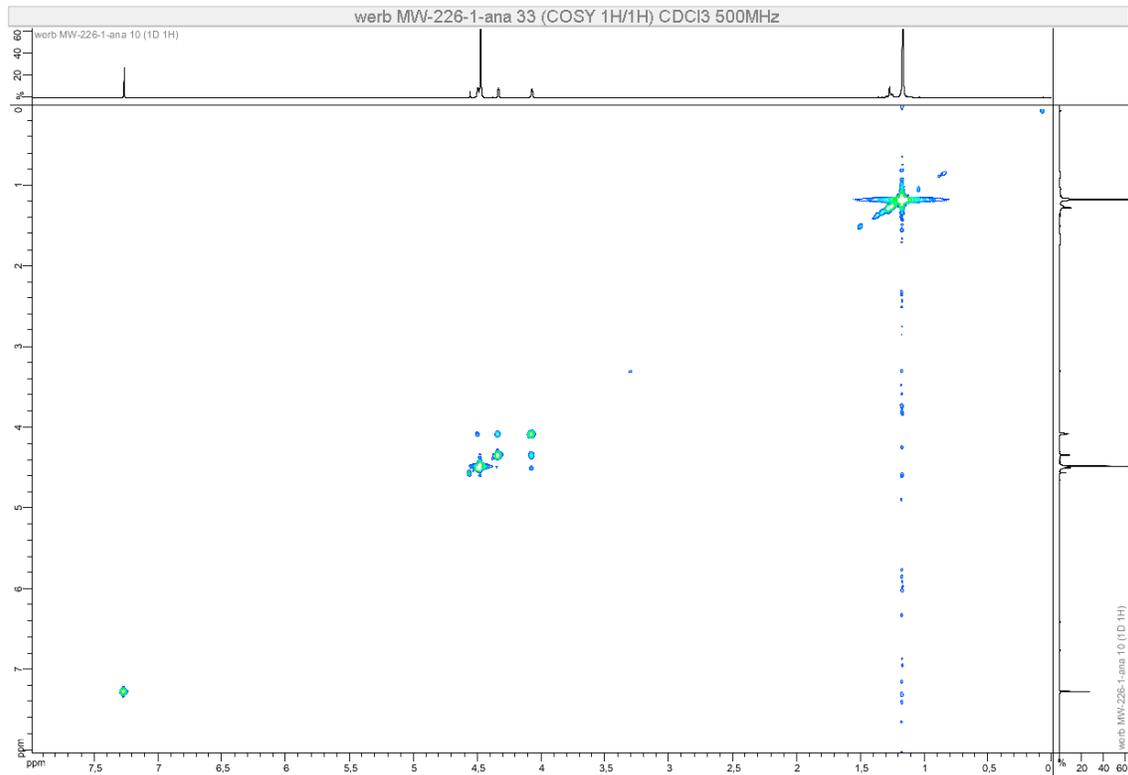
^{13}C NMR (126 MHz, CDCl_3)



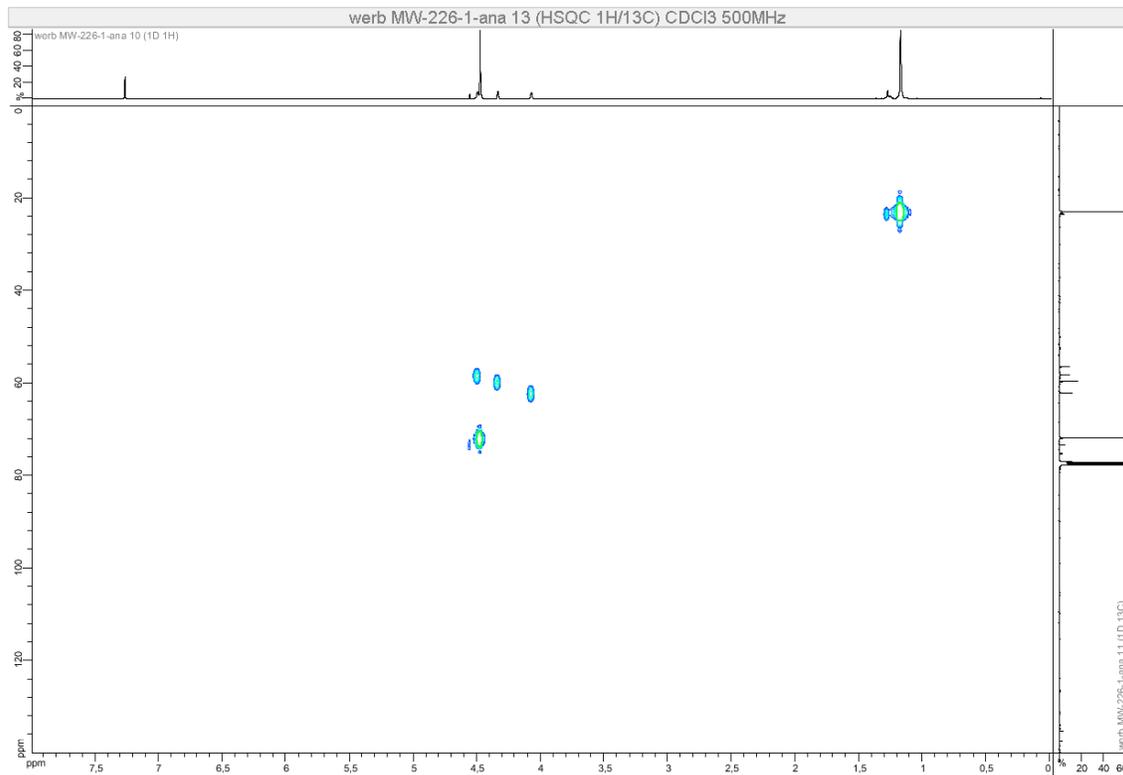
DEPT 135 (126 MHz, CDCl₃)



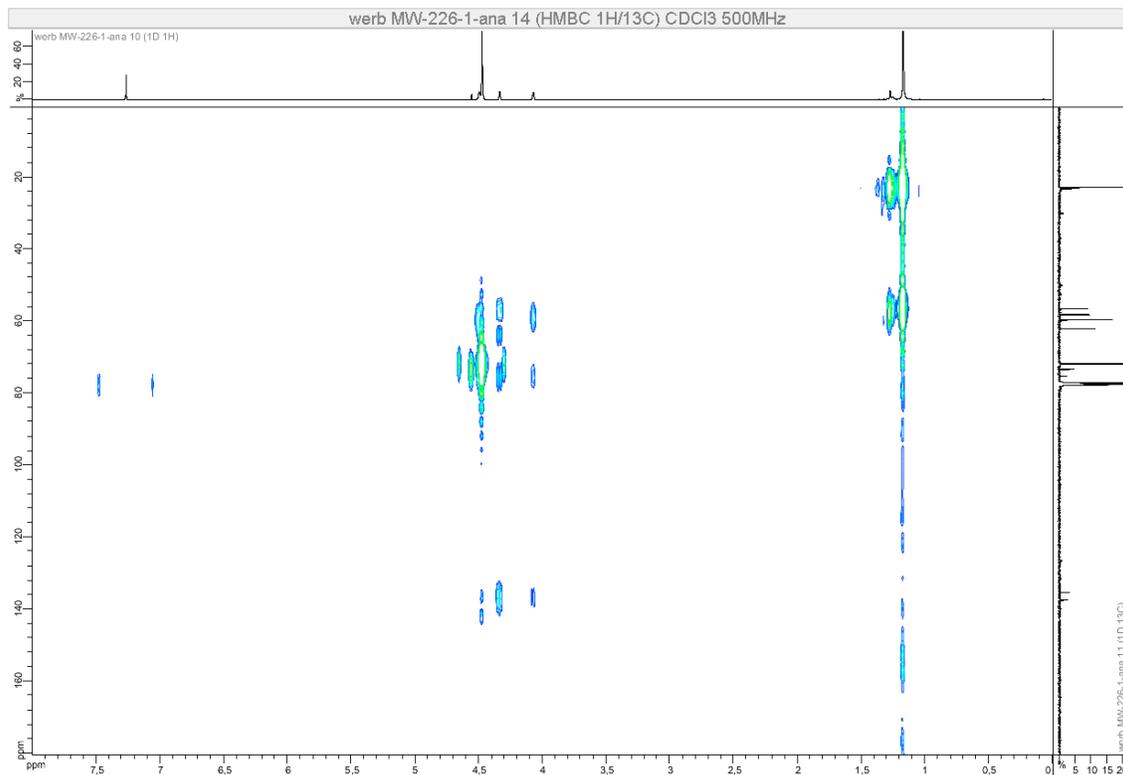
COSY (500 MHz, CDCl₃)



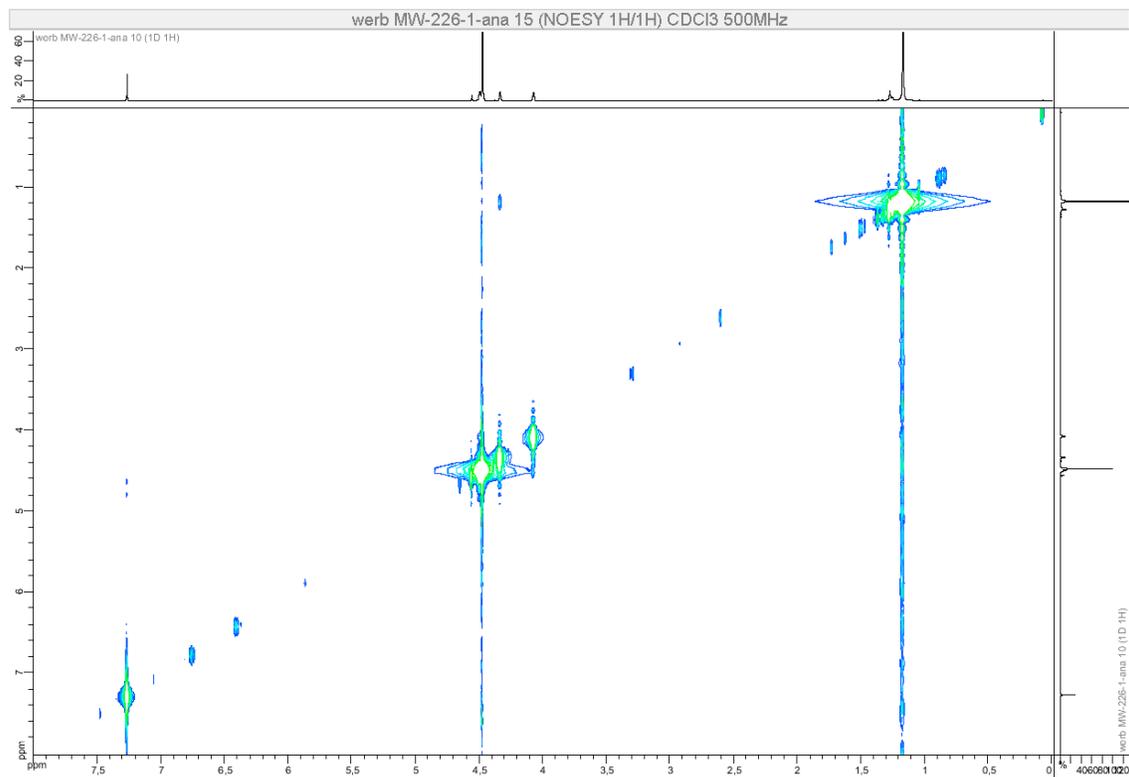
HSQC (500 MHz, CDCl₃)



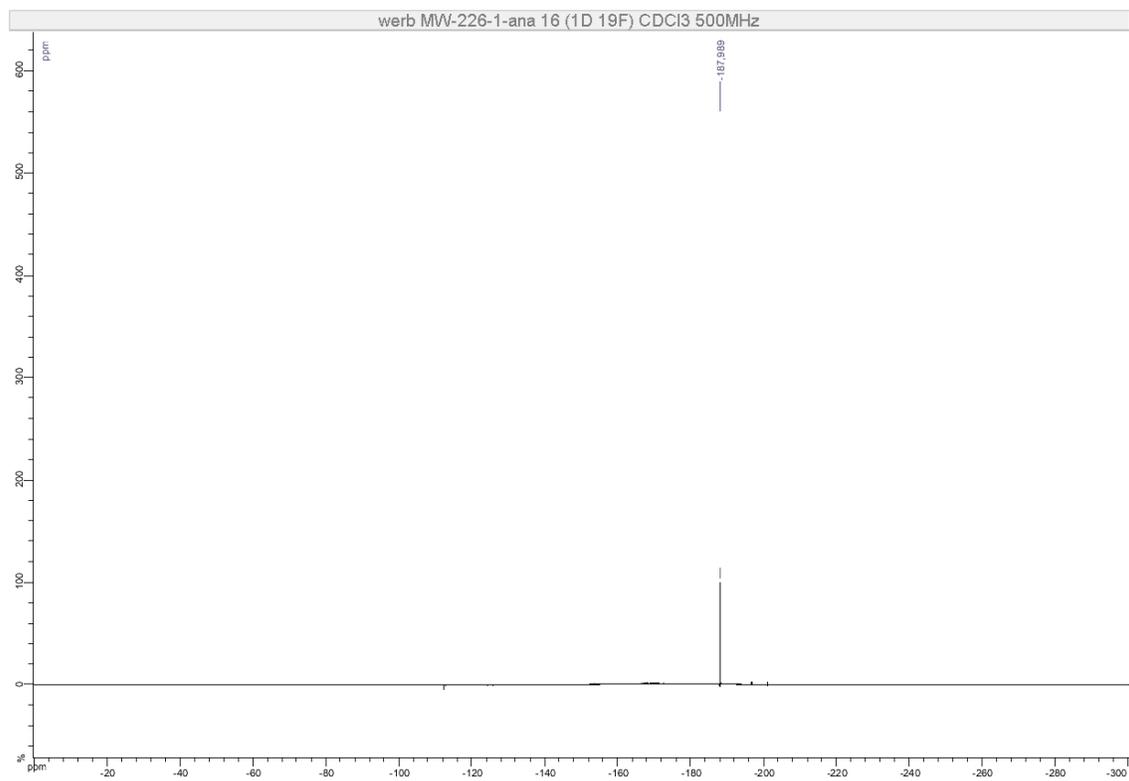
HMBC (500 MHz, CDCl₃)



NOESY (500 MHz, CDCl₃)

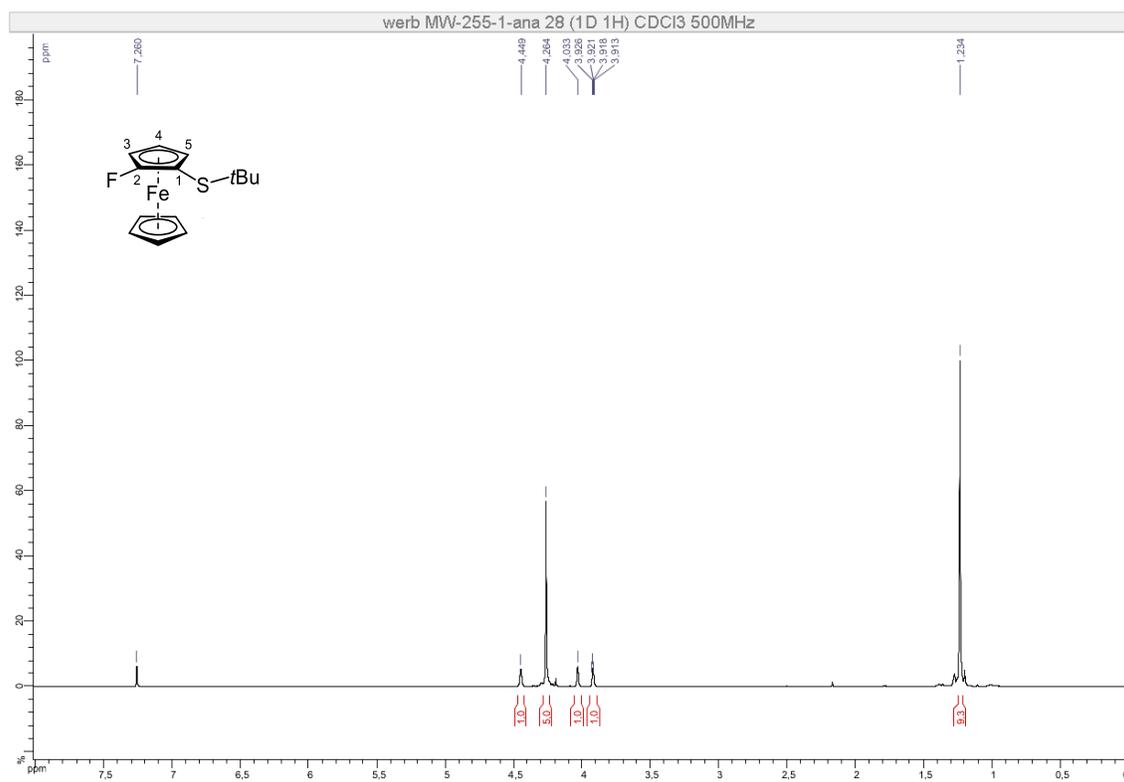


¹⁹F NMR (471 MHz, CDCl₃)

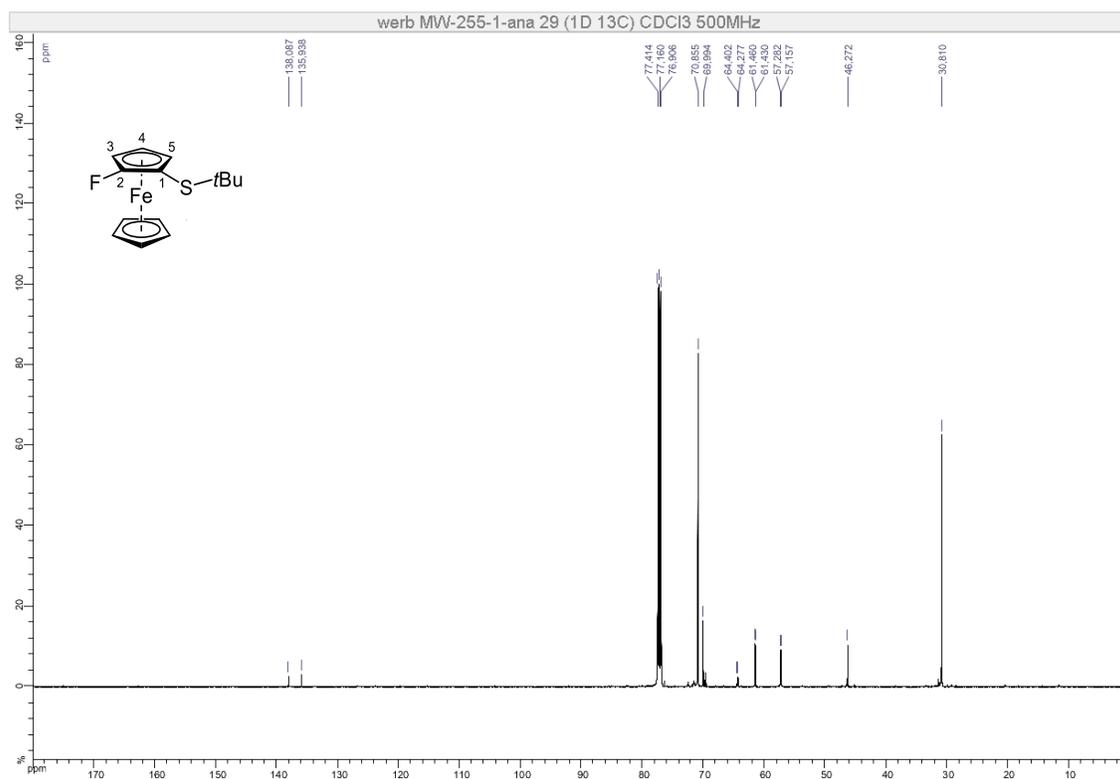


(*R_P*)-1-(*tert*-Butylthio)-2-fluoroferrrocene (*R_P*-8i)

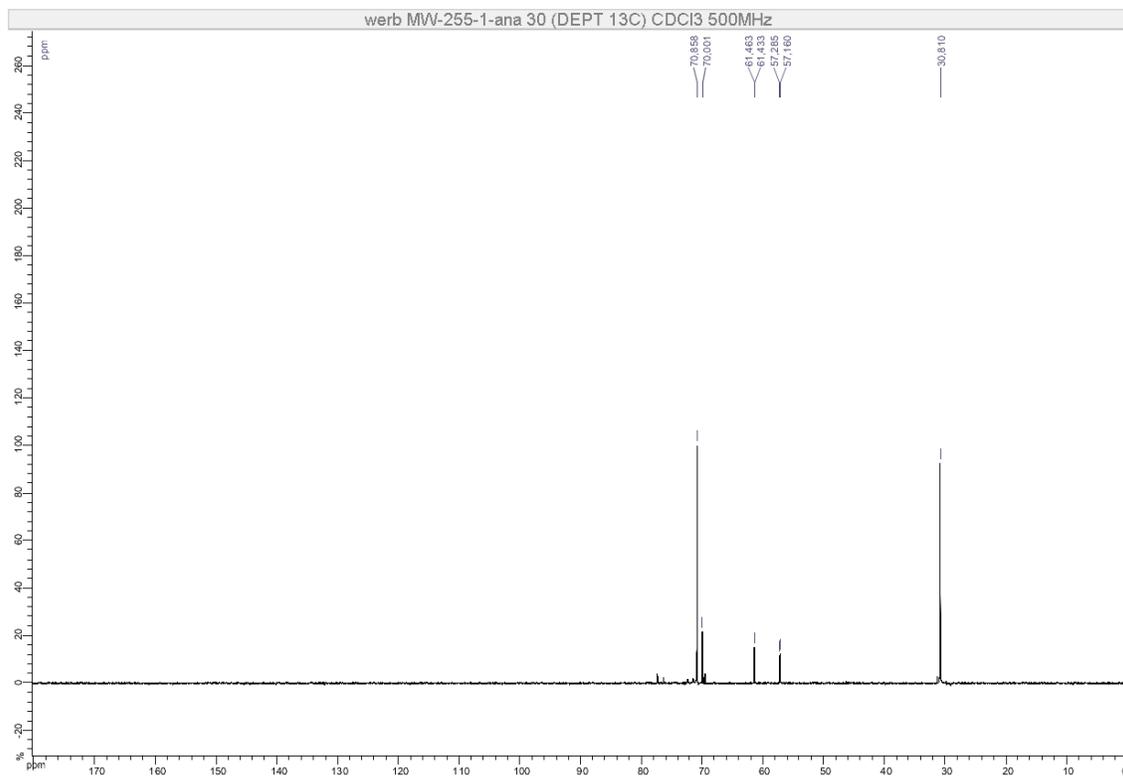
¹H NMR (500 MHz, CDCl₃)



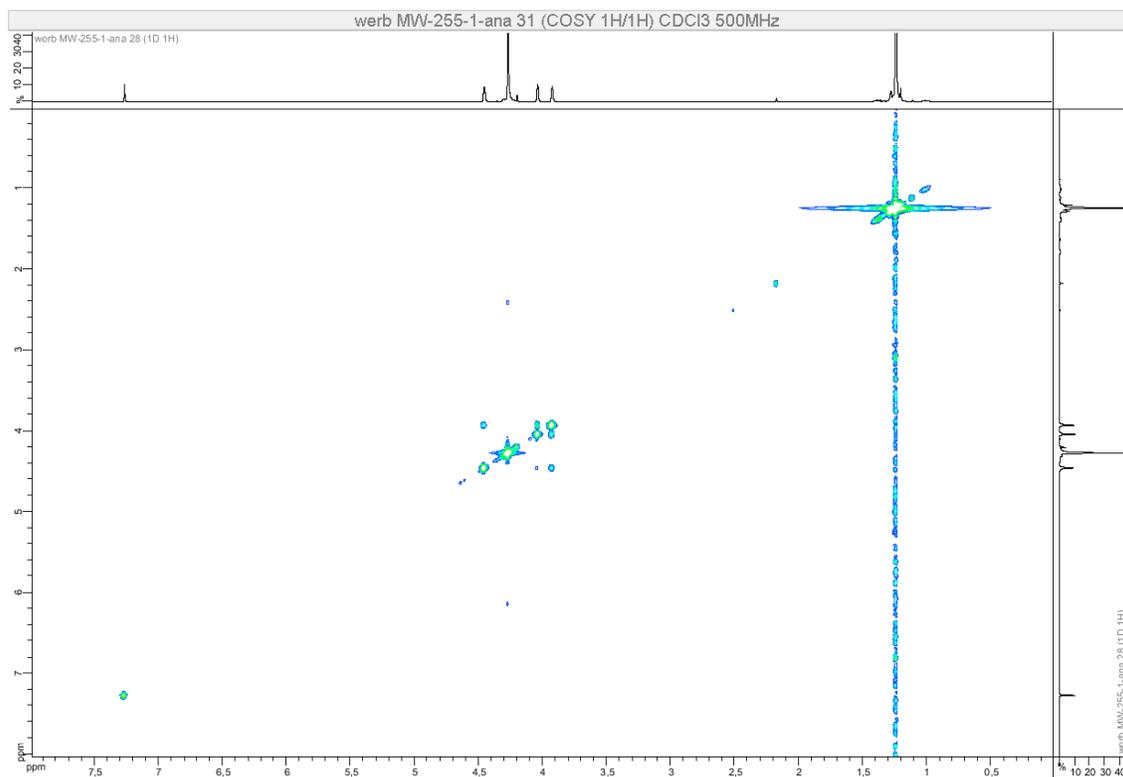
¹³C NMR (126 MHz, CDCl₃)



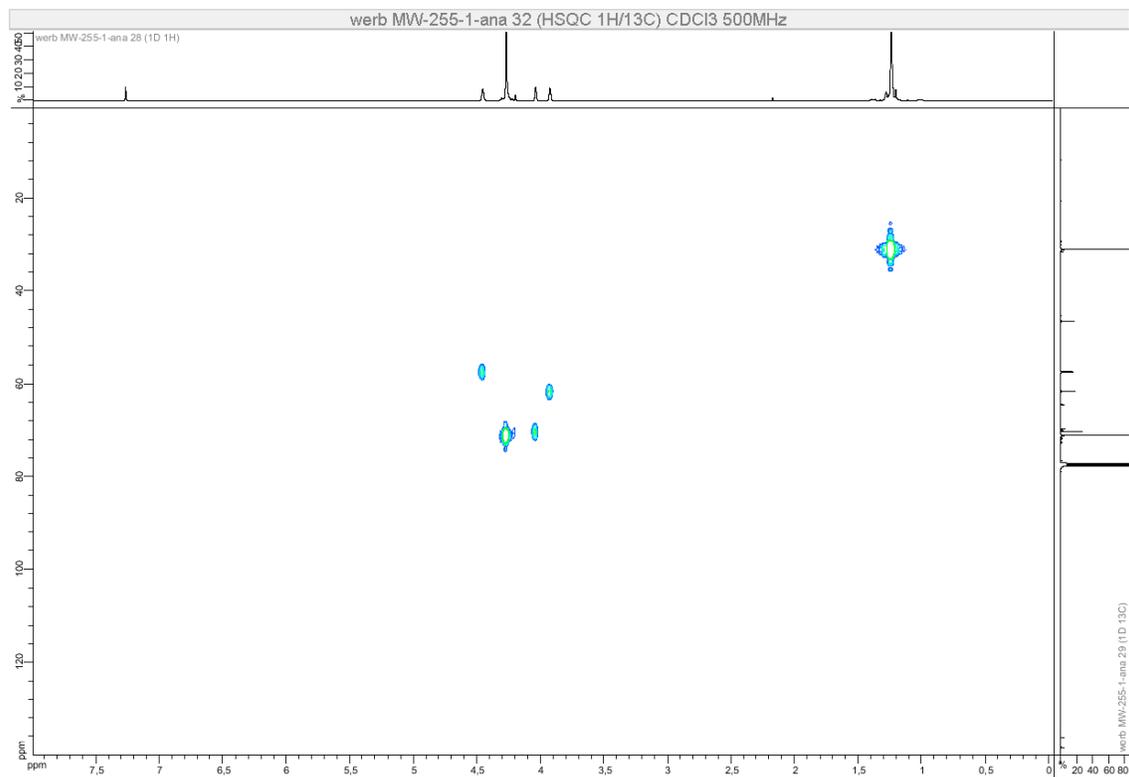
DEPT 135 (126 MHz, CDCl₃)



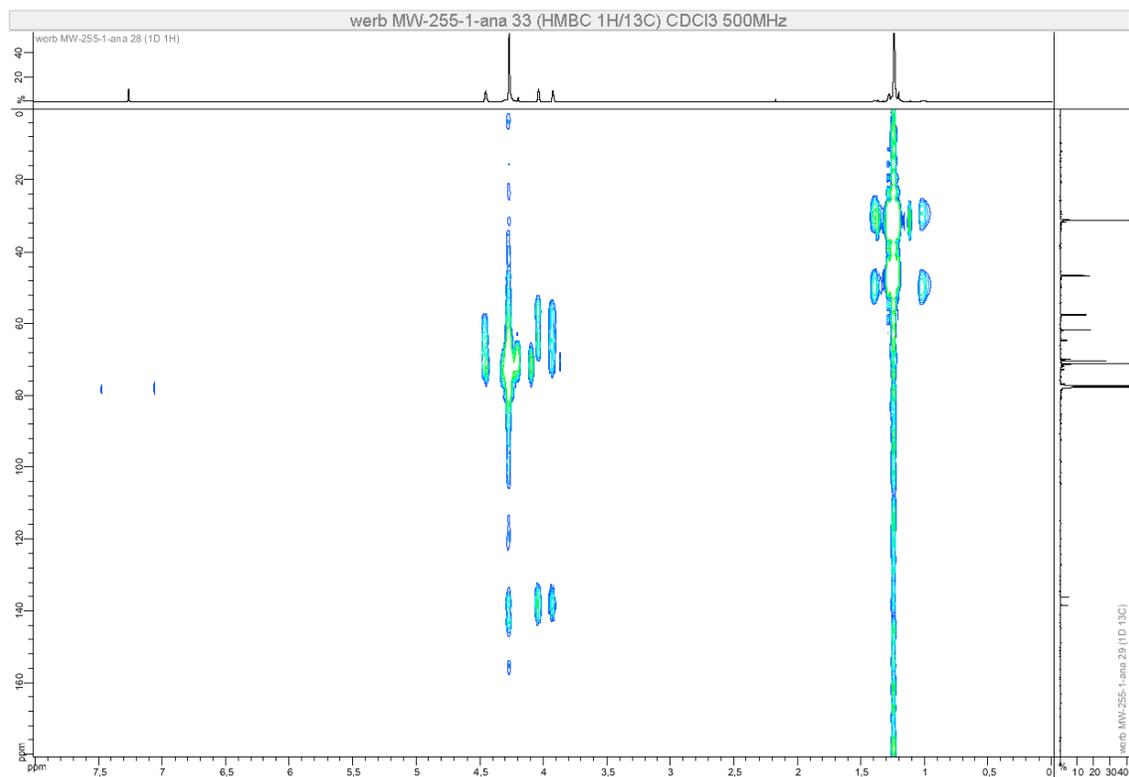
COSY (500 MHz, CDCl₃)



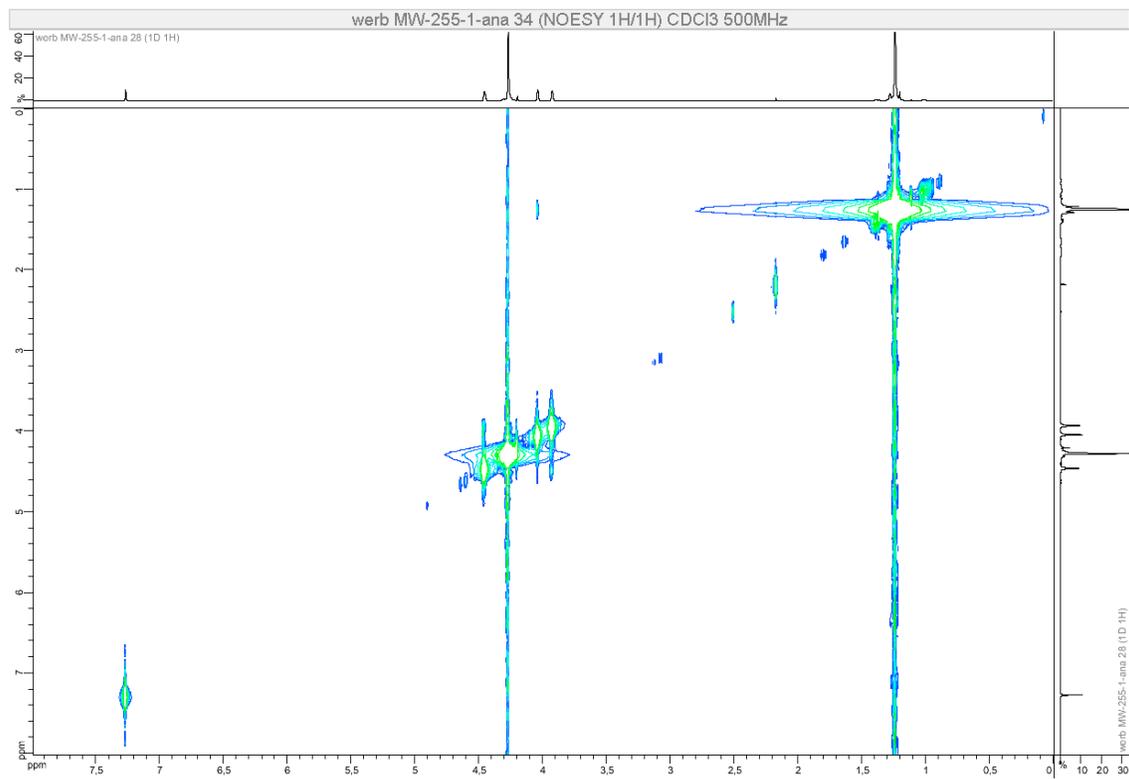
HSQC (500 MHz, CDCl₃)



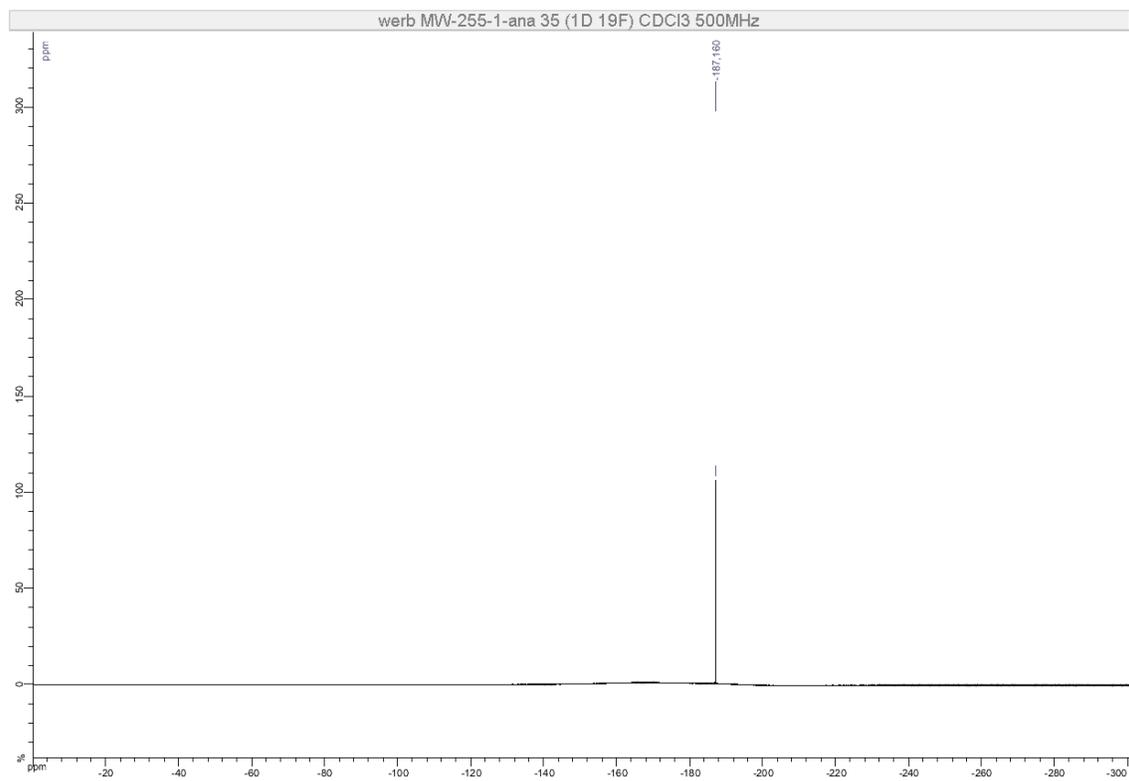
HMBC (500 MHz, CDCl₃)



NOESY (500 MHz, CDCl₃)

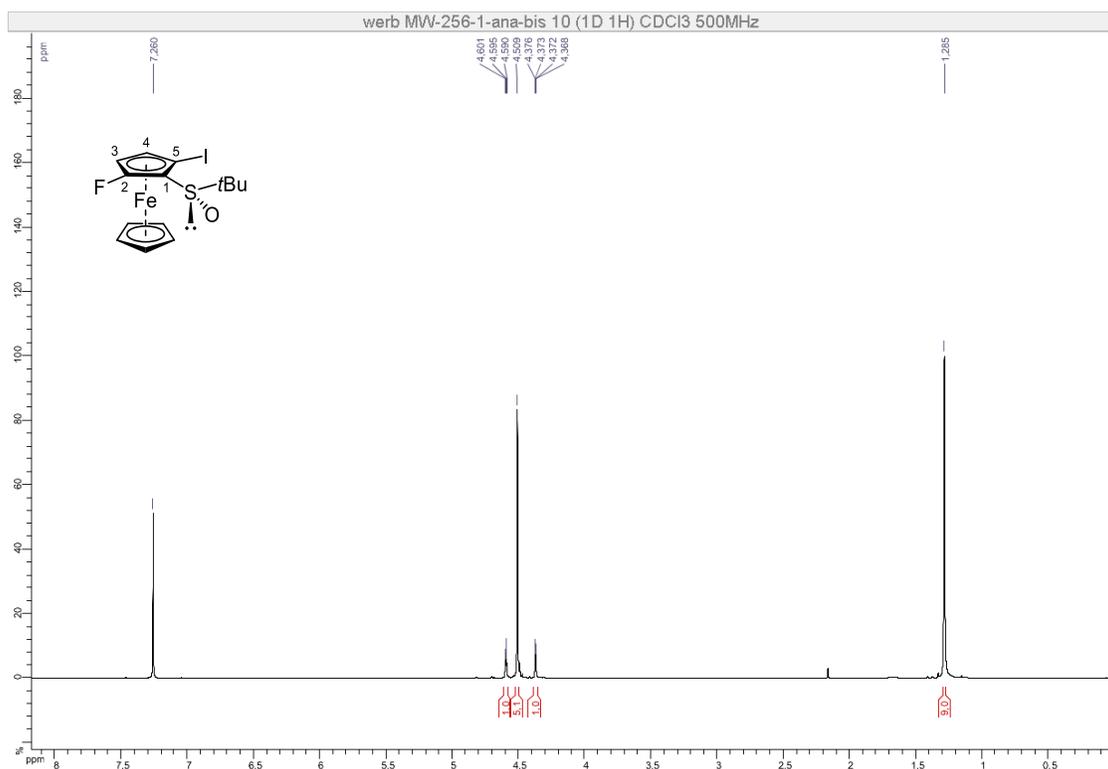


¹⁹F NMR (471 MHz, CDCl₃)

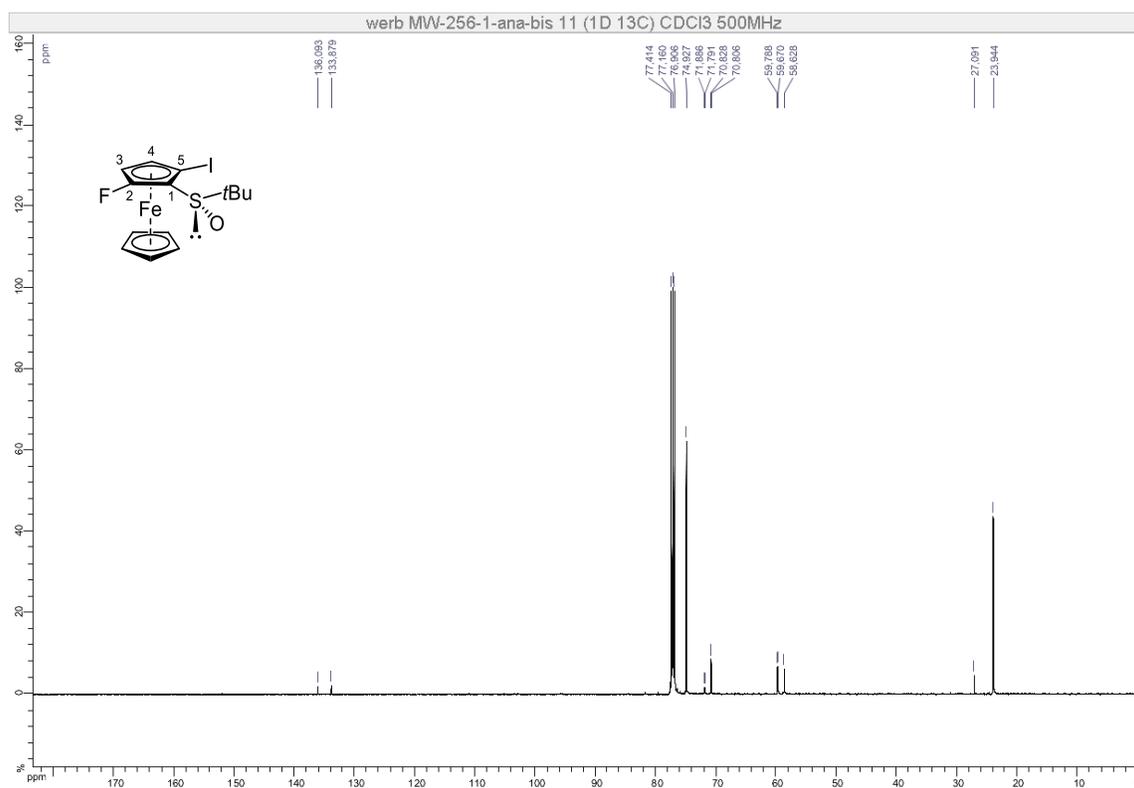


(*S,R*_P)-*S*-tert-Butyl-2-fluoro-5-iodoferrocenesulfoxide (*S,R*_P-2bi)

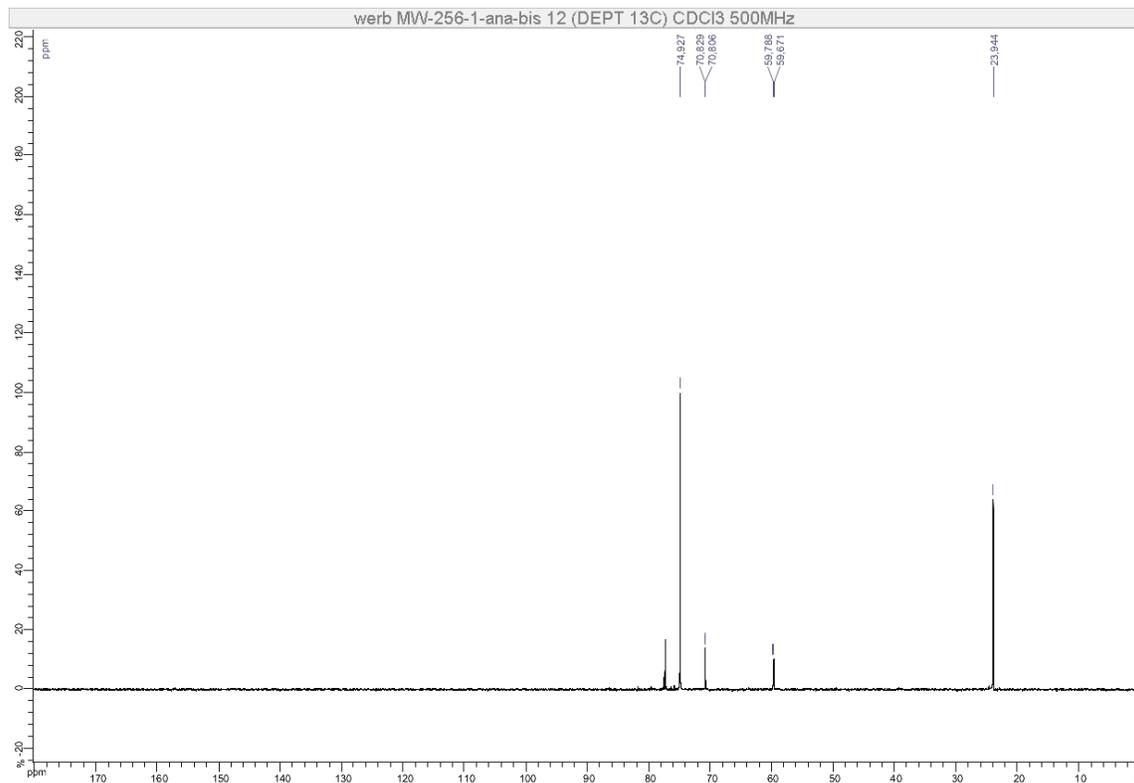
¹H NMR (500 MHz, CDCl₃)



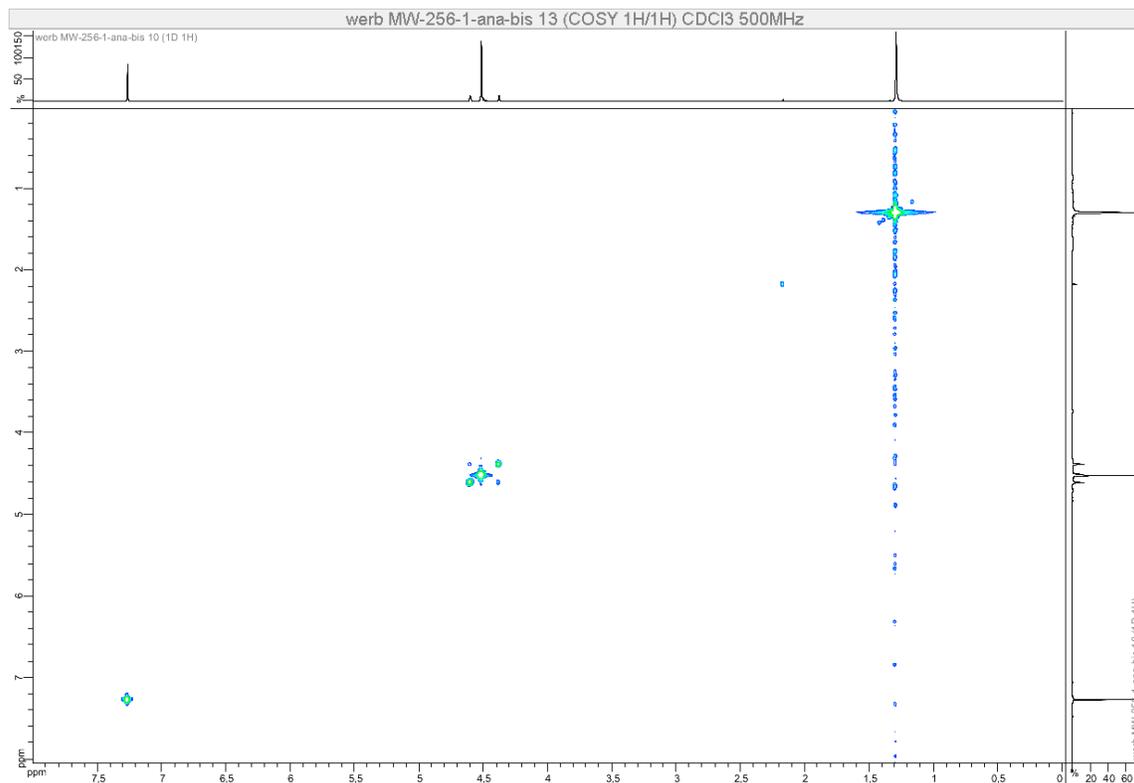
¹³C NMR (126 MHz, CDCl₃)



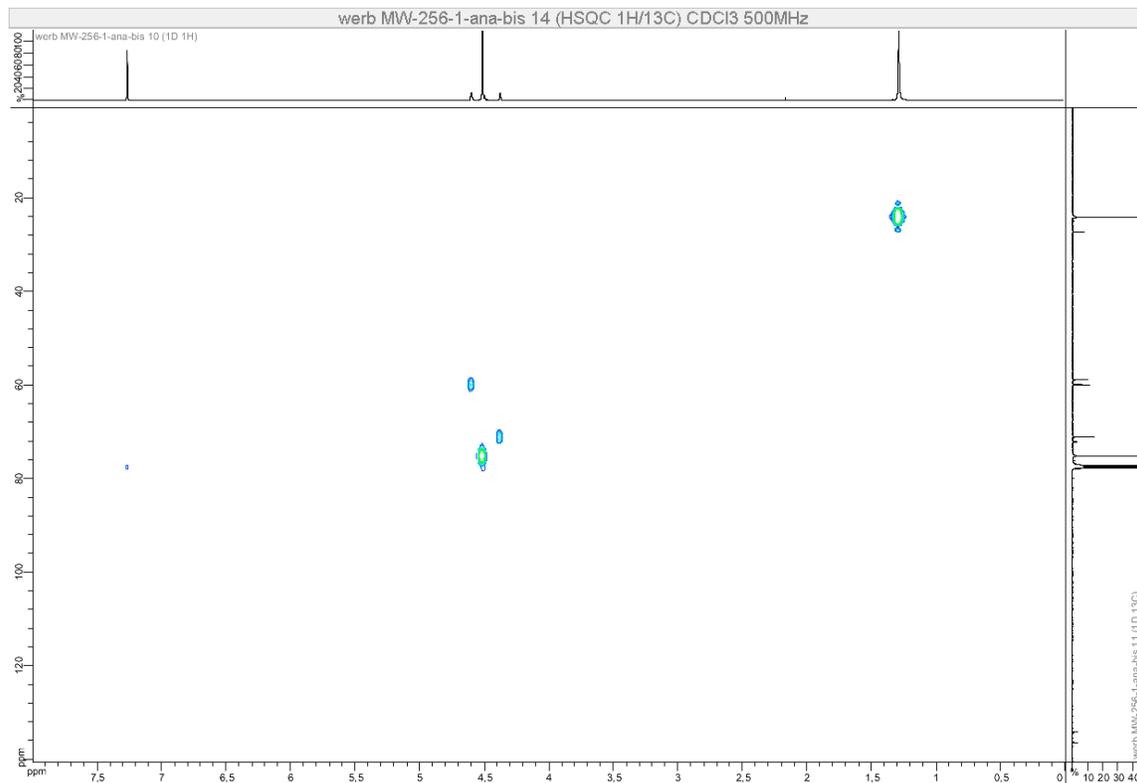
DEPT 135 (126 MHz, CDCl₃)



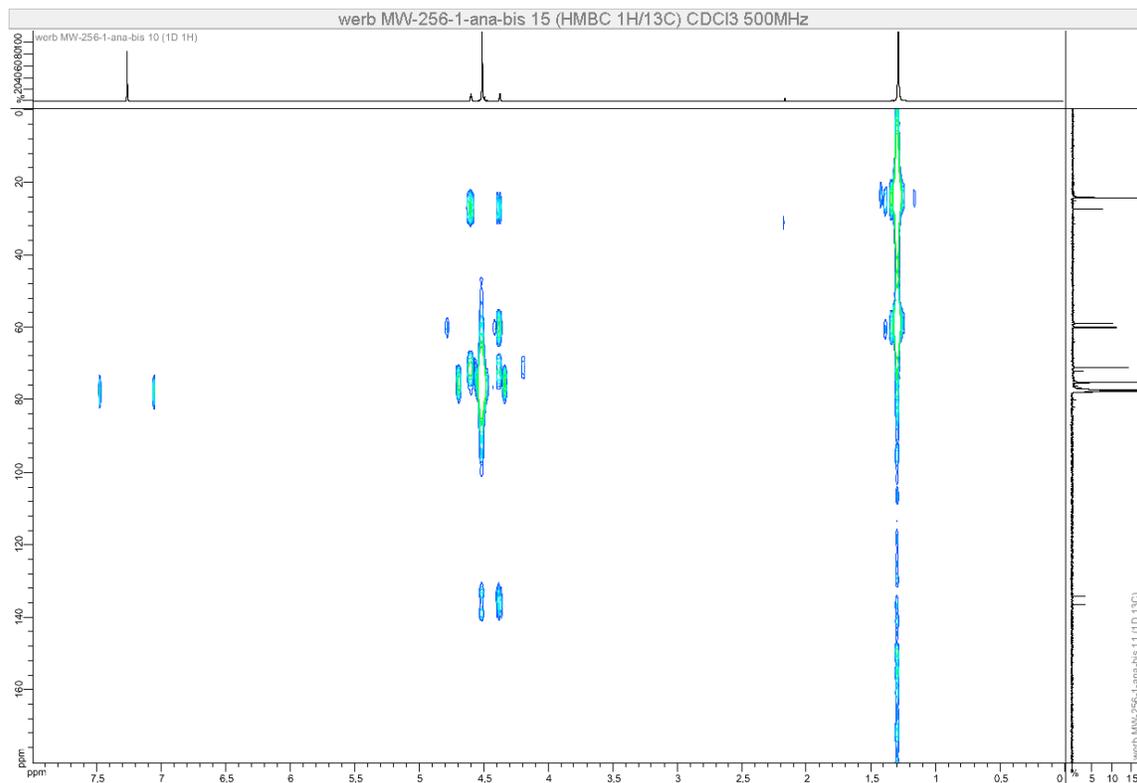
COSY (500 MHz, CDCl₃)



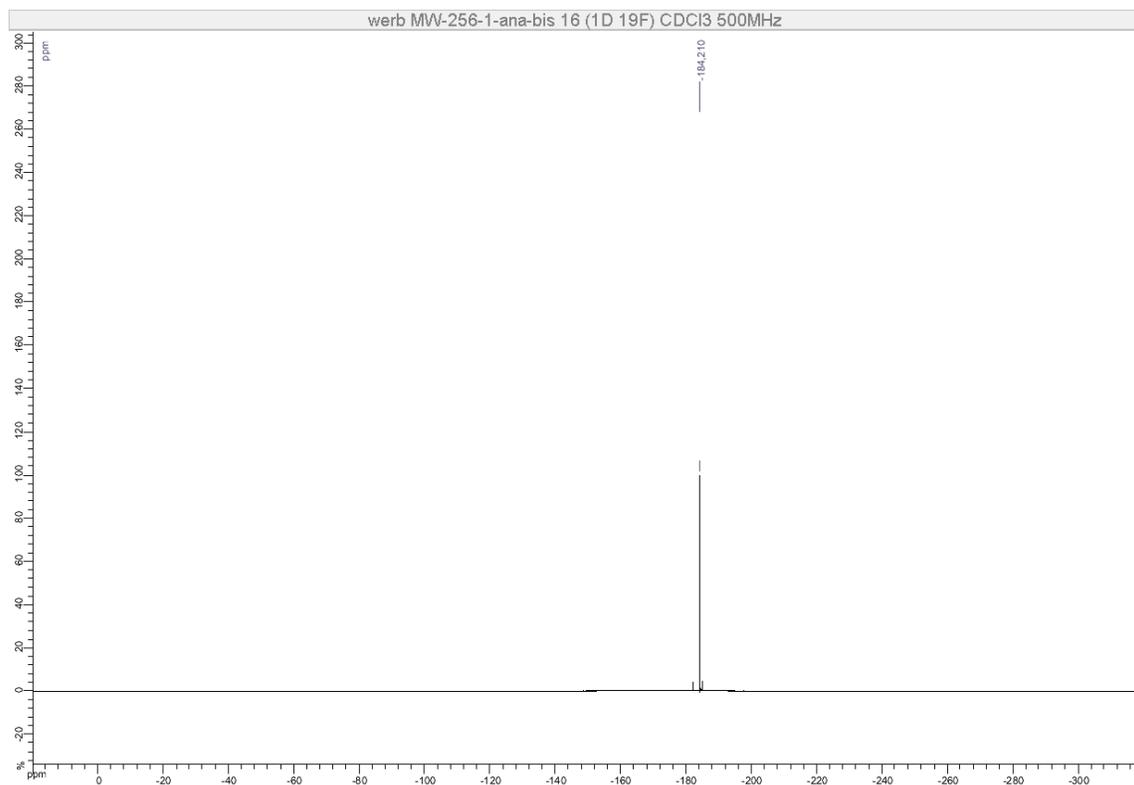
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

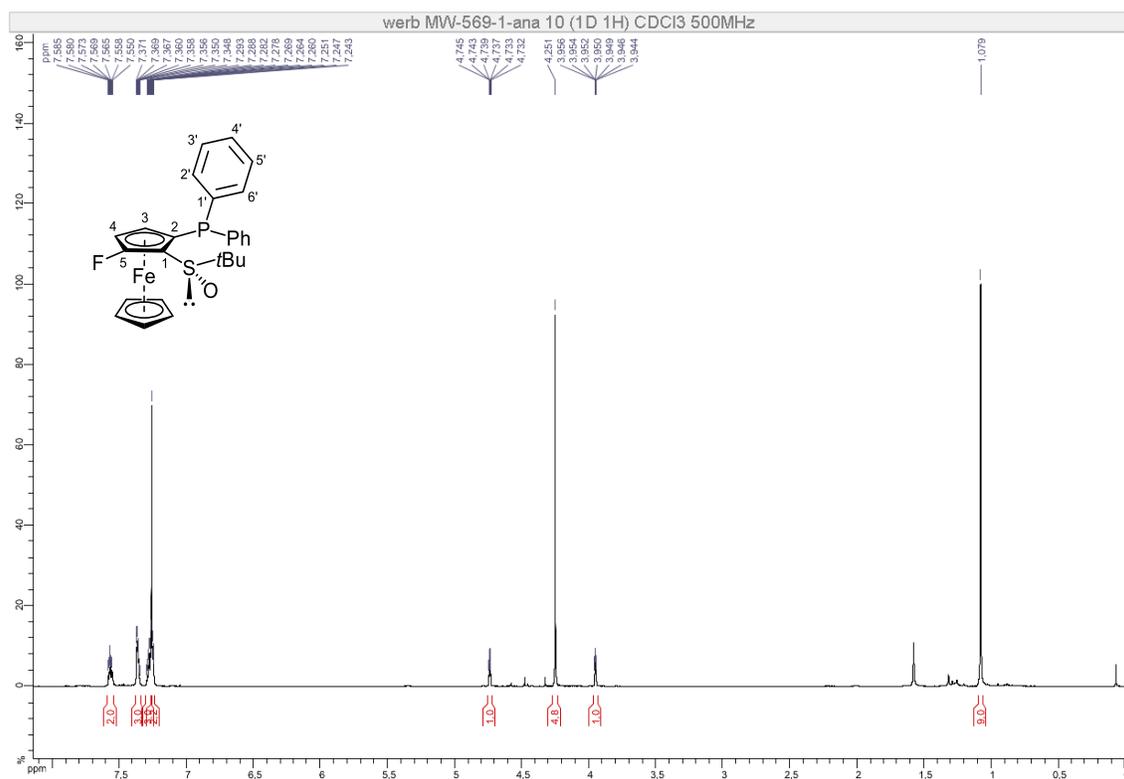


^{19}F NMR (471 MHz, CDCl_3)

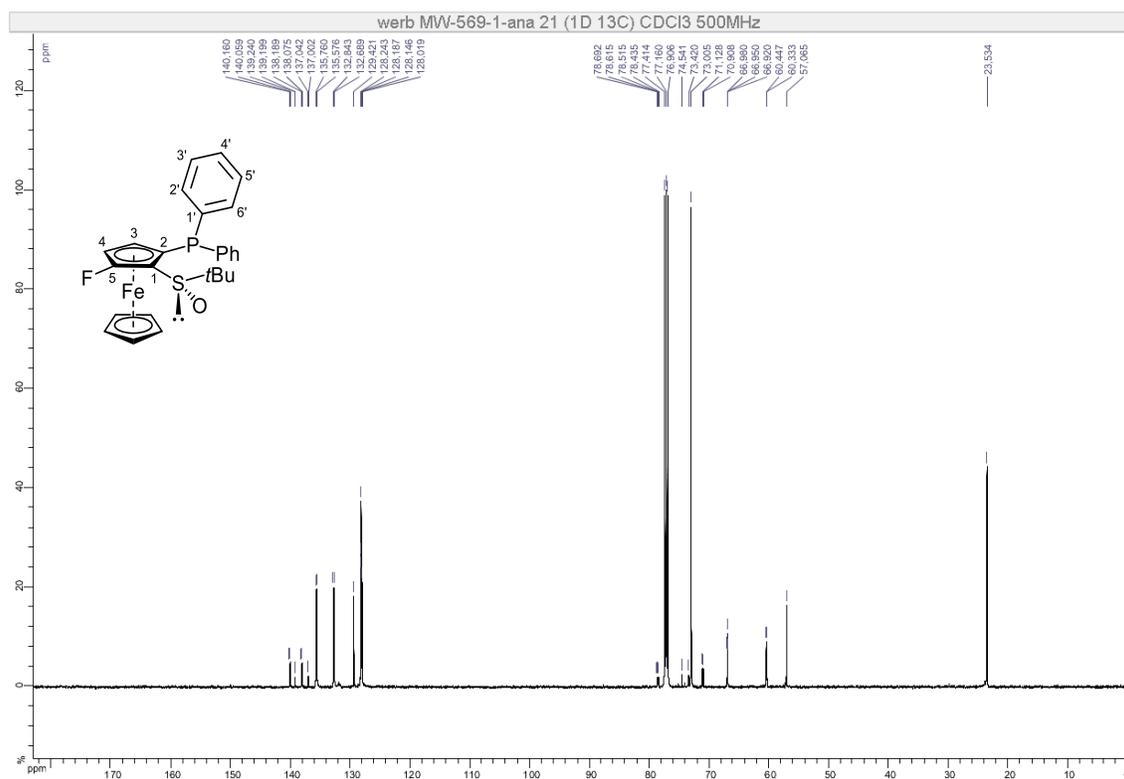


(*S,S*_P)-*S*-tert-Butyl-2-(diphenylphosphino)-5-fluoroferroenesulfoxide (*S,S*_P-2ei)

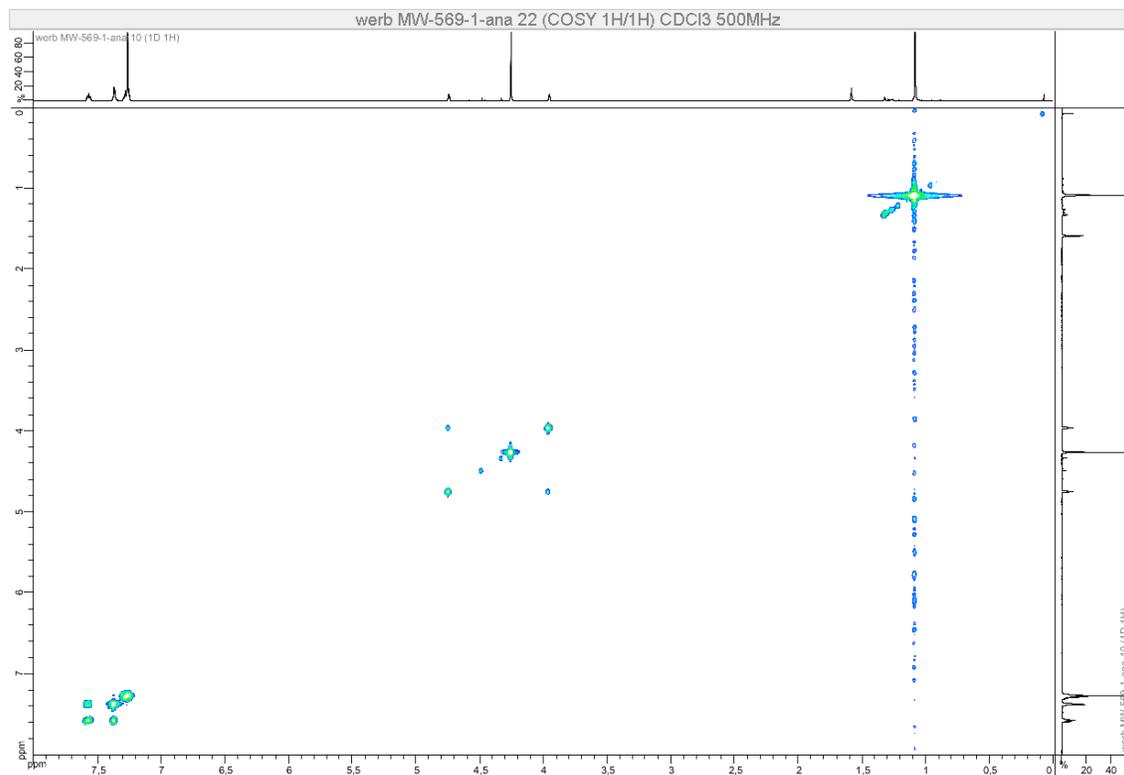
¹H NMR (500 MHz, CDCl₃)



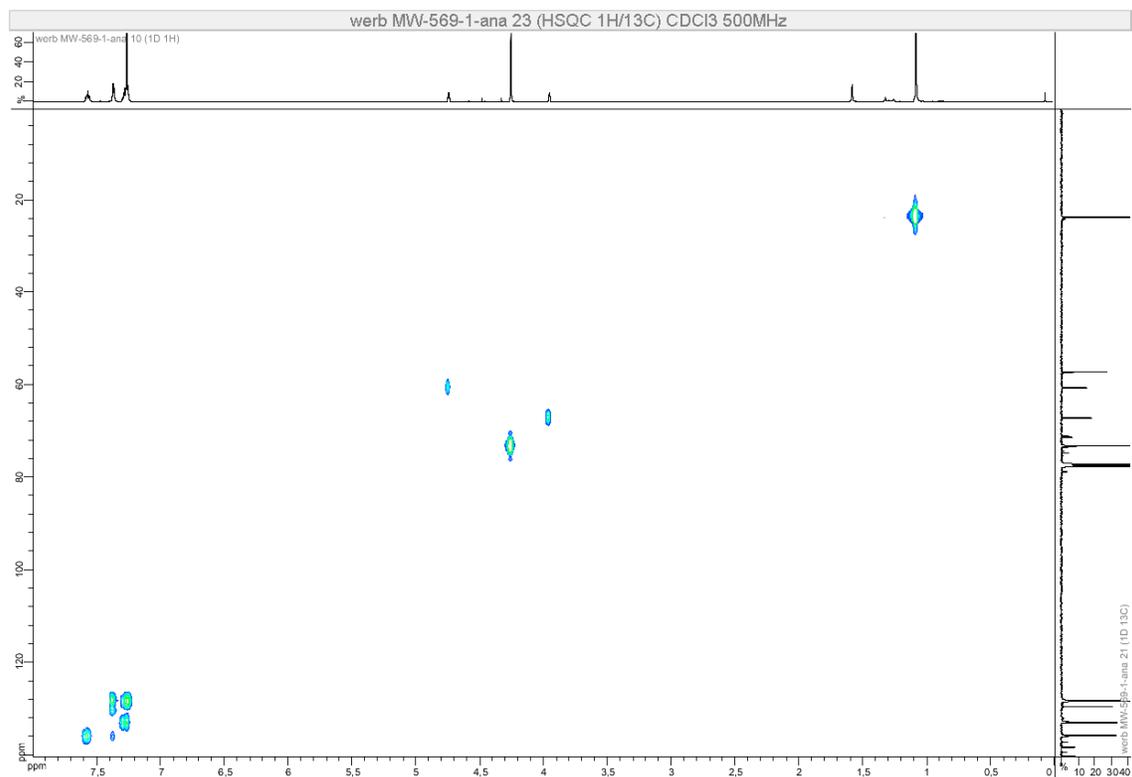
¹³C NMR (126 MHz, CDCl₃)



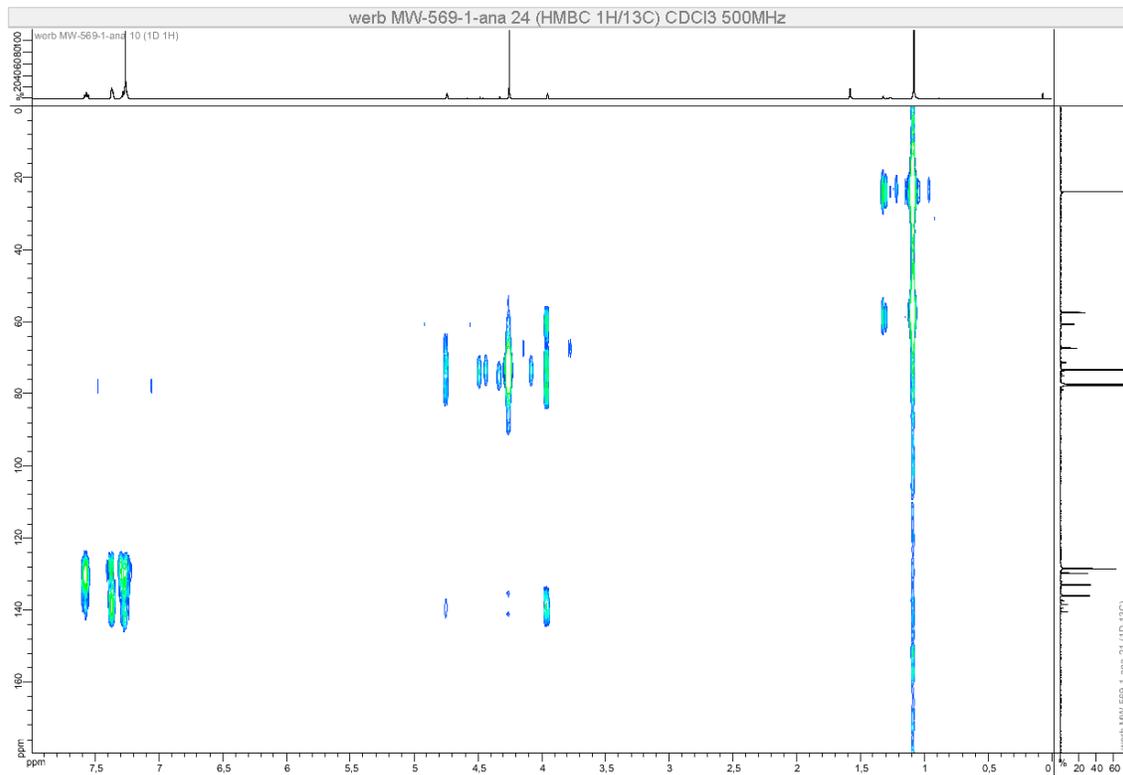
COSY (500 MHz, CDCl₃)



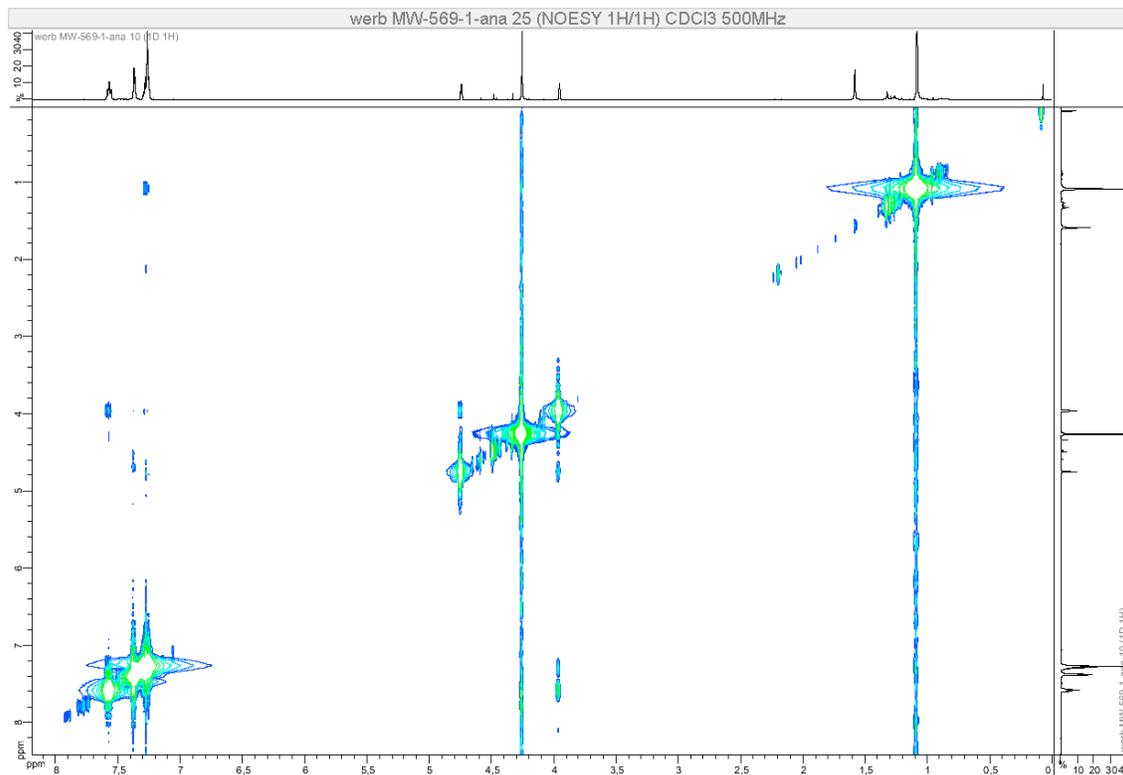
HSQC (500 MHz, CDCl₃)



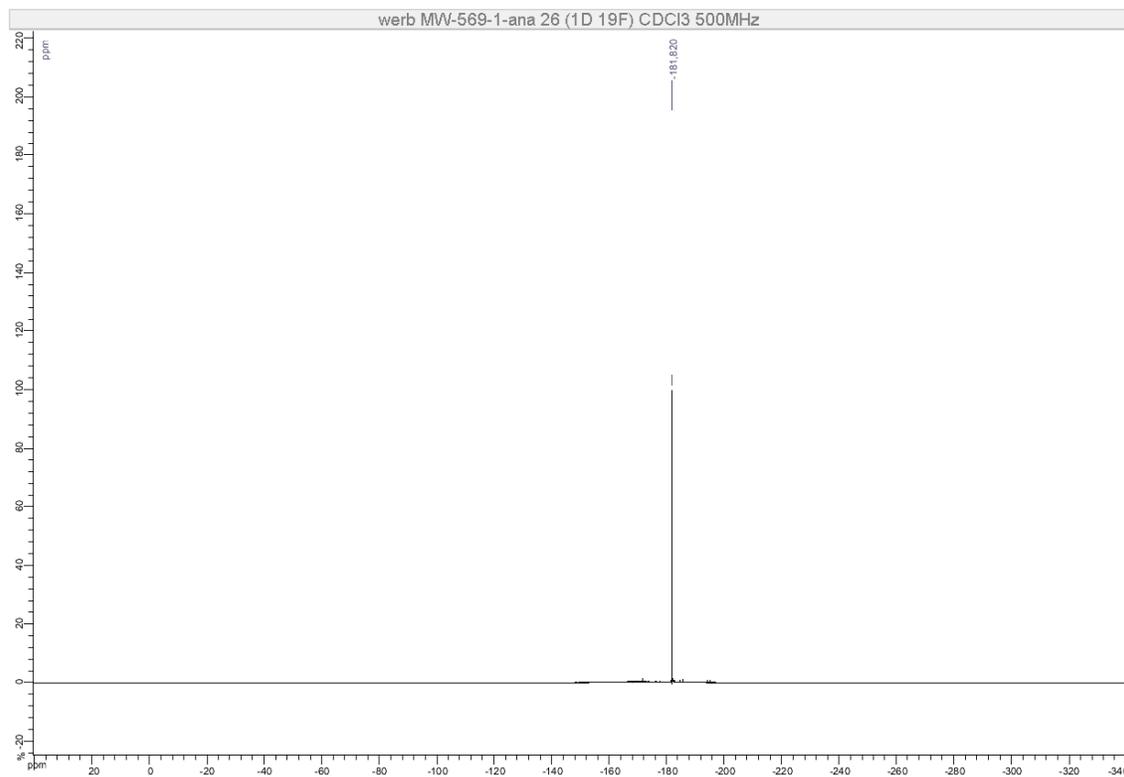
HMBC (500 MHz, CDCl₃)



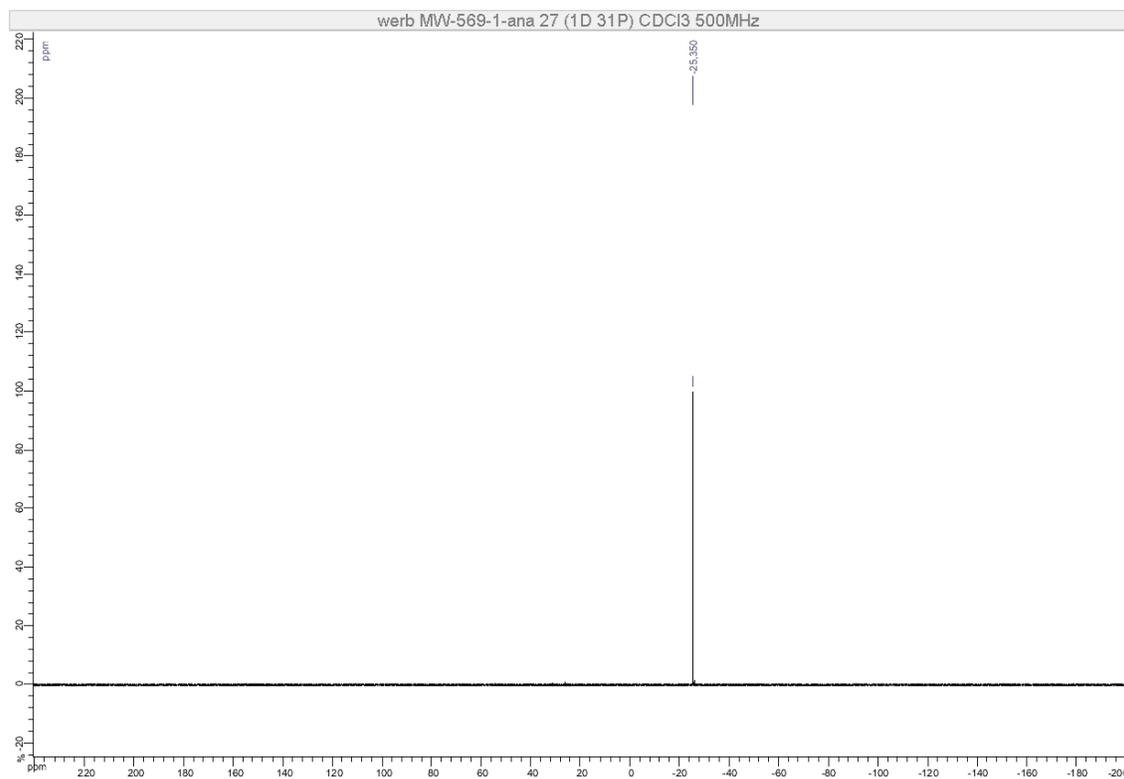
NOESY (500 MHz, CDCl₃)



^{19}F NMR (471 MHz, CDCl_3)

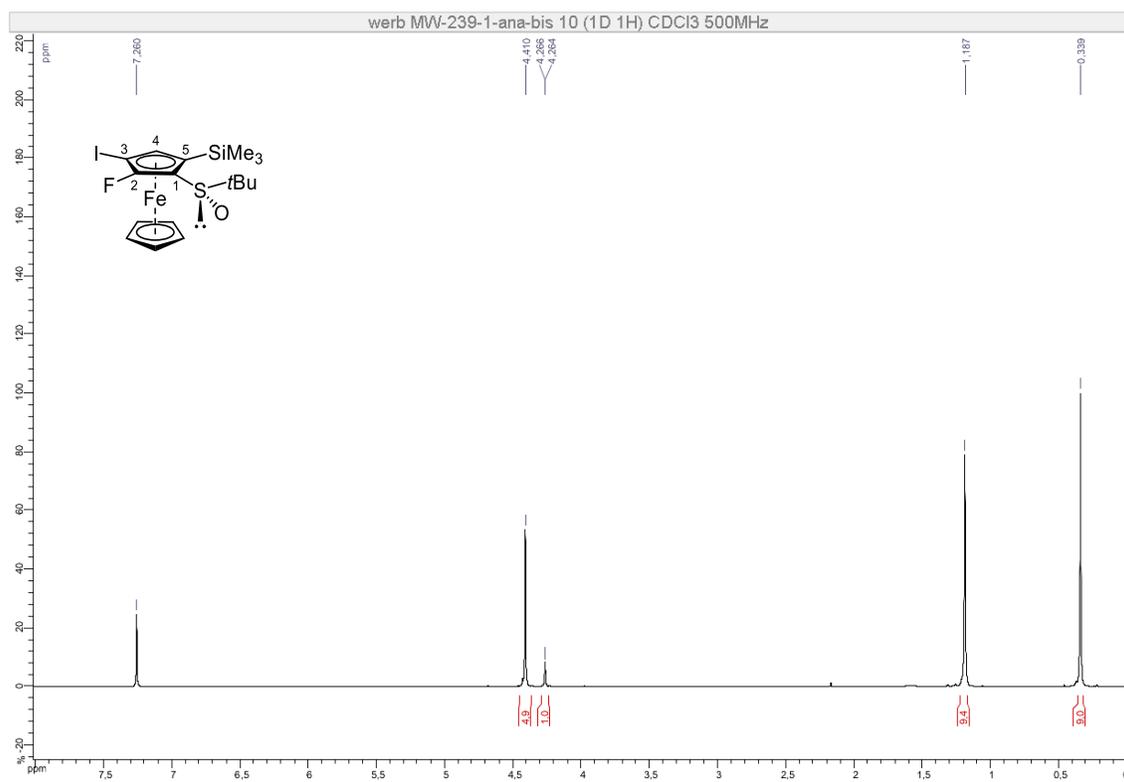


^{31}P NMR (202 MHz, CDCl_3)

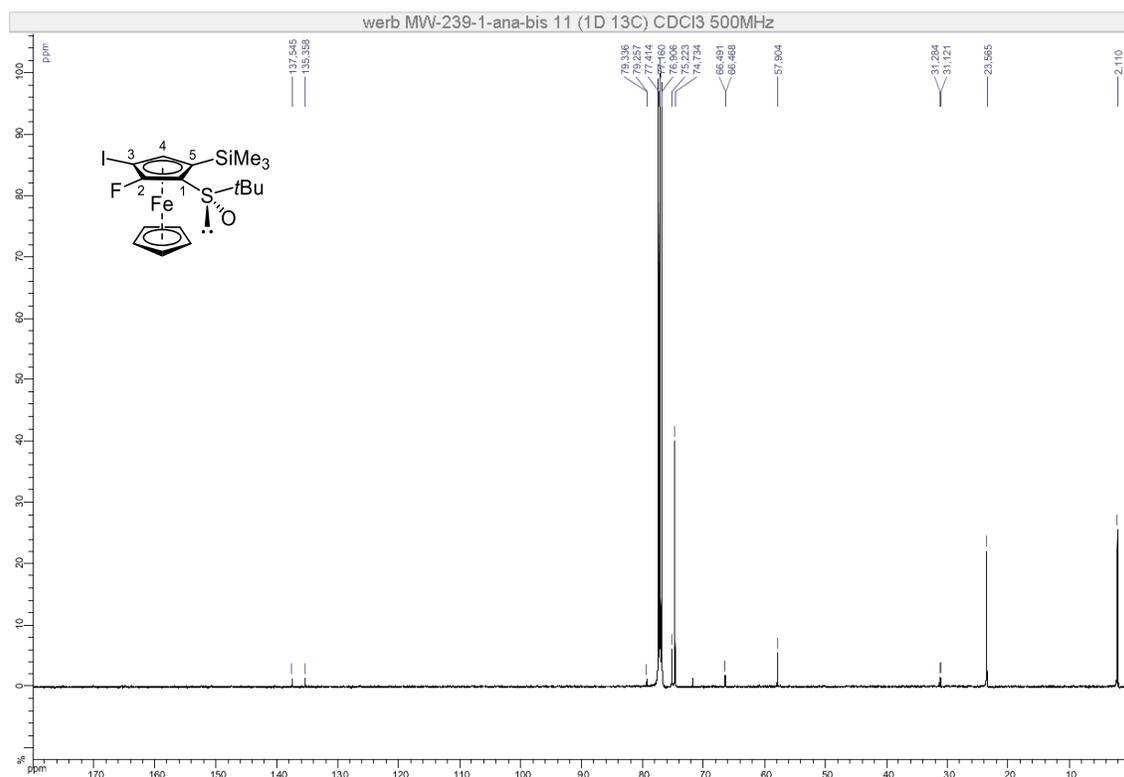


(*S,S*)-*S*-tert-Butyl-2-fluoro-3-iodo-5-(trimethylsilyl)ferrocenesulfoxide (*S,S*P-9b)

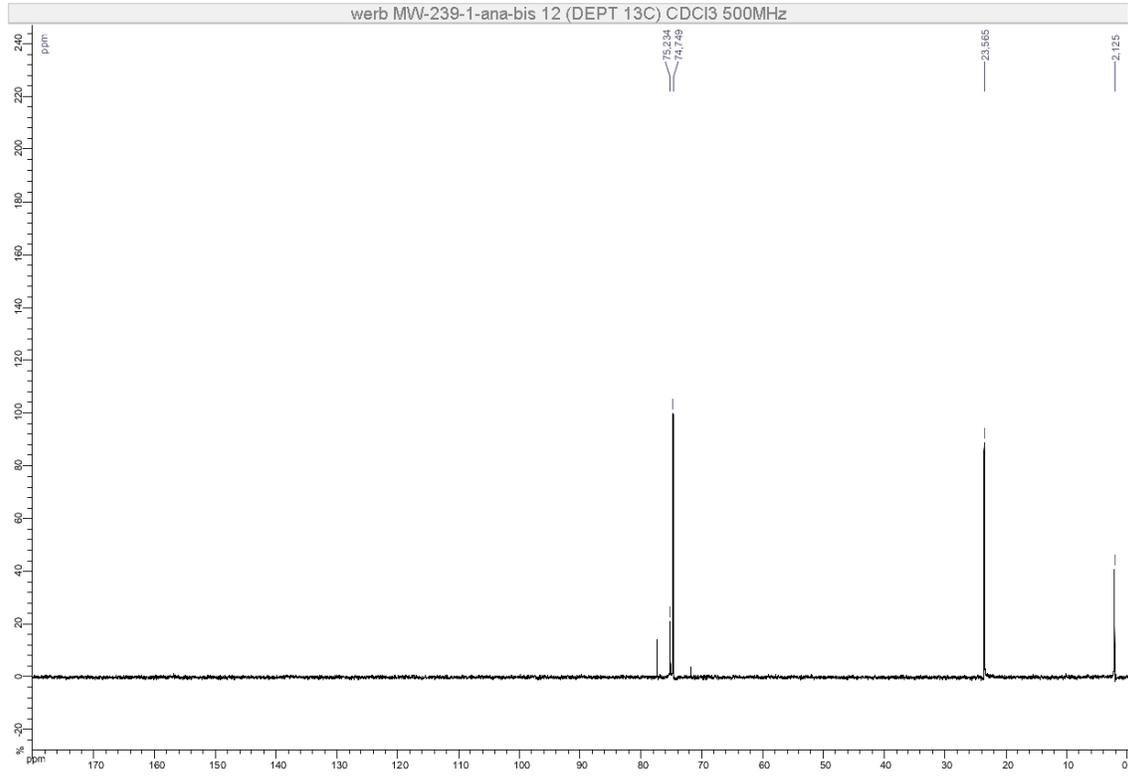
^1H NMR (500 MHz, CDCl_3)



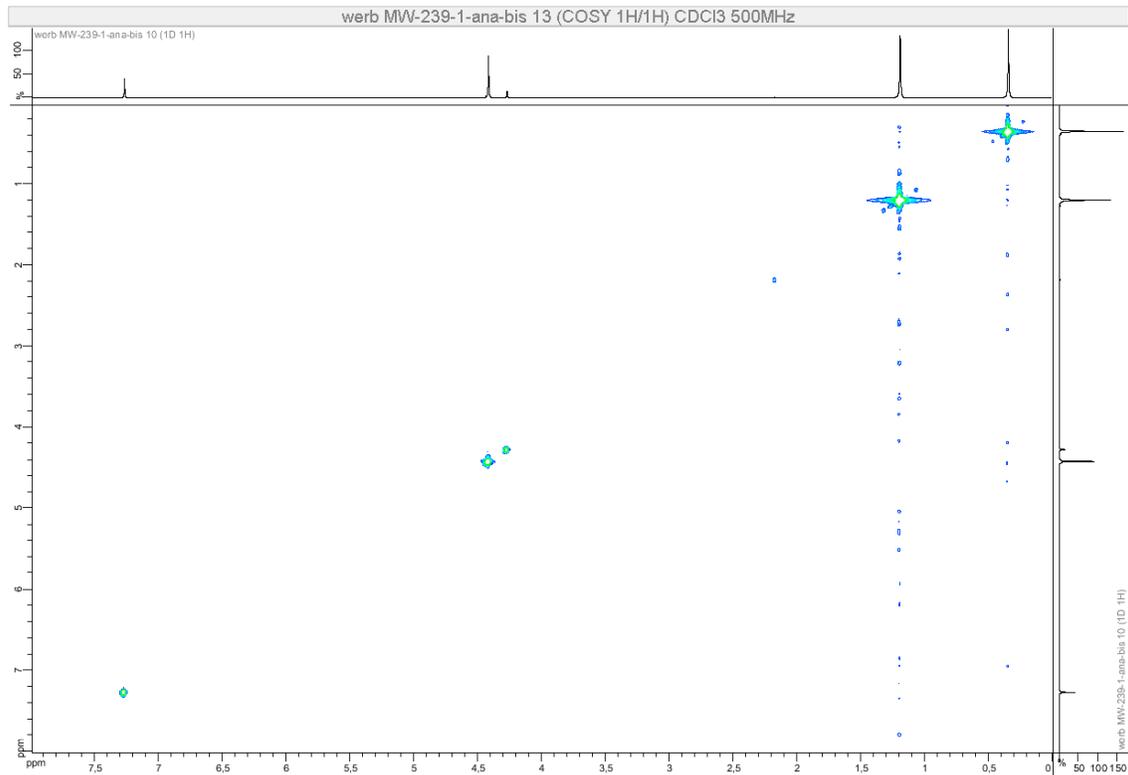
^{13}C NMR (126 MHz, CDCl_3)



DEPT 135 (126 MHz, CDCl₃)



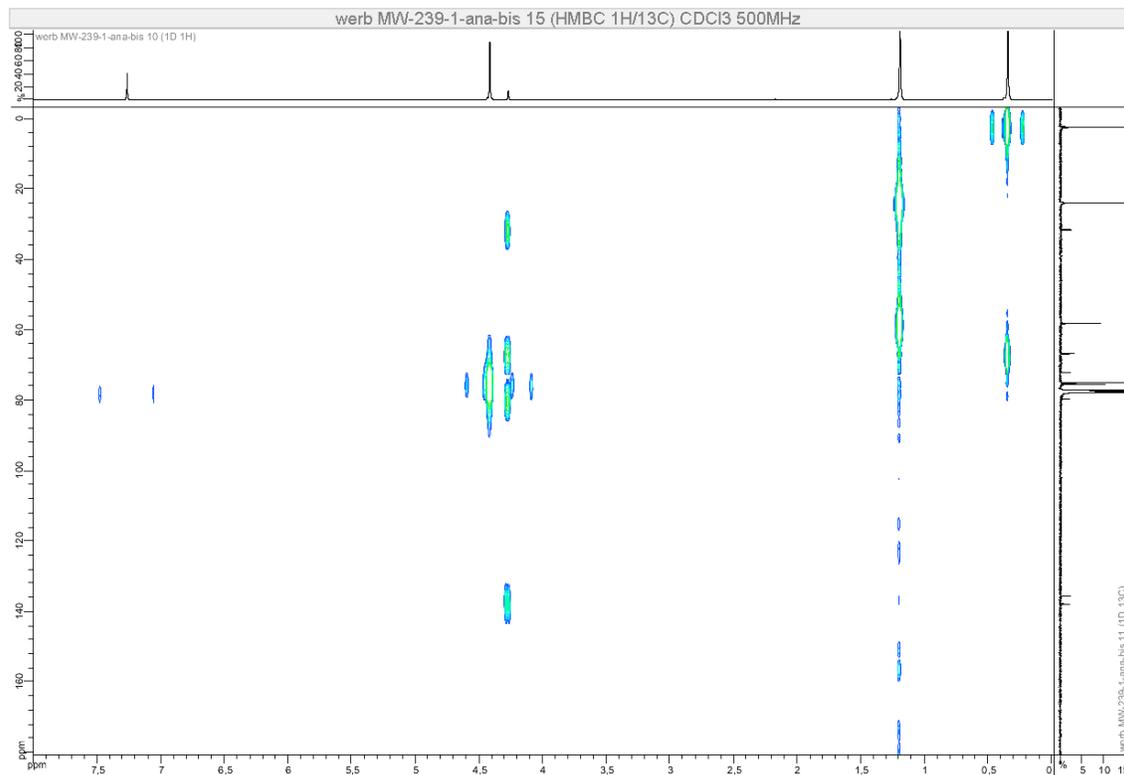
COSY (500 MHz, CDCl₃)



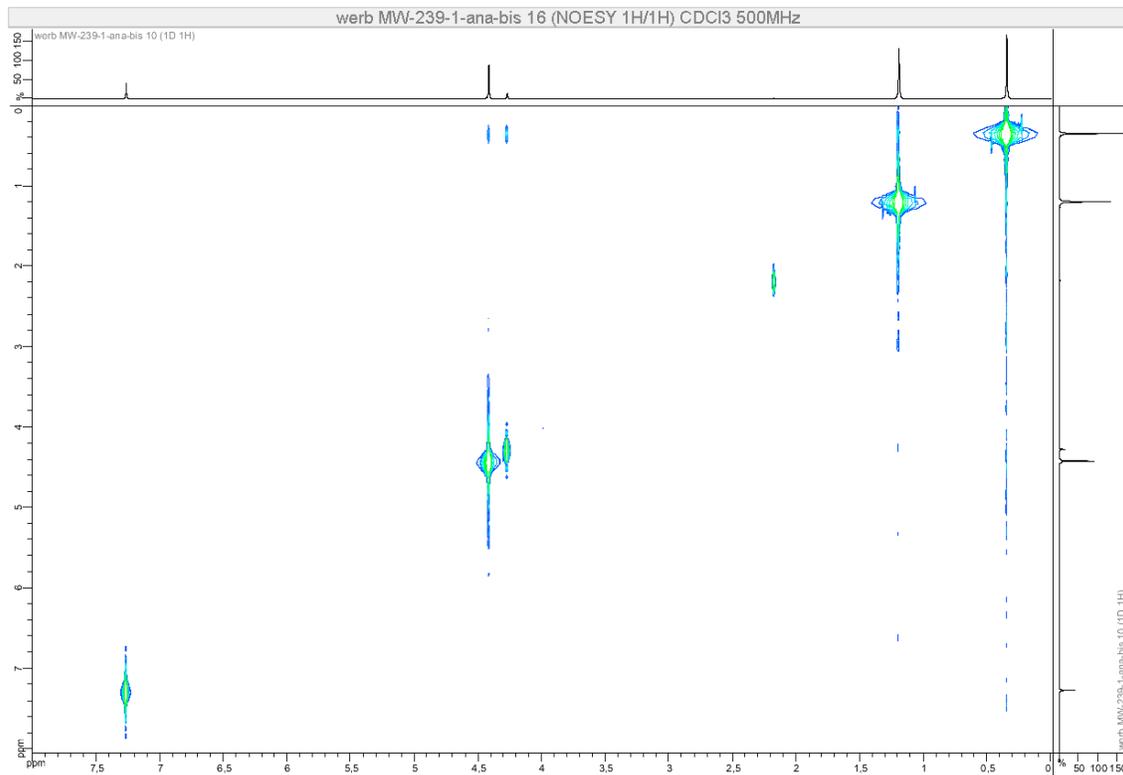
HSQC (500 MHz, CDCl₃)



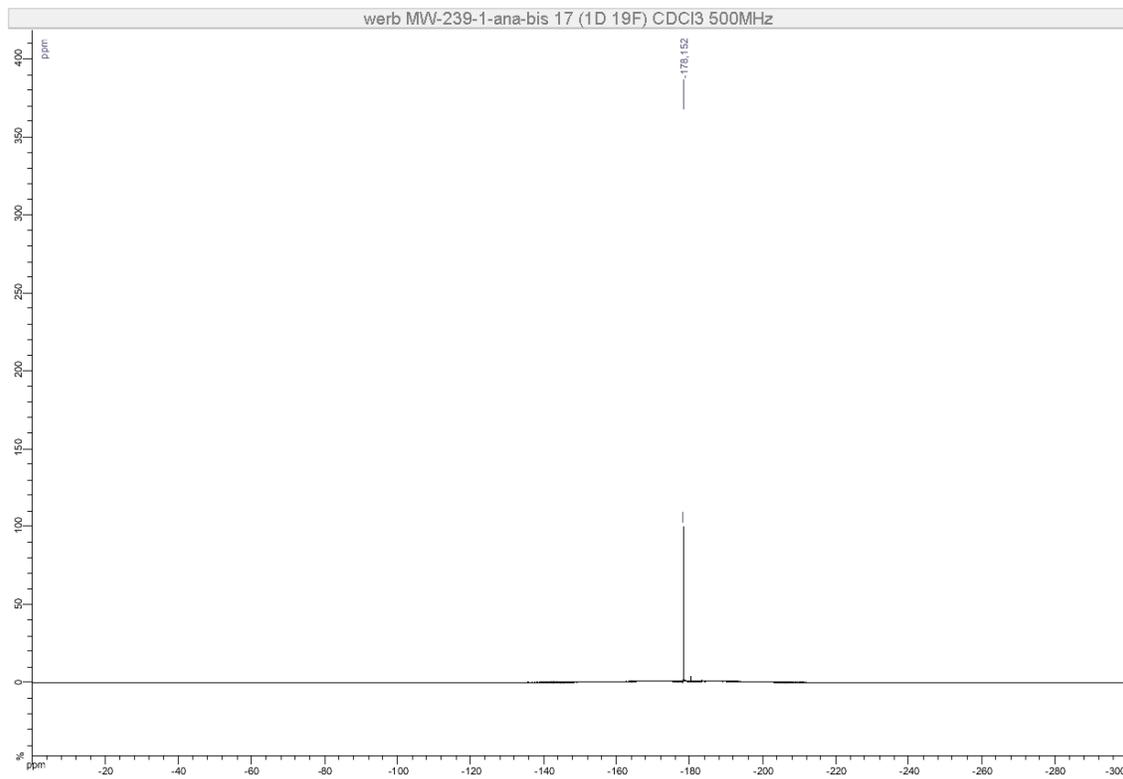
HMBC (500 MHz, CDCl₃)



NOESY (500 MHz, CDCl₃)

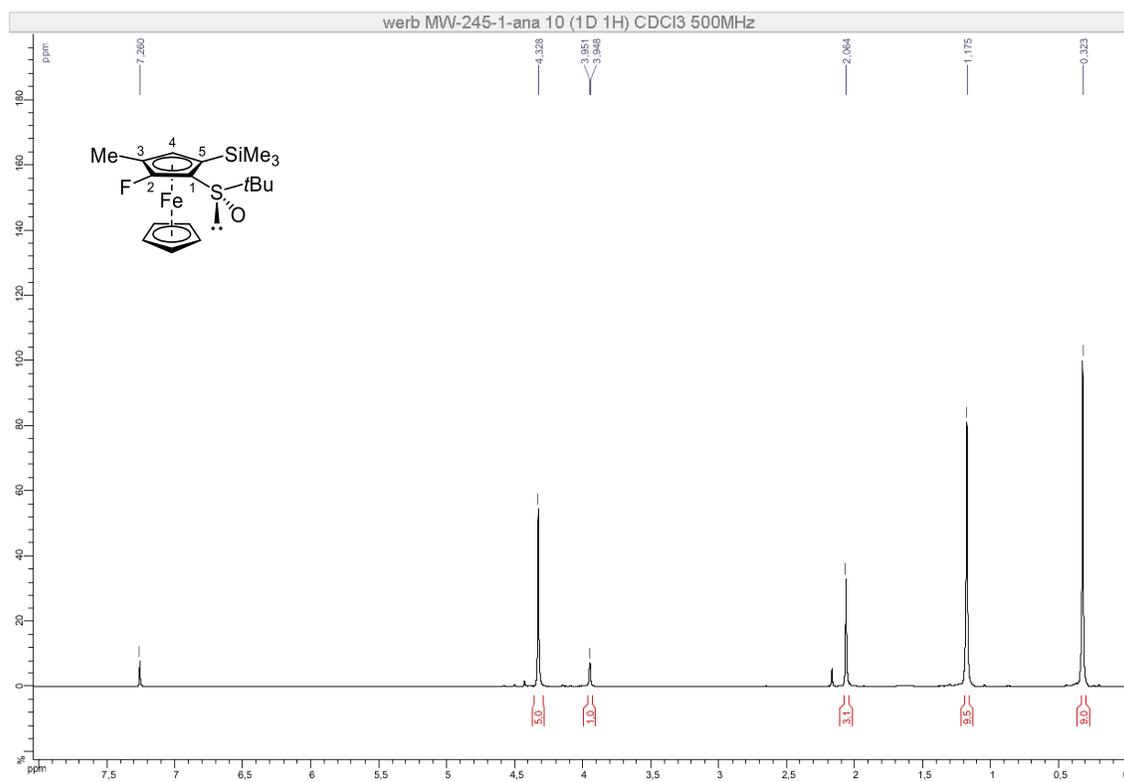


¹⁹F NMR (471 MHz, CDCl₃)

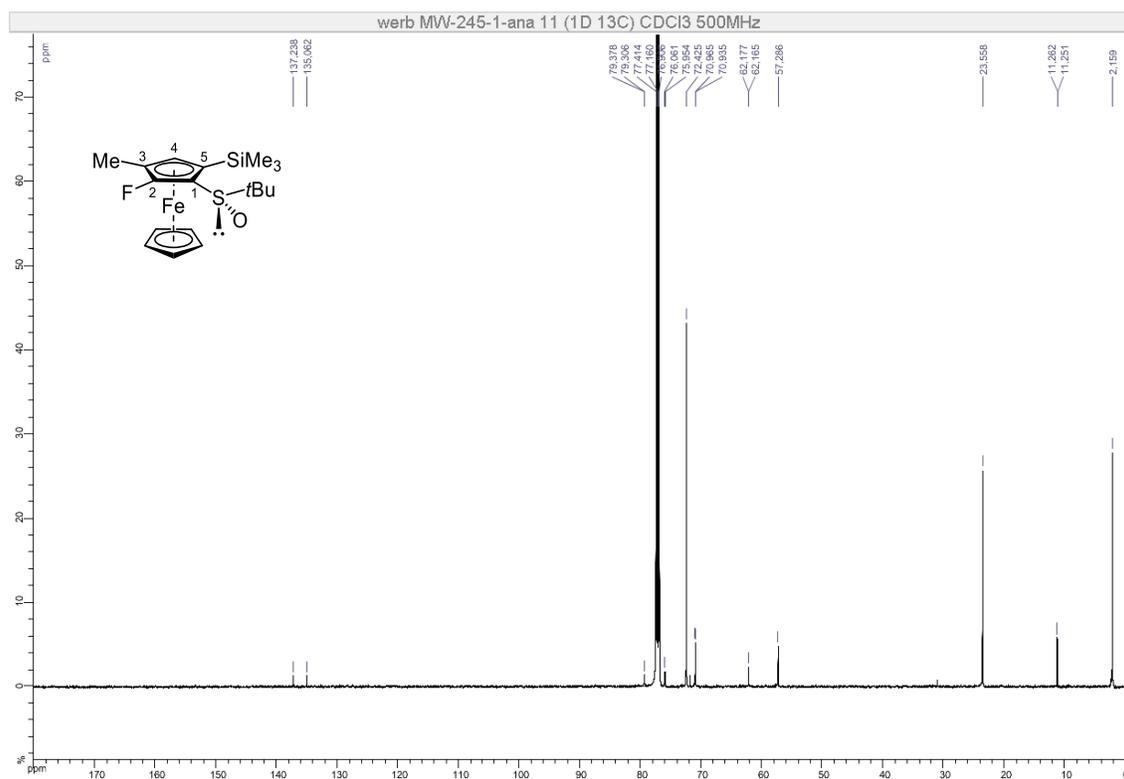


(*S,S*)-*S*-tert-Butyl-2-fluoro-3-methyl-5-(trimethylsilyl)ferrocenesulfoxide (*S,S*_P-9d)

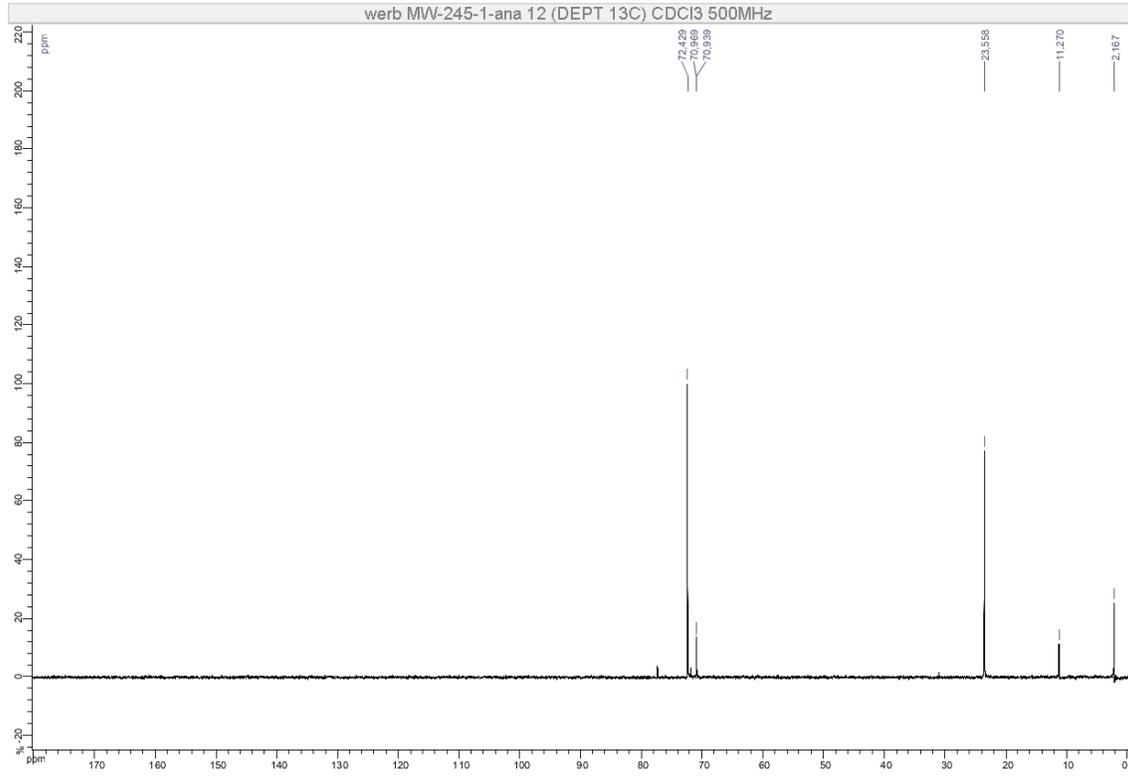
¹H NMR (500 MHz, CDCl₃)



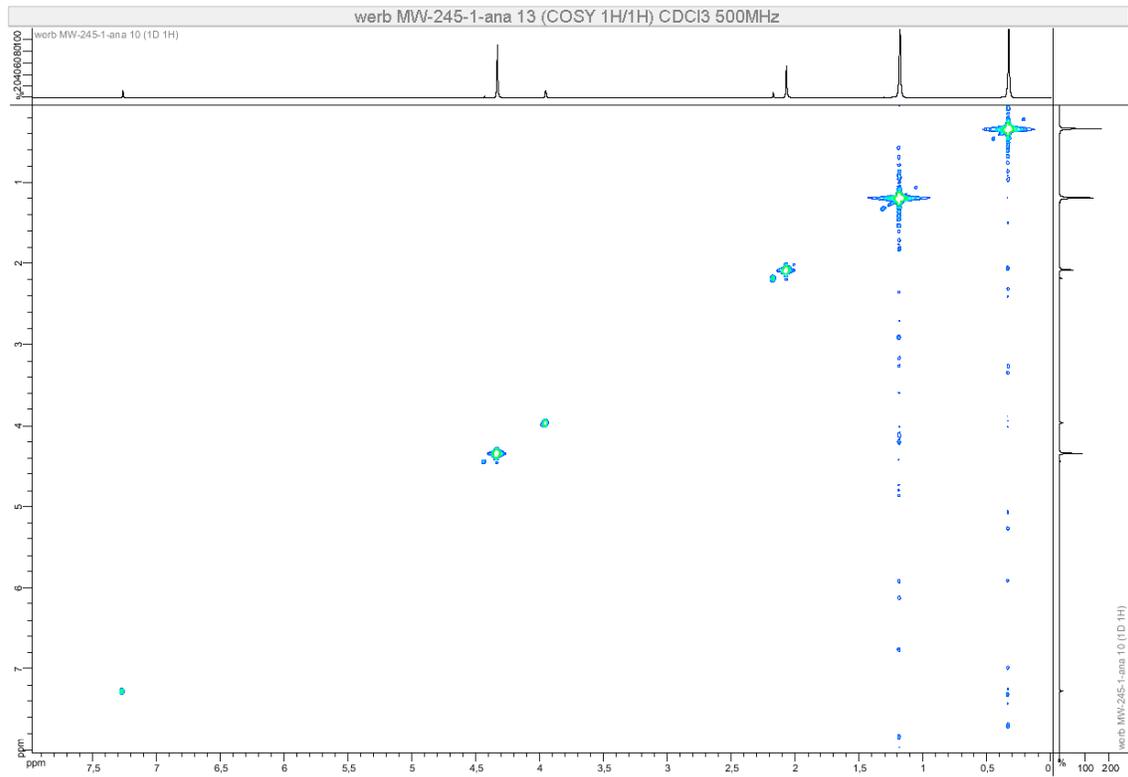
¹³C NMR (126 MHz, CDCl₃)



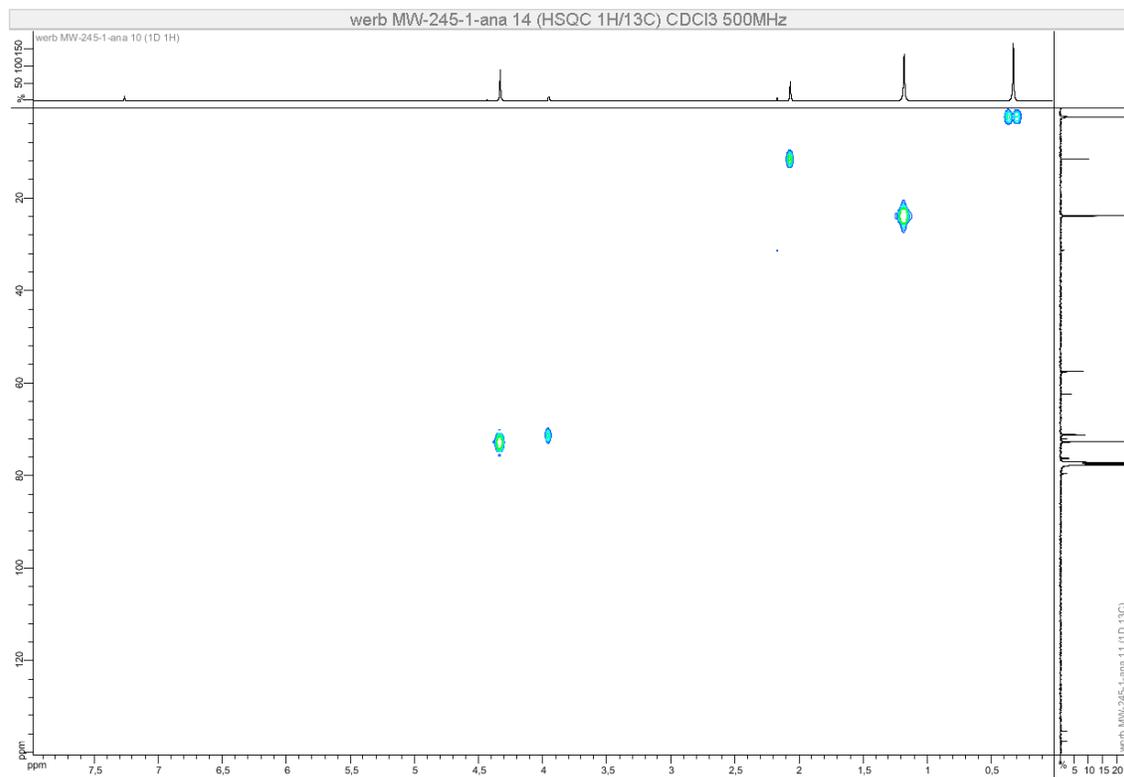
DEPT 135 (126 MHz, CDCl₃)



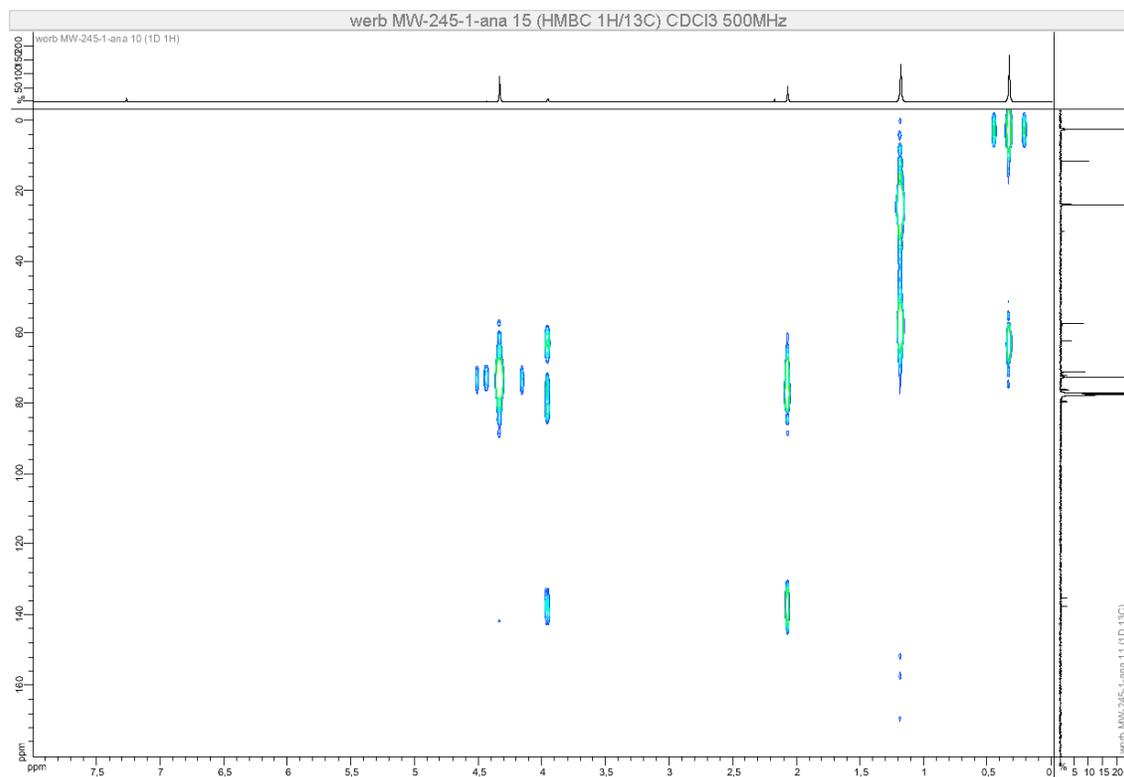
COSY (500 MHz, CDCl₃)



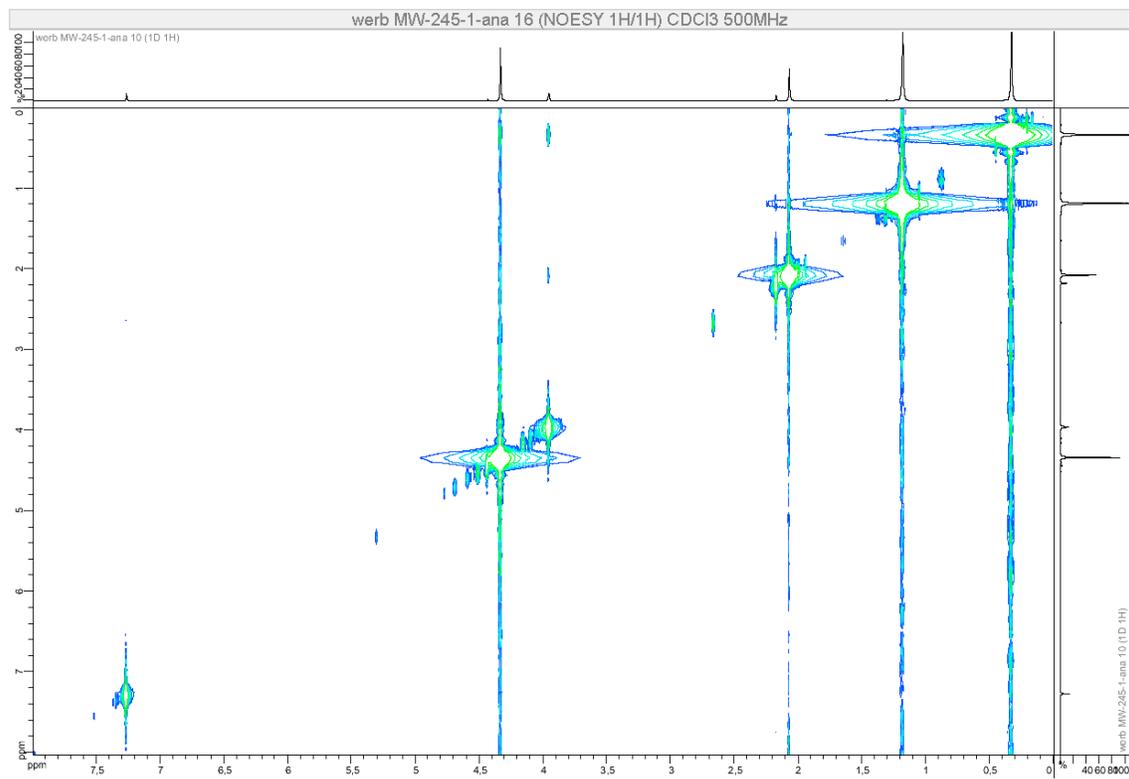
HSQC (500 MHz, CDCl₃)



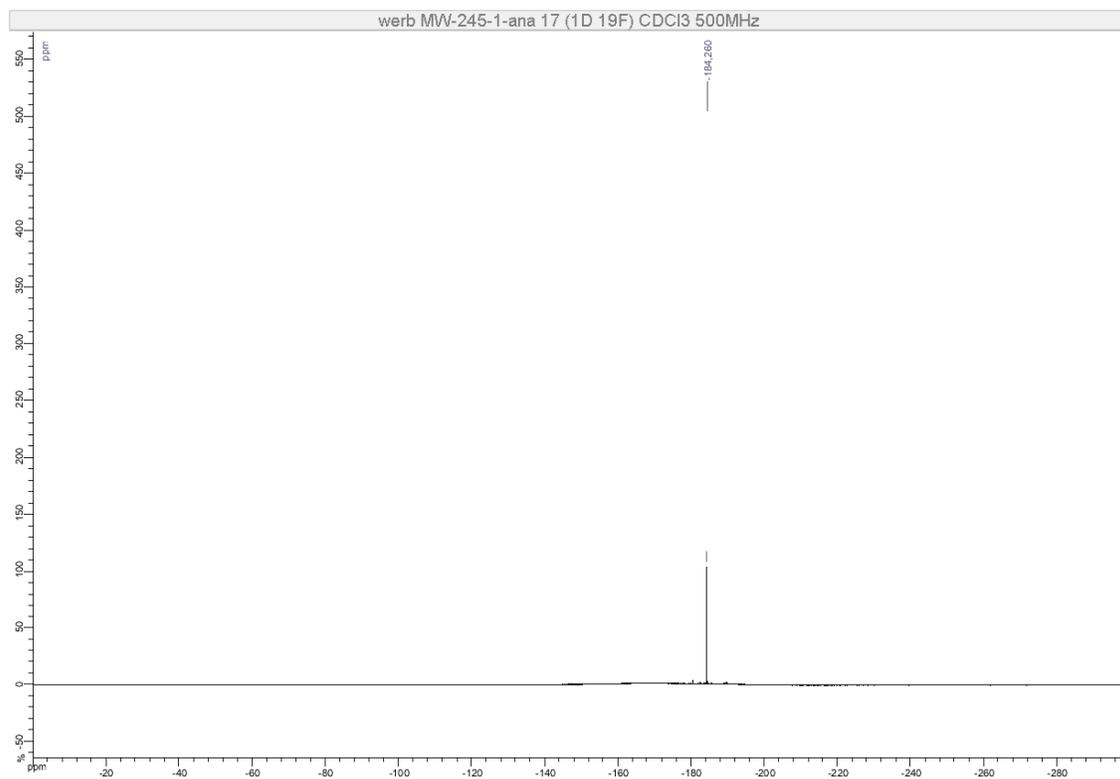
HMBC (500 MHz, CDCl₃)



NOESY (500 MHz, CDCl₃)

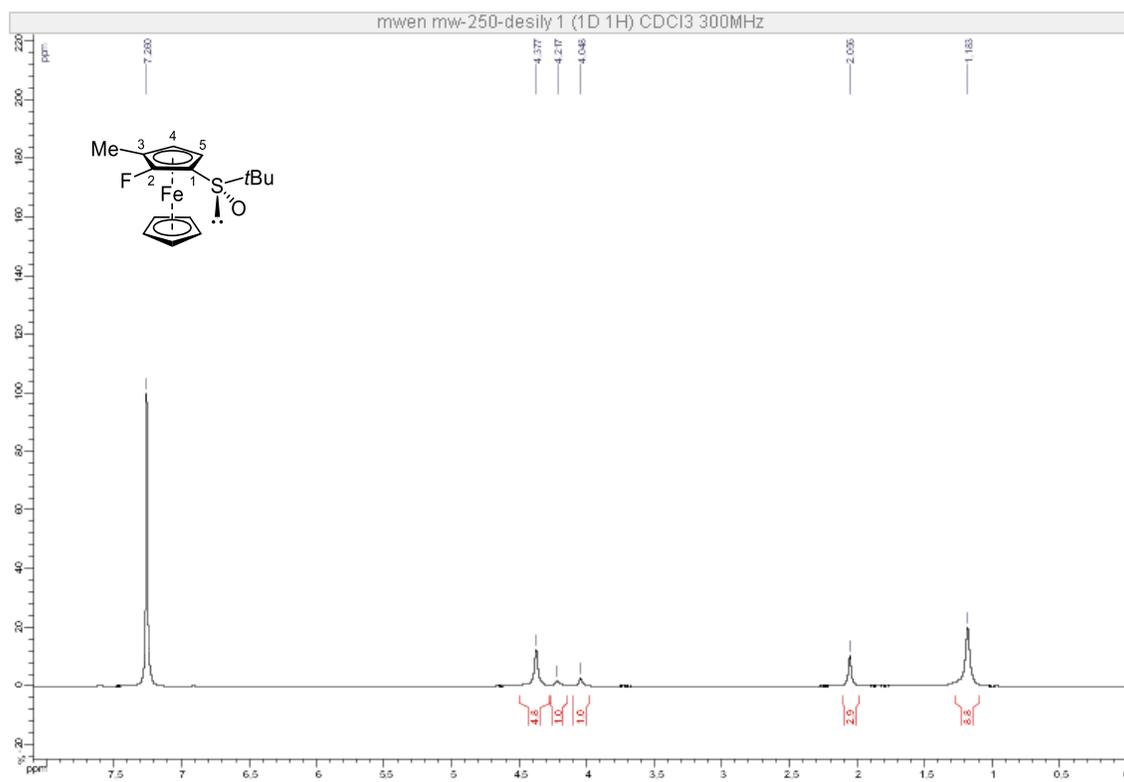


¹⁹F NMR (471 MHz, CDCl₃)



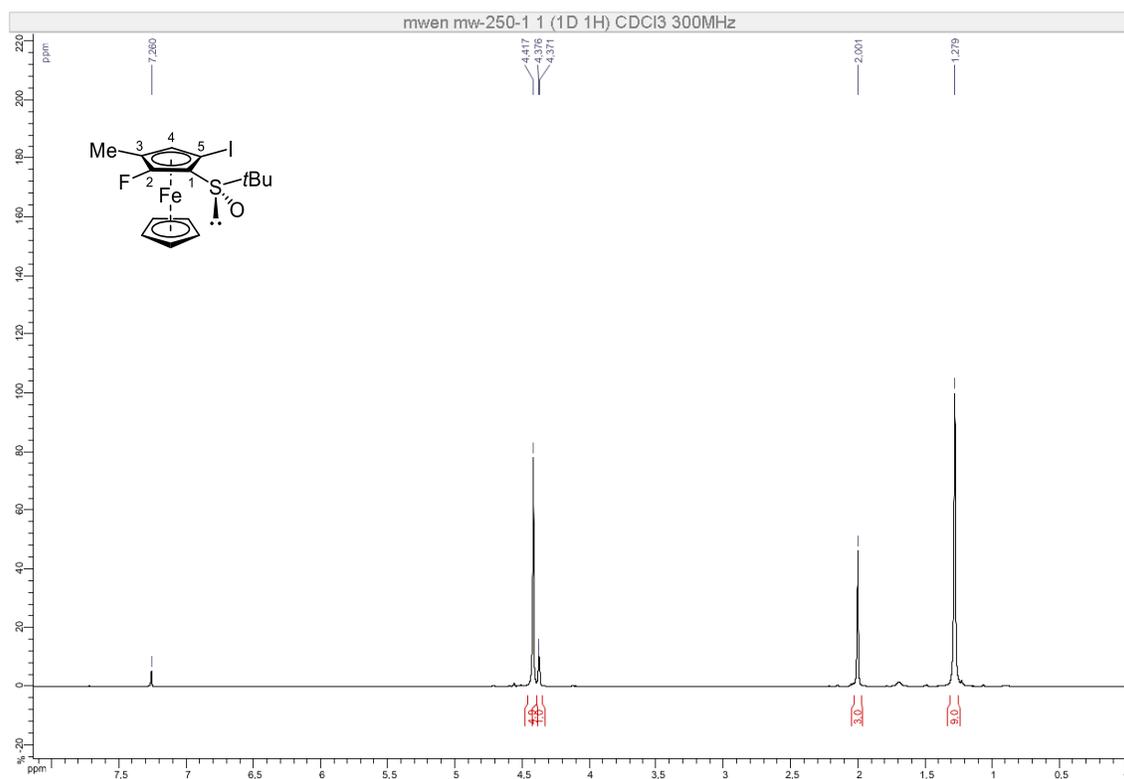
(*S,R*_P)-*S*-*tert*-Butyl-2-fluoro-3-methylferrocenesulfoxide (*S,R*_P-10)

¹H NMR (300 MHz, CDCl₃)



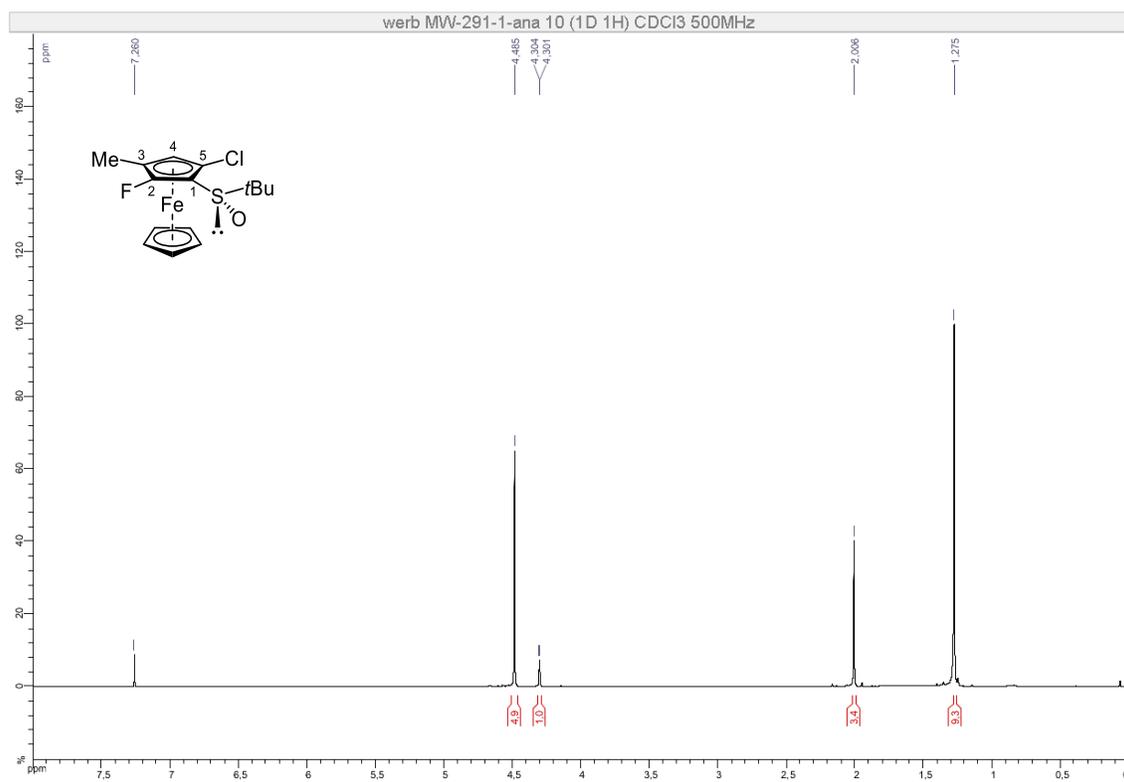
(*S,R*_P)-*S*-*tert*-Butyl-2-fluoro-5-iodo-3-methylferrocenesulfoxide (*S,R*_P-11b)

¹H NMR (300 MHz, CDCl₃)

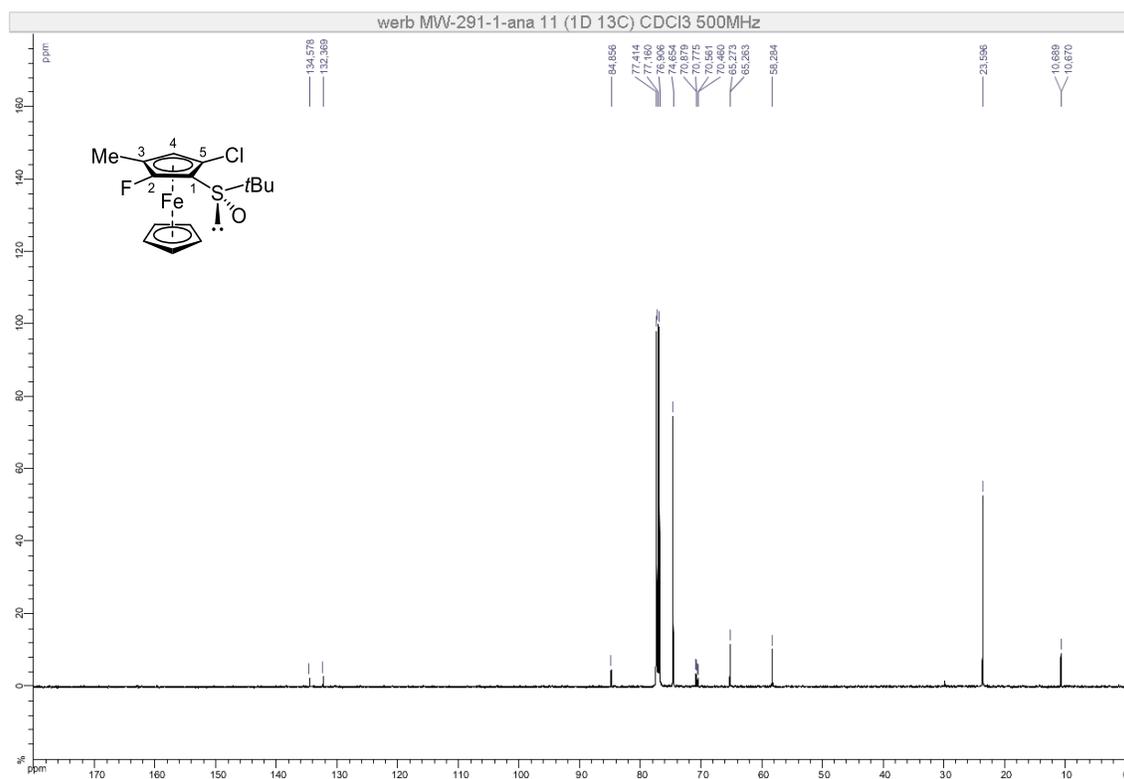


(*S,R*_P)-*S*-tert-Butyl-5-chloro-2-fluoro-3-methylferrocenesulfoxide (*S,R*_P-11k)

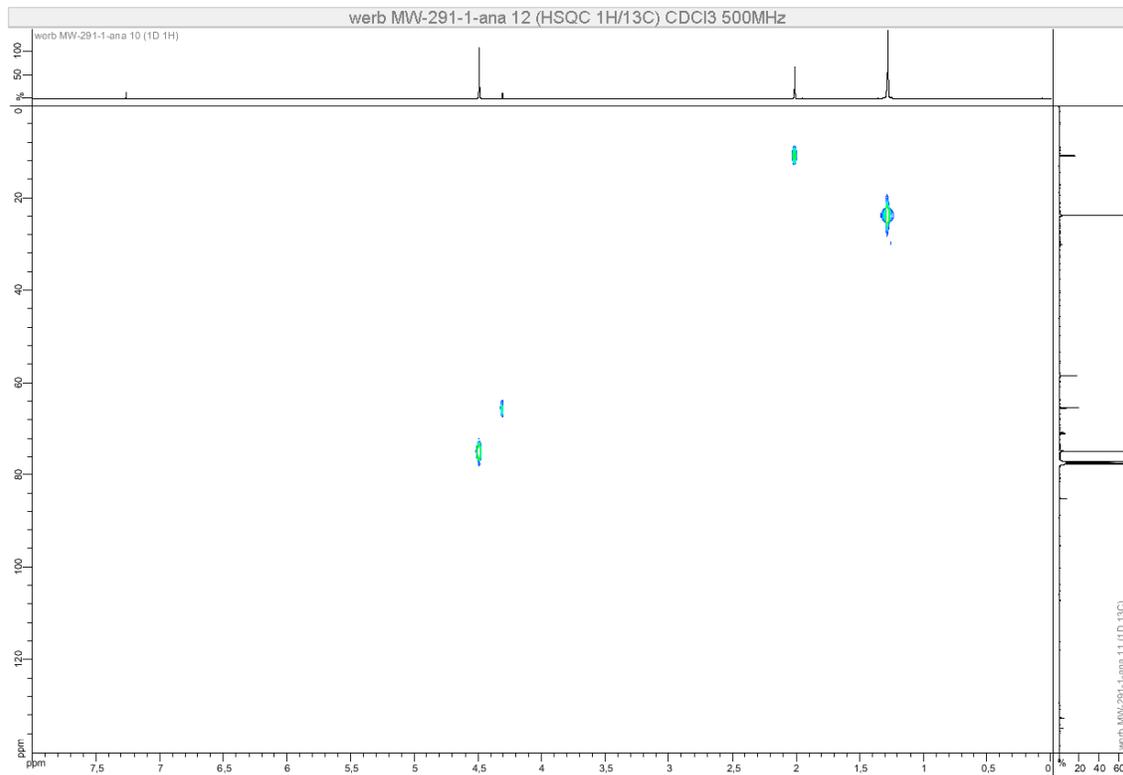
¹H NMR (500 MHz, CDCl₃)



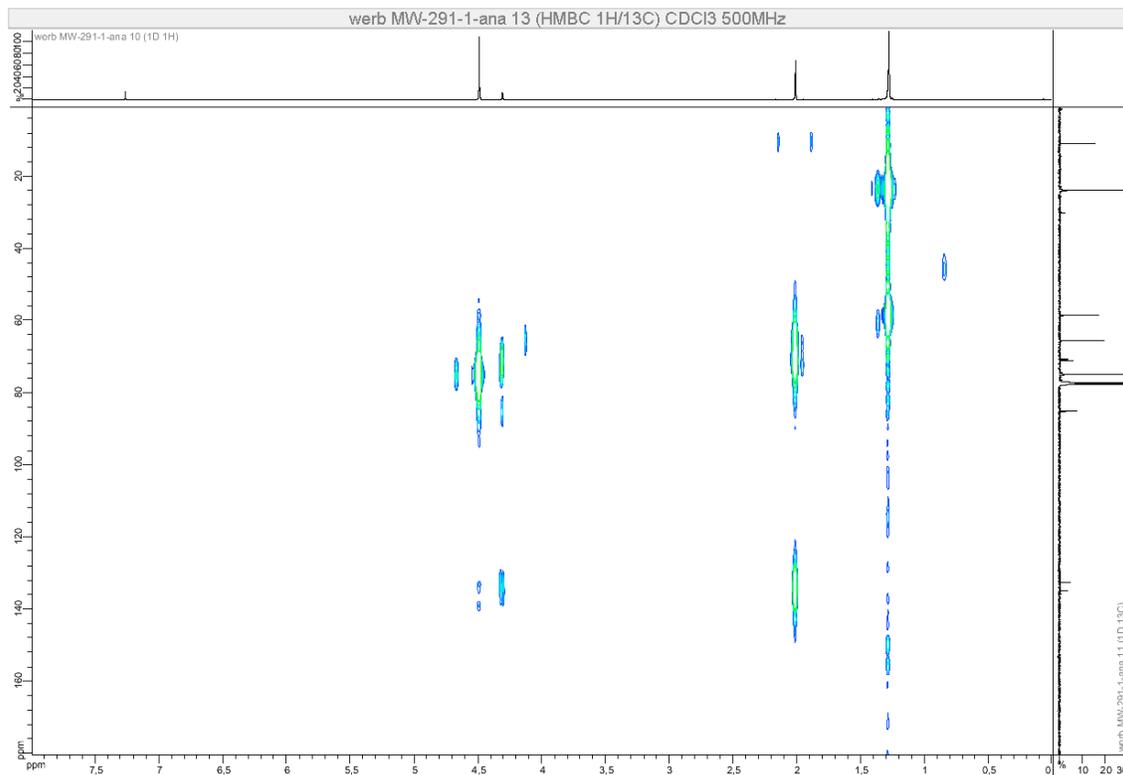
¹³C NMR (126 MHz, CDCl₃)



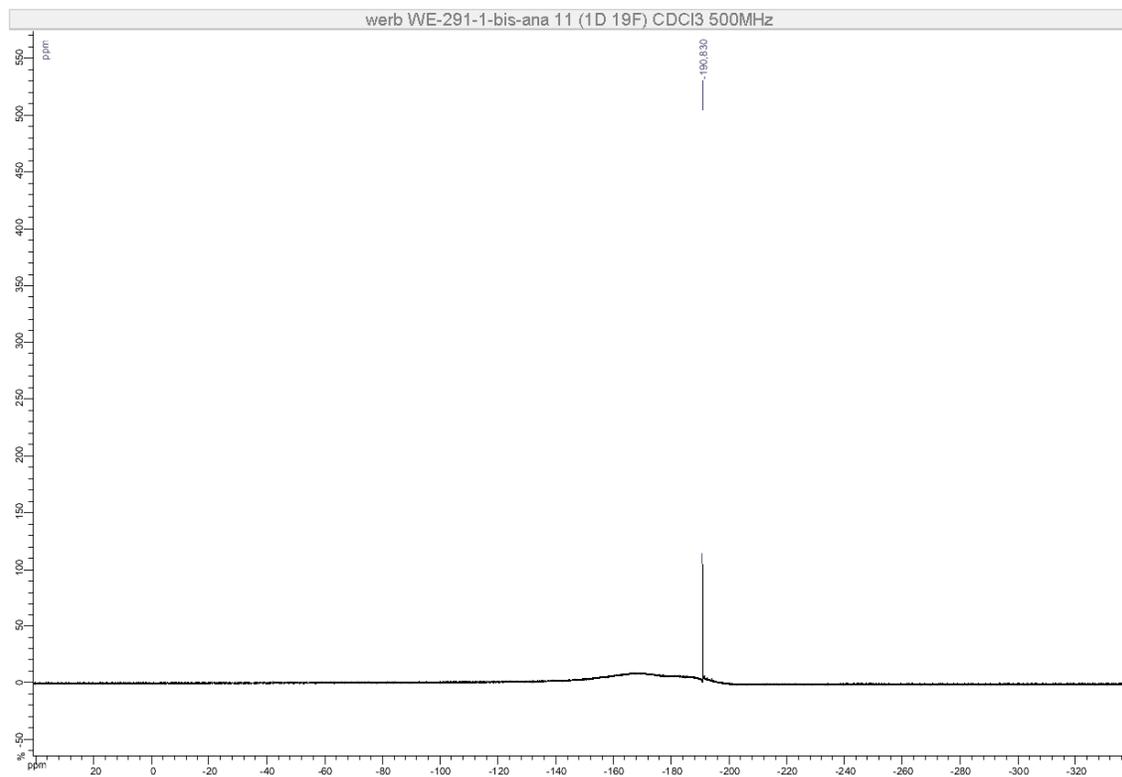
HSQC (500 MHz, CDCl₃)



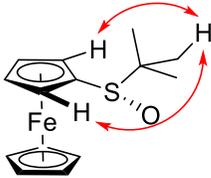
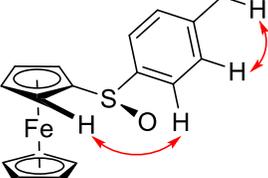
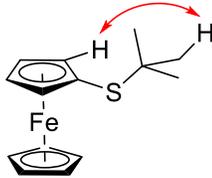
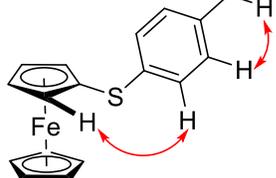
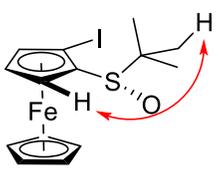
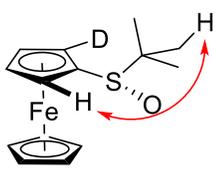
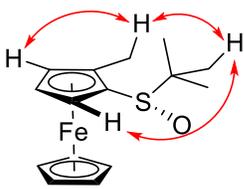
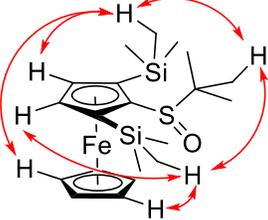
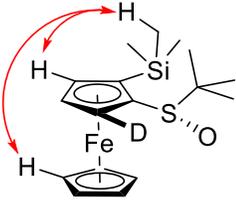
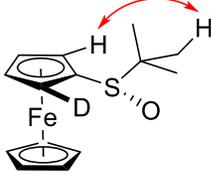
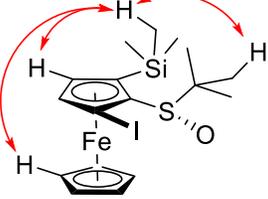
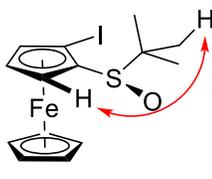
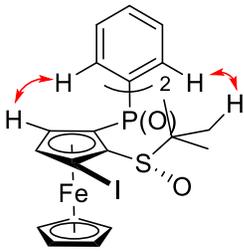
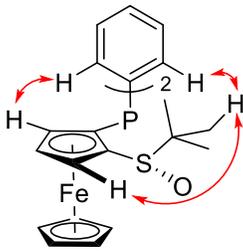
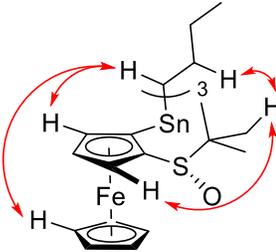
HMBC (500 MHz, CDCl₃)



^{19}F NMR (471 MHz, CDCl_3)



Selected NOESY correlations

		
<p>S-FcSOtBu</p>	<p>R-FcSO-p-tol</p>	<p>(tert-Butylthio)ferrocene</p>
		
<p>(4-Tolylthio)ferrocene</p>	<p>S,R_p-1b</p>	<p>S,S_p-1c</p>
		
<p>S,S_p-1d</p>	<p>rac-2aa</p>	<p>S,S_p-2ac</p>
		
<p>S,R_p-1c</p>	<p>R,R_p-2ab</p>	<p>R,R_p-1b</p>
		
<p>S,S_p-2eb</p>	<p>S,S_p-1e</p>	<p>S,R_p-1f</p>

S,S_p-2ag	S,S_p-2ea	S,S_p-7
S,S_p-12	R,R_p/S,S_p-3a	R,R_p/S,S_p-3a' (*)
R,S_p/S,R_p-3b	S,S_p-3c	R,R_p/S,S_p-4
rac-5	R,S_p/S,R_p-6	S,R_p-1d
S,R_p-2ae	S,S_p-2ah	S,R_p-1h

(*) Not resolved enough for attribution.

<p>S,S_p-2ai</p>	<p>S,R_p-1i</p>	<p>R_p-8i</p>
<p>S,R_p-1a</p>	<p>S,S_p-9b</p>	<p>S,S_p-9d</p>

Calculated values of the Gibbs energies ΔG_{acid} [kcal·mol⁻¹] for deprotonation

