

Supplementary Materials

Synthesis of polysubstituted ferrocenesulfoxides

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

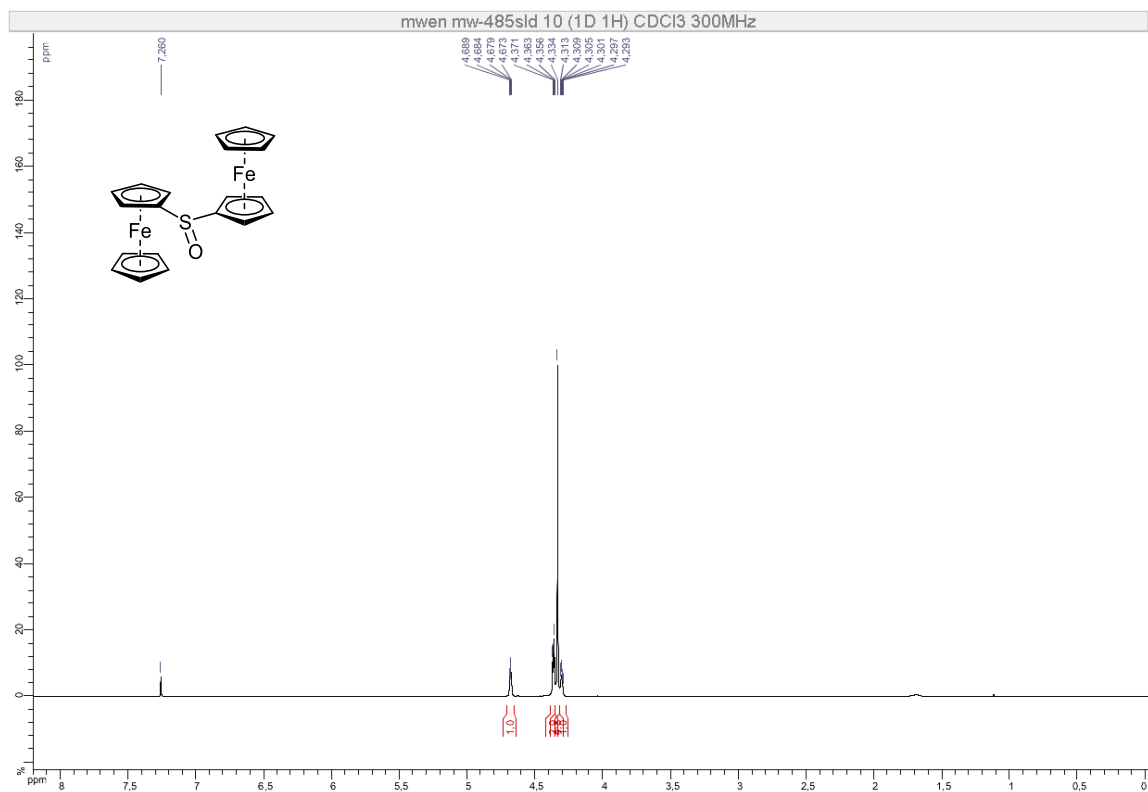
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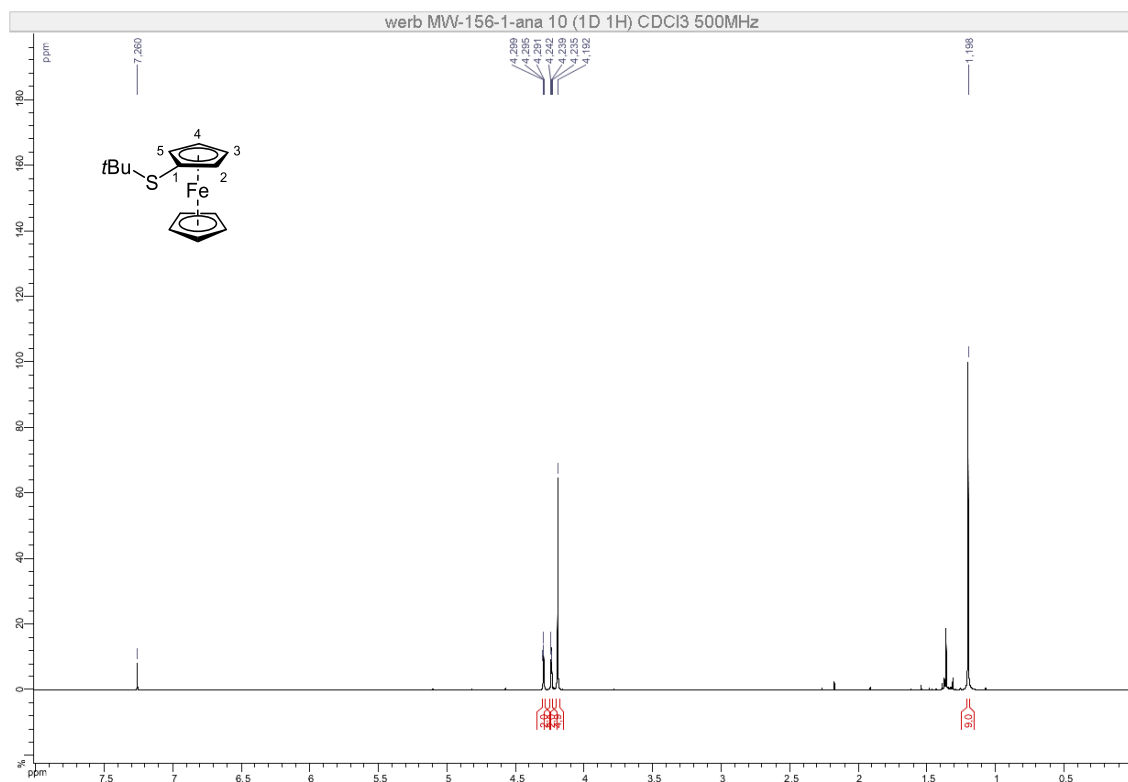
NMR Spectra

Diferrocenesulfoxide (FcSOFc)

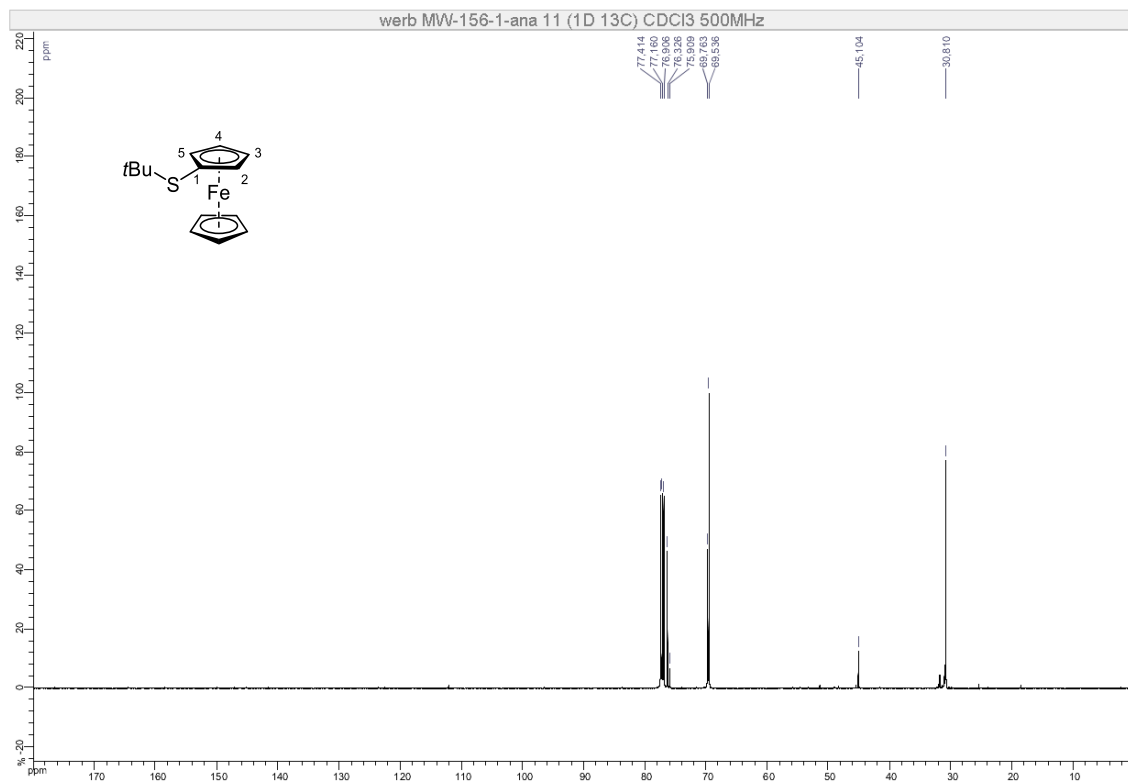


(*tert*-Butylthio)ferrocene

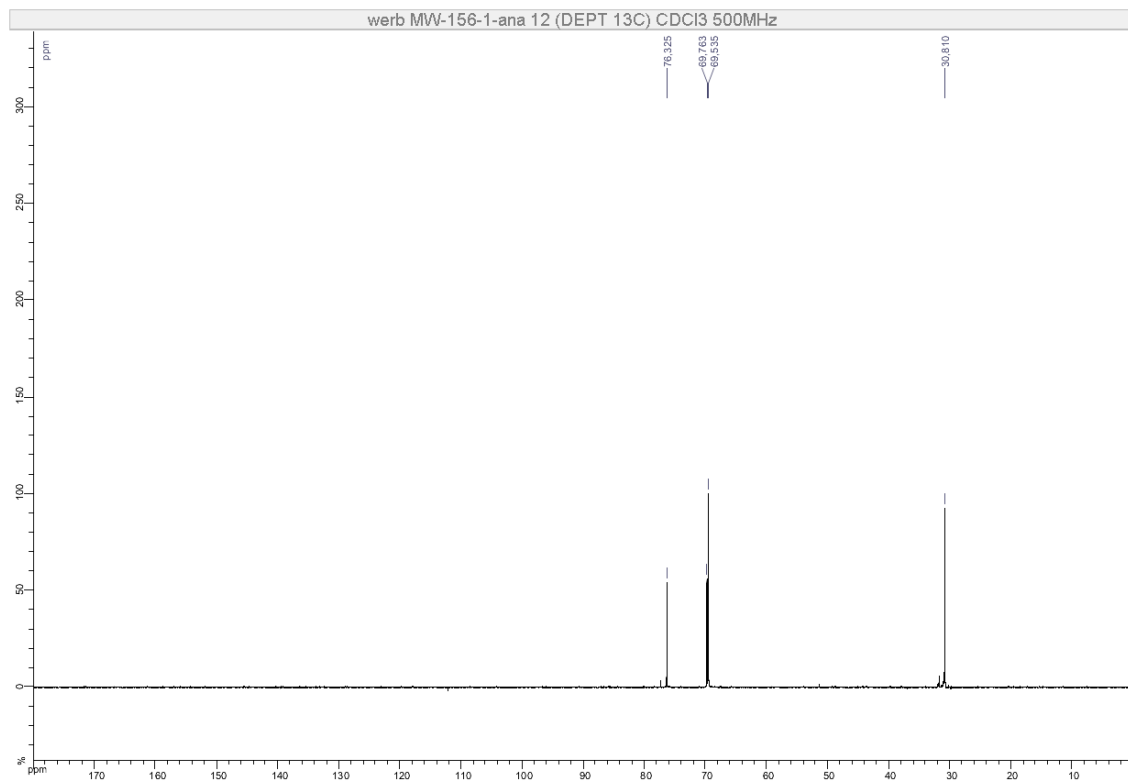
^1H NMR (500 MHz, CDCl_3)



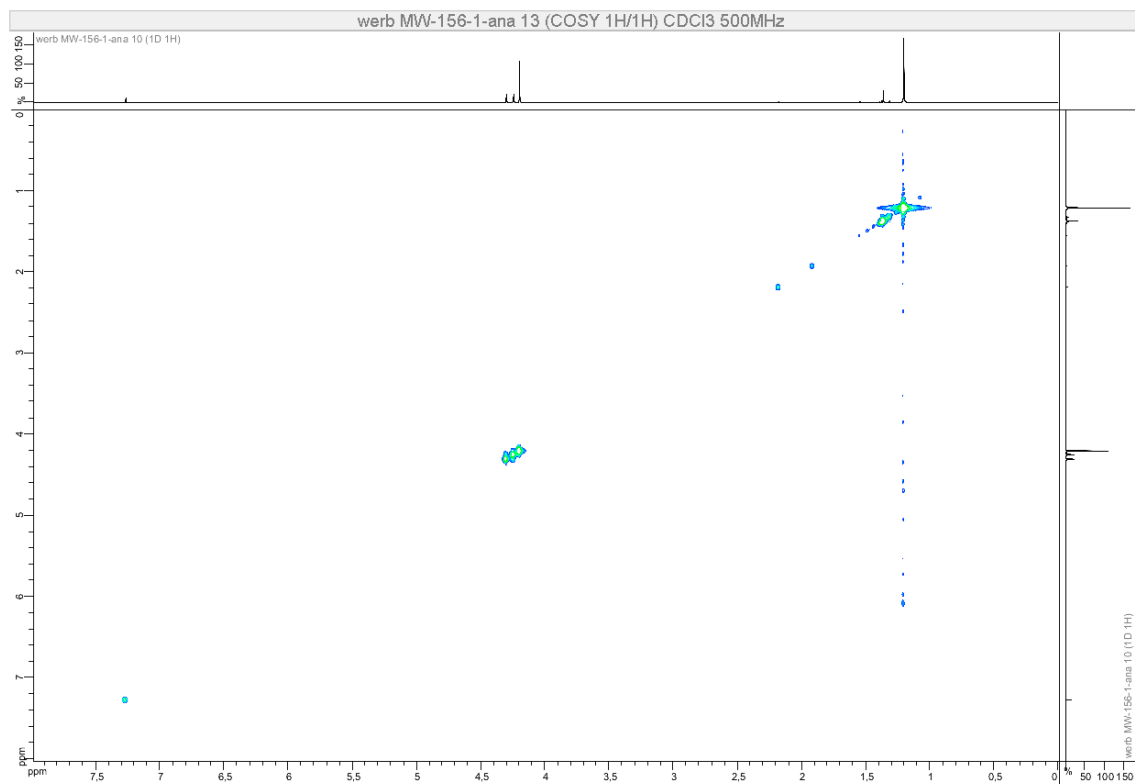
^{13}C NMR (126 MHz, CDCl_3)



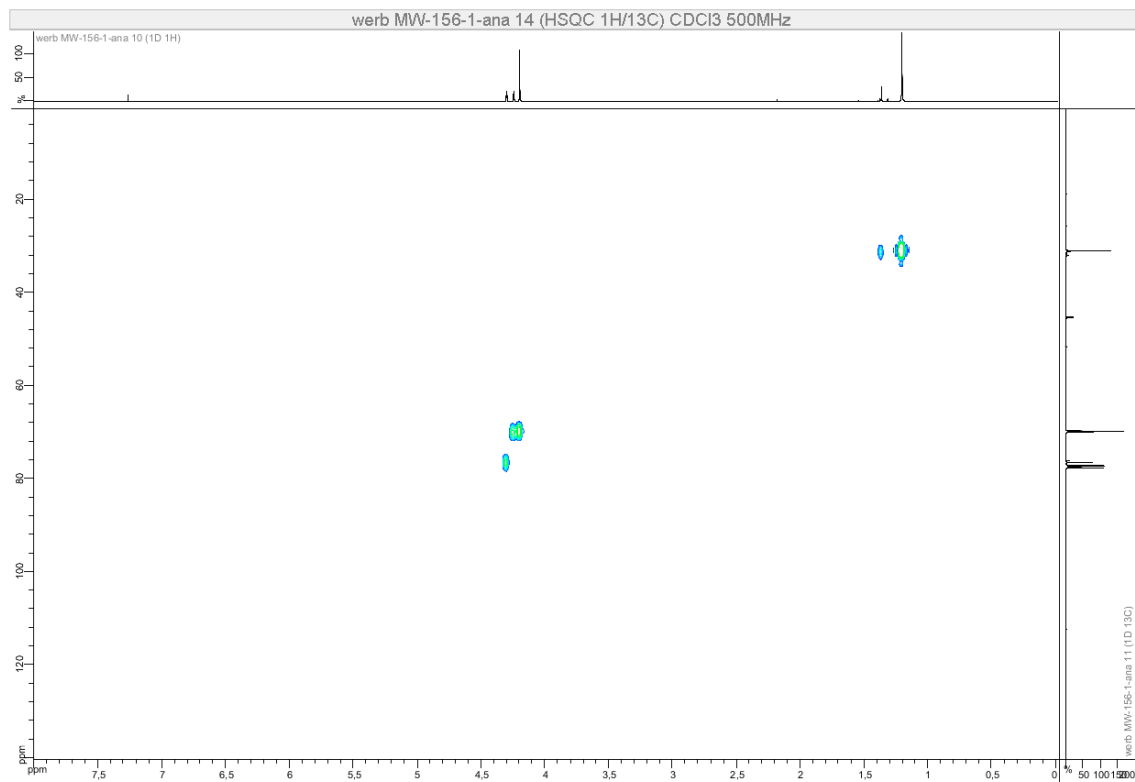
DEPT 135 (126 MHz, CDCl₃)



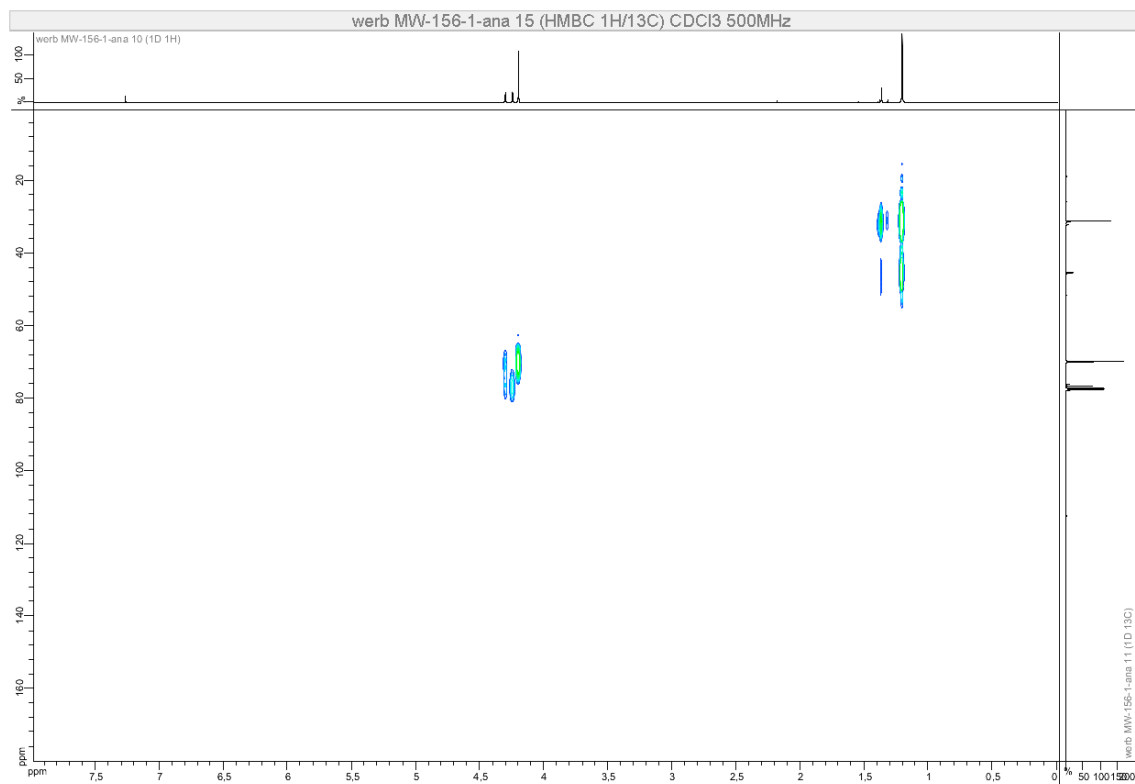
COSY (500 MHz, CDCl₃)



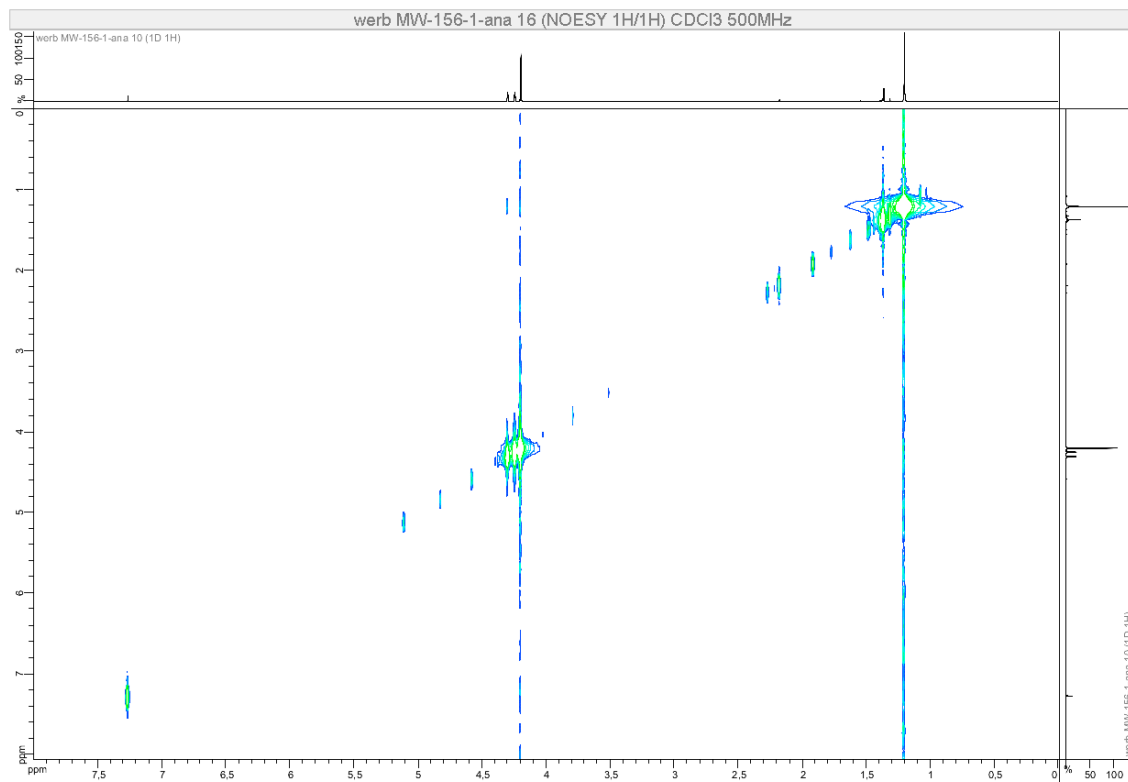
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

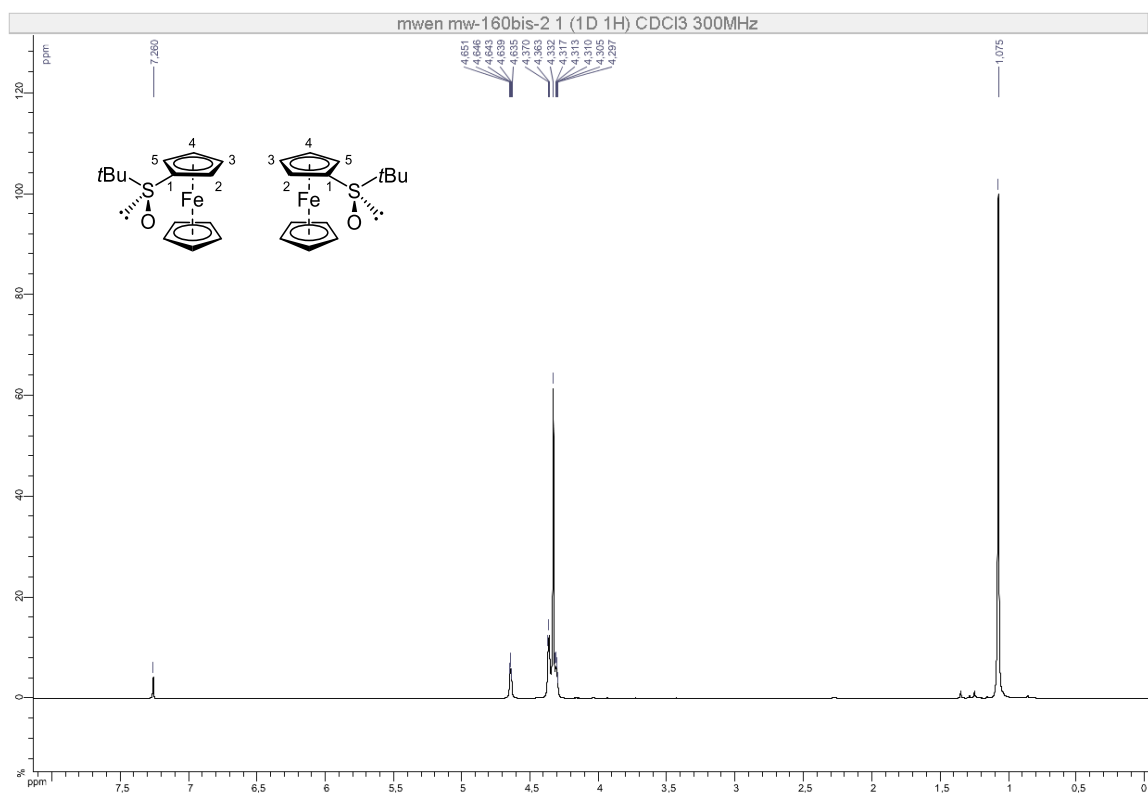


NOESY (500 MHz, CDCl₃)



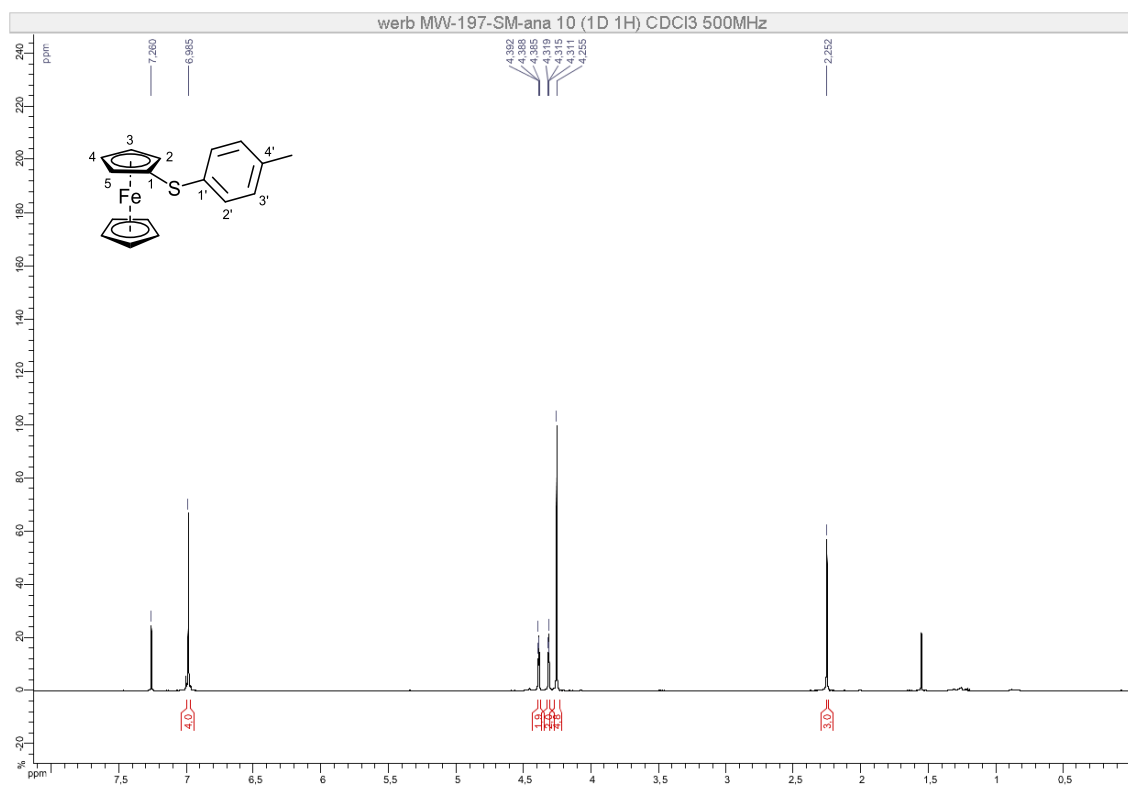
Racemic *S-tert*-Butylferrocenesulfoxide (*rac*-FcSO*t*Bu)

^1H NMR (300 MHz, CDCl_3)

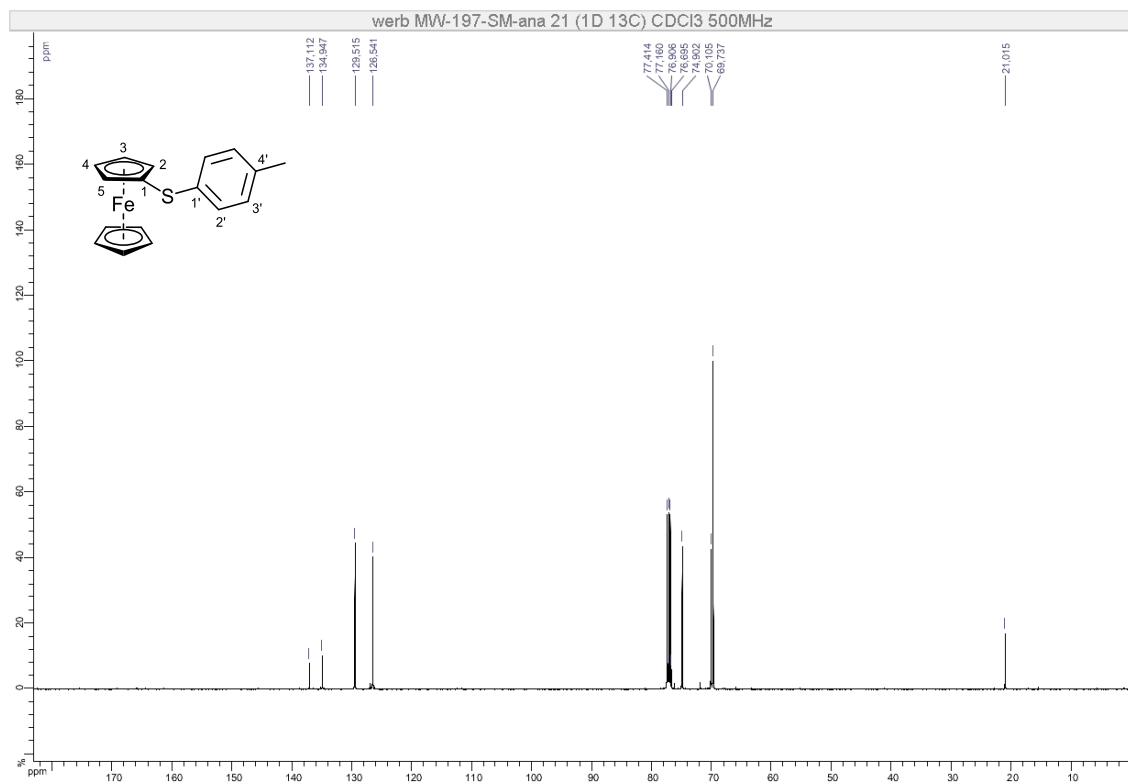


(4-Tolylthio)ferrocene

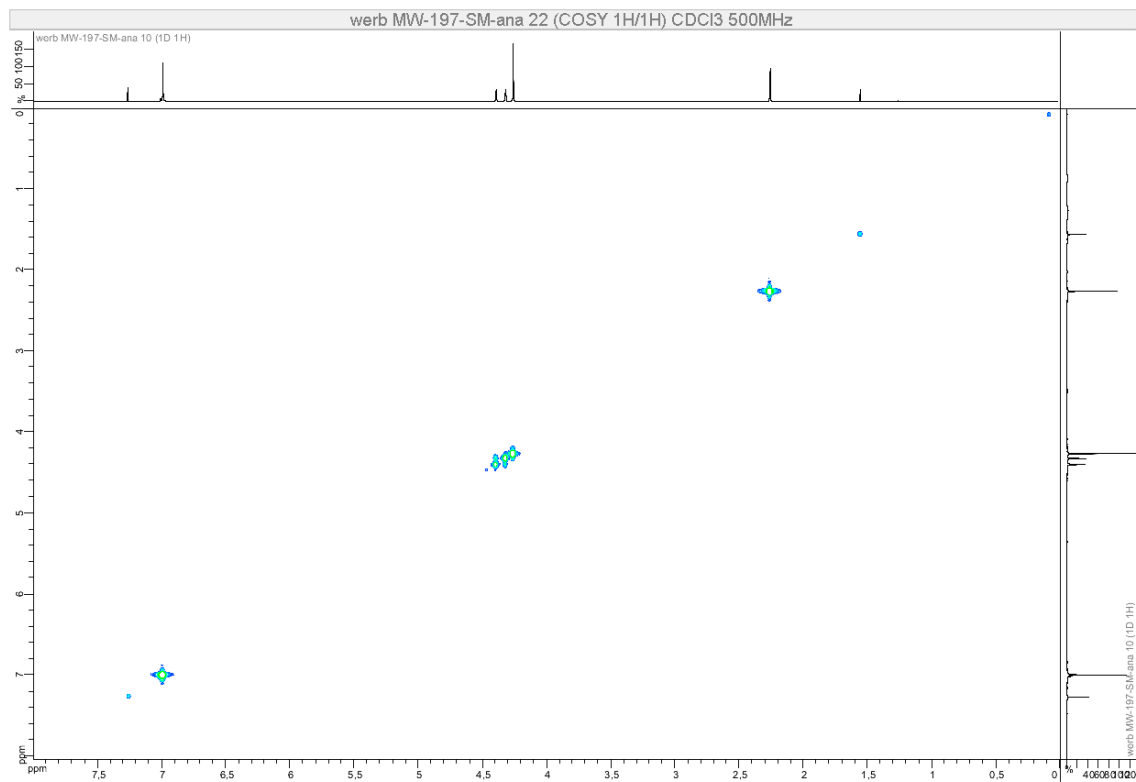
^1H NMR (500 MHz, CDCl_3)



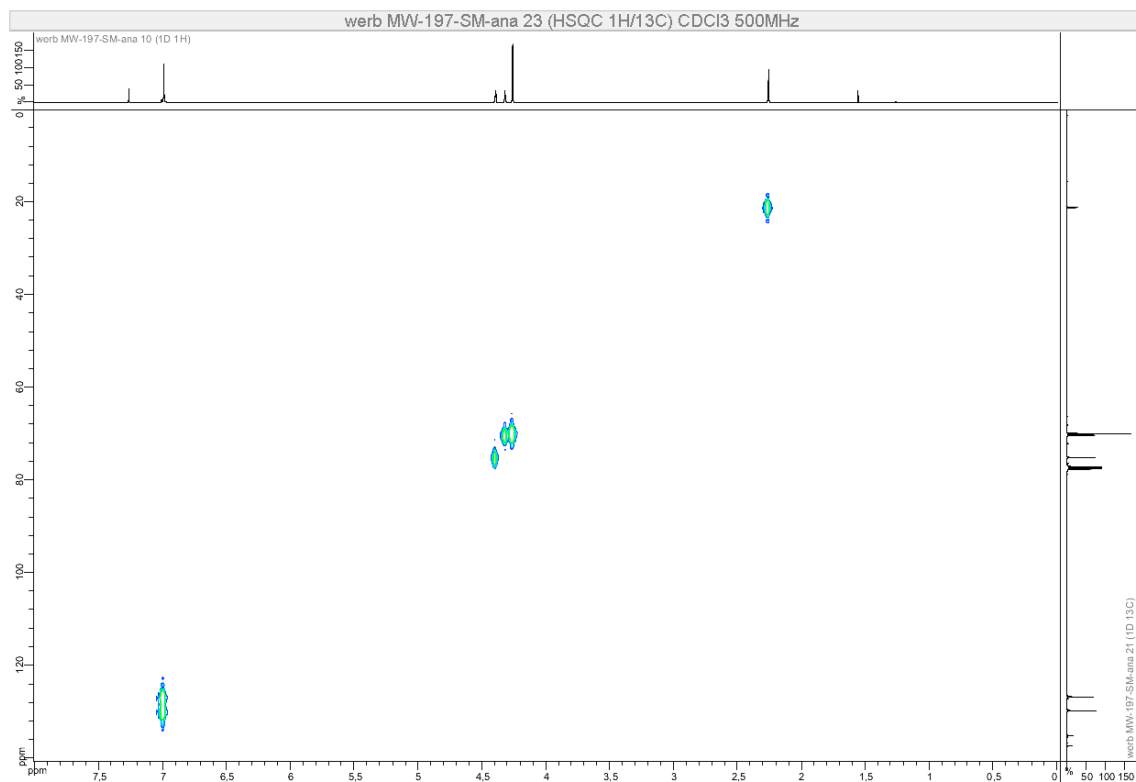
^{13}C NMR (126 MHz, CDCl_3)



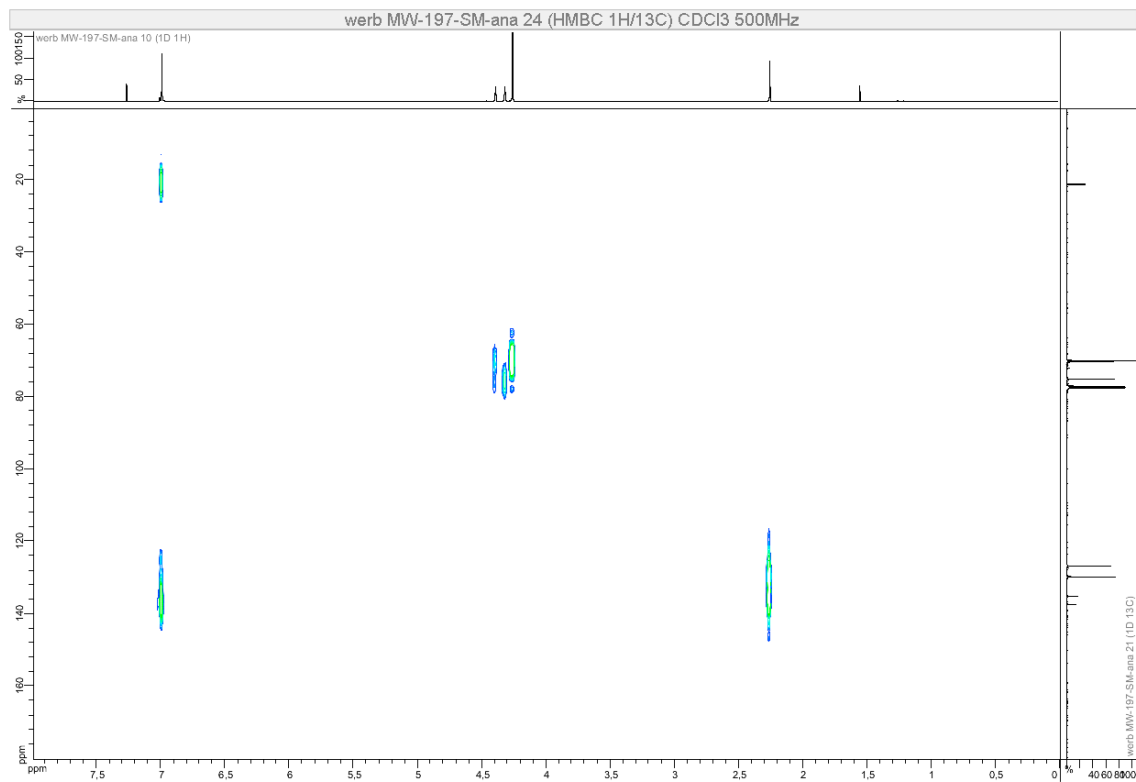
COSY (500 MHz, CDCl₃)



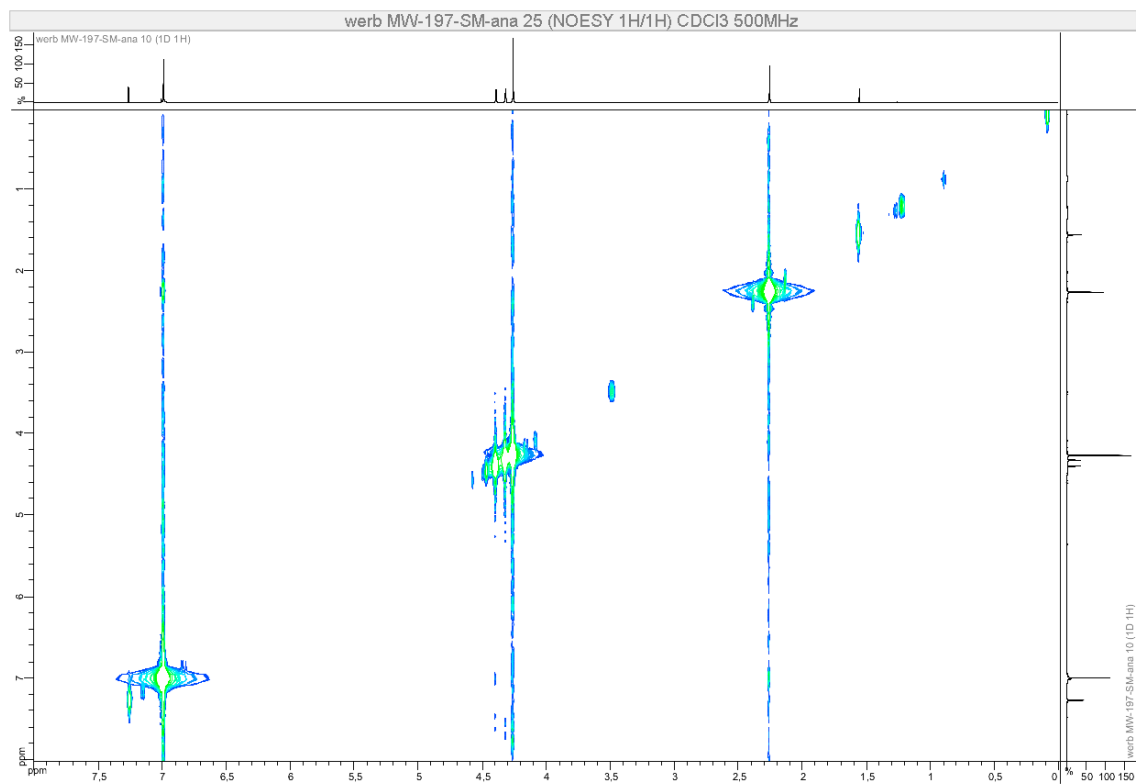
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

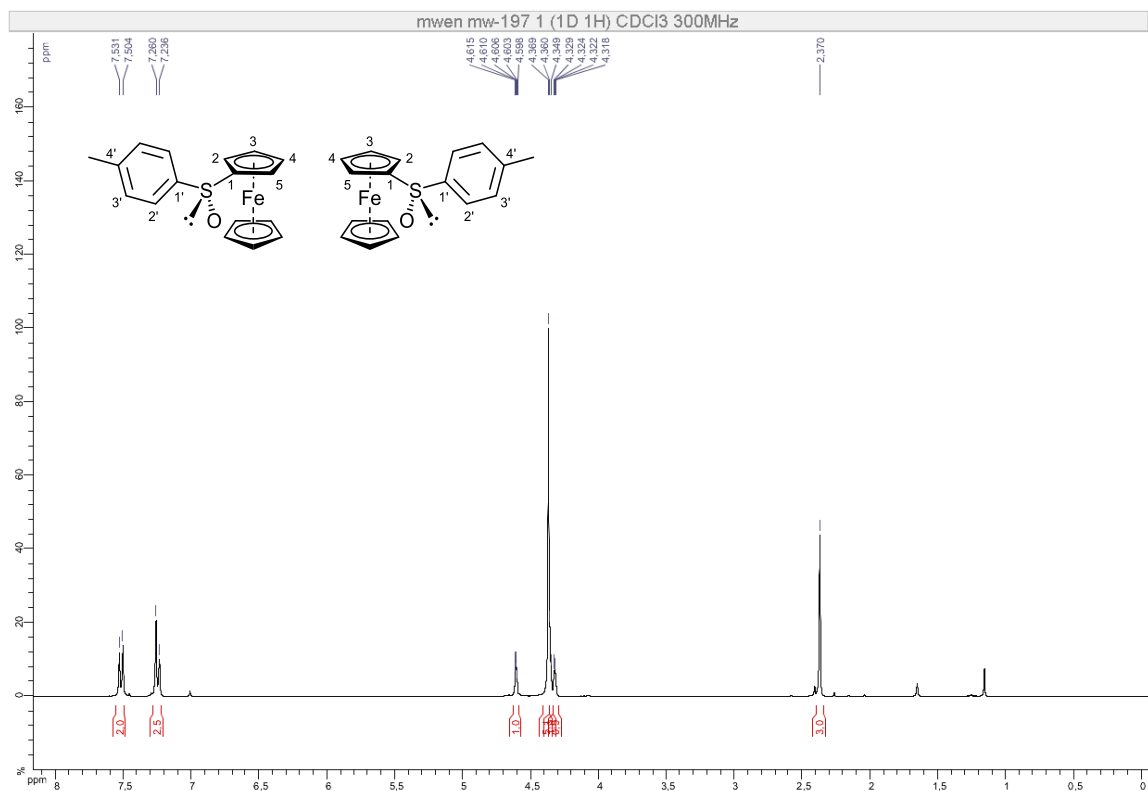


NOESY (500 MHz, CDCl₃)



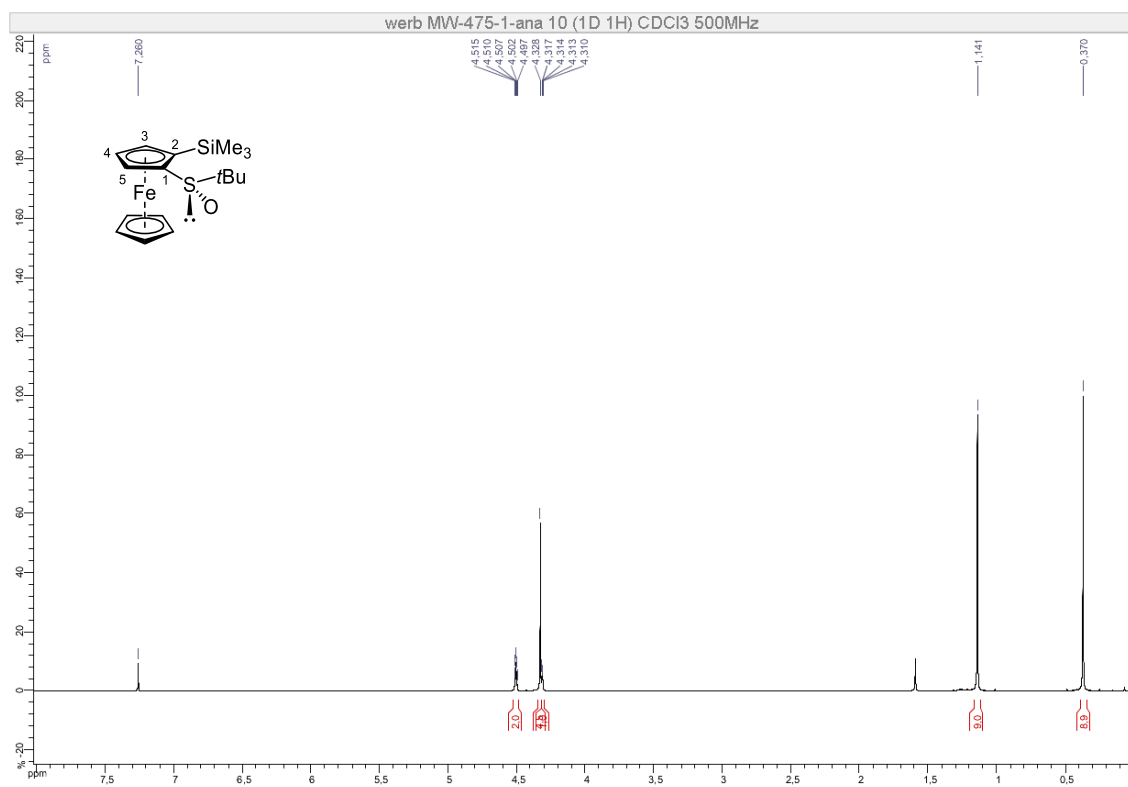
Racemic *S*-(4-Tolyl)ferrocenesulfoxide (*rac*-FcSO-*p*-Tol)

^1H NMR (300 MHz, CDCl_3)

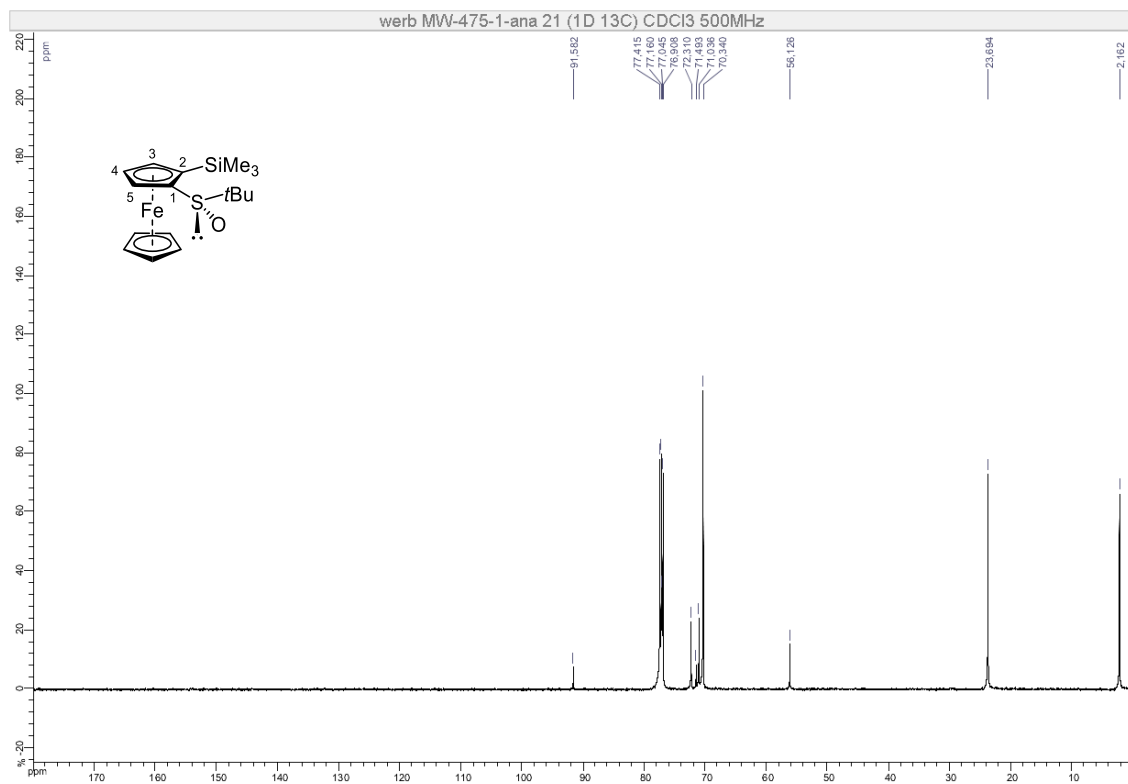


(*S,S*)-*S*-tert-Butyl-2-(trimethylsilyl)ferrocenesulfoxide (*S,S*-1a)

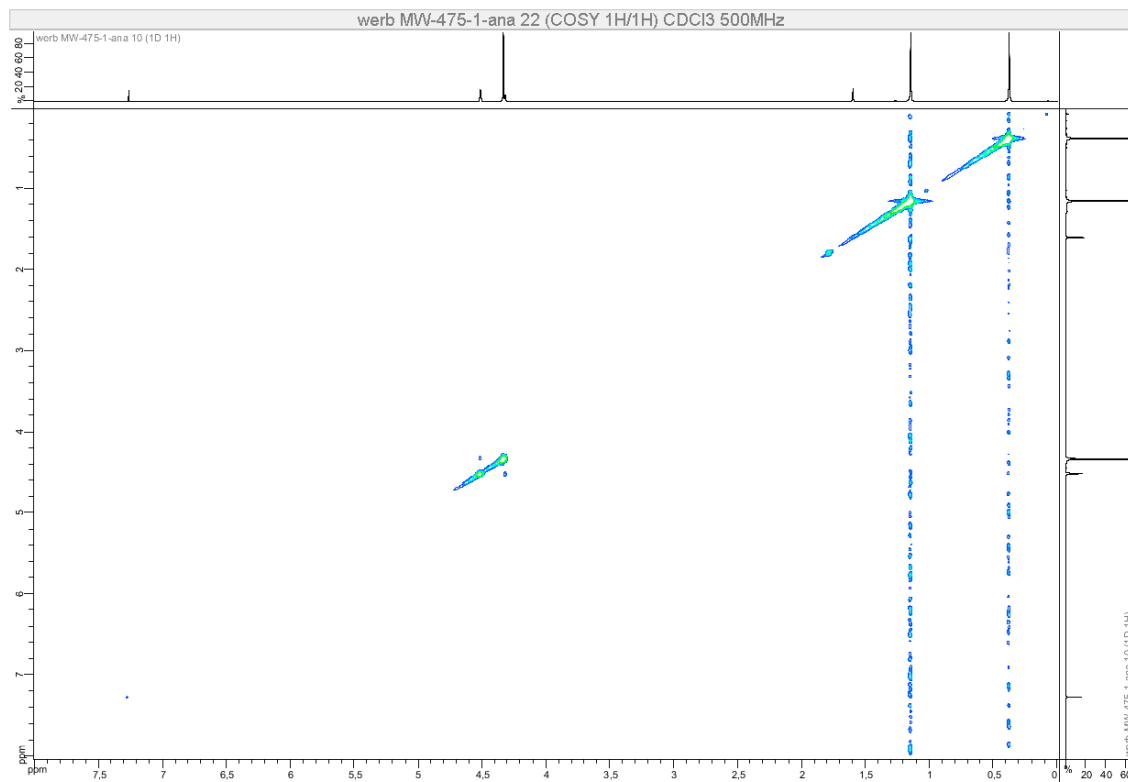
^1H NMR (500 MHz, CDCl_3)



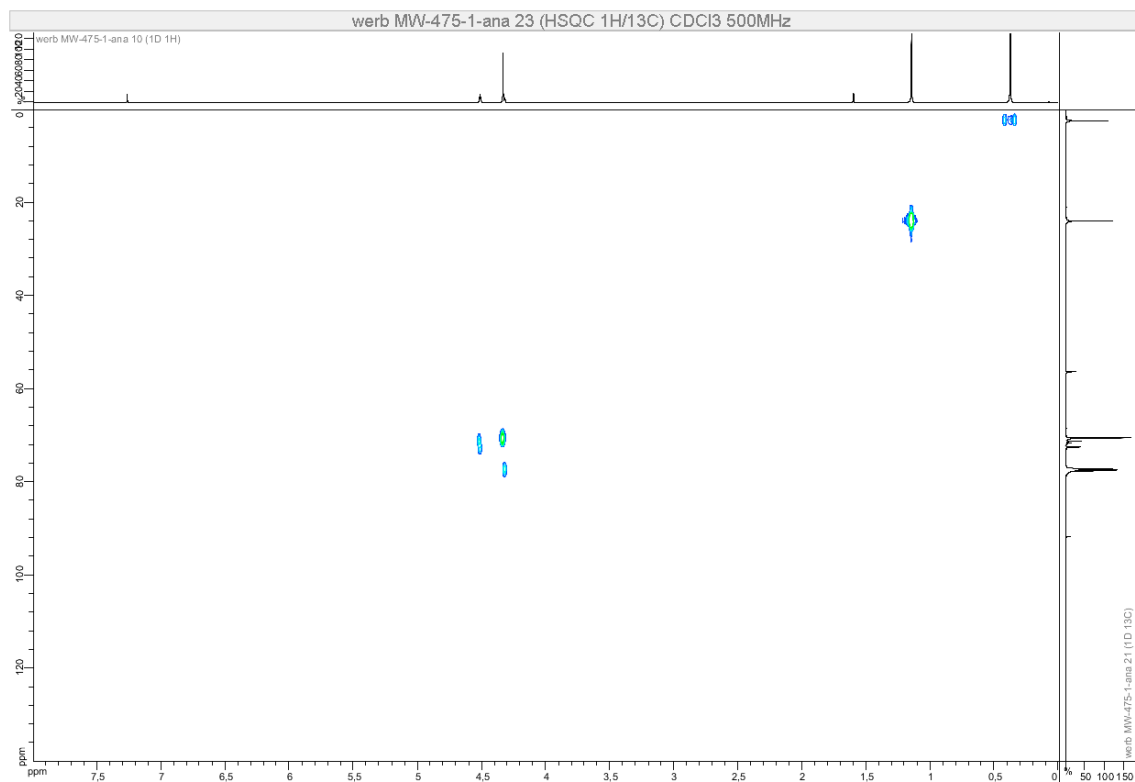
^{13}C NMR (126 MHz, CDCl_3)



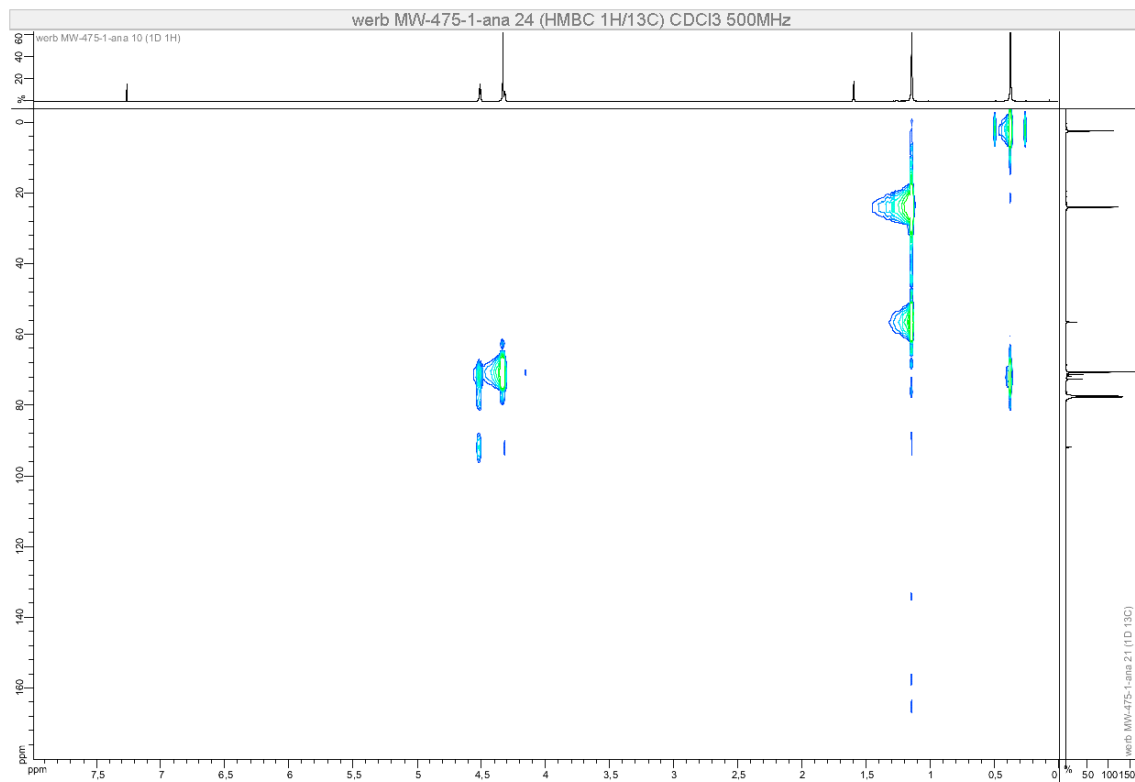
COSY (500 MHz, CDCl₃)



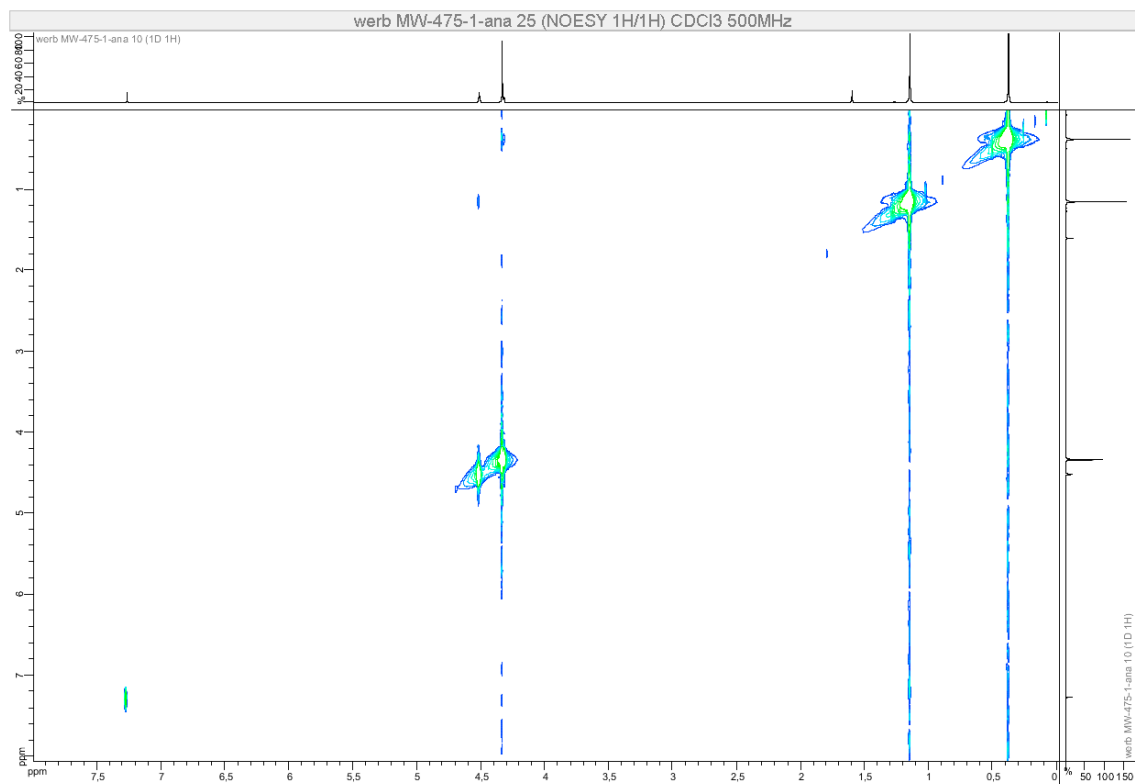
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

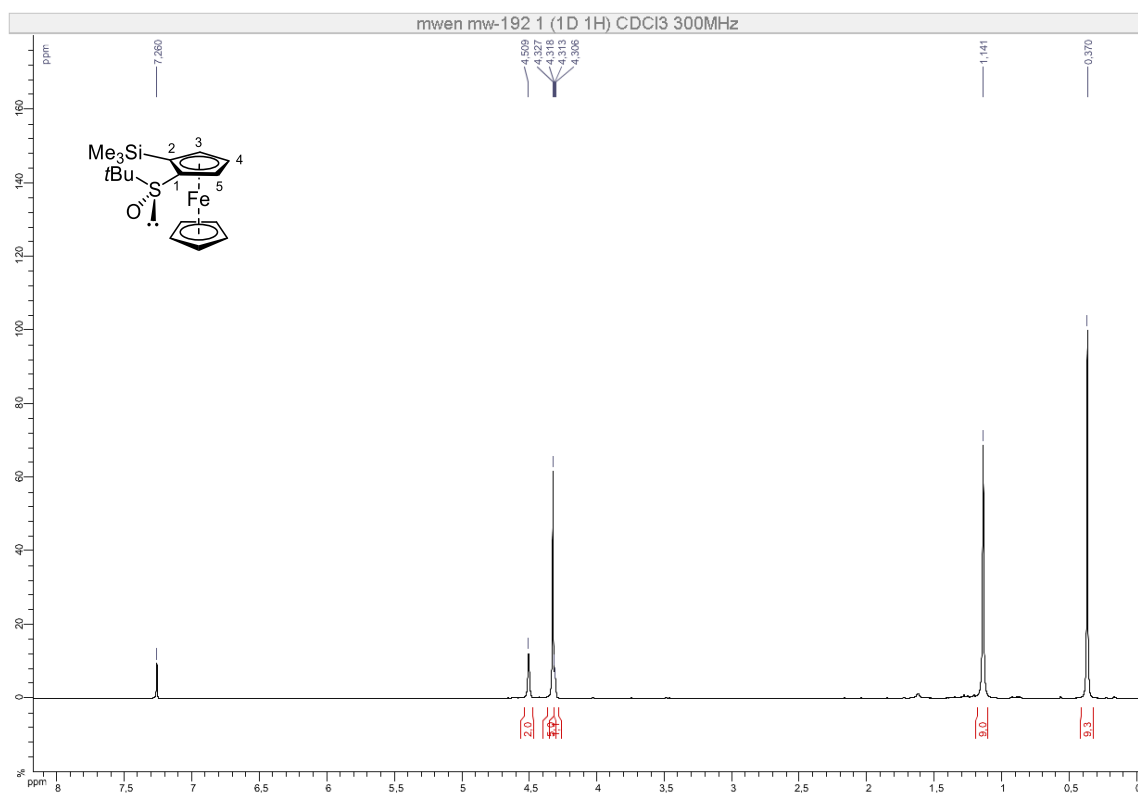


NOESY (500 MHz, CDCl₃)



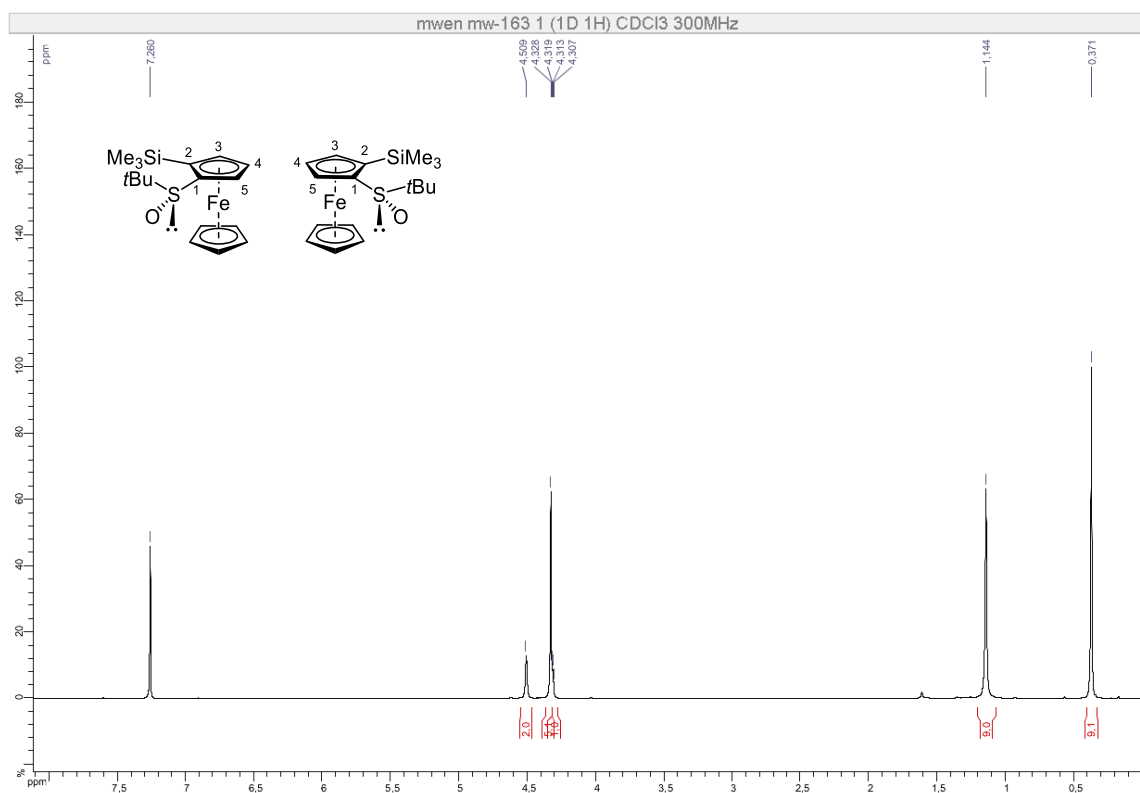
(*R,R*)-*S*-*tert*-Butyl-2-(trimethylsilyl)ferrocenesulfoxide (*R,R*-1a)

^1H NMR (300 MHz, CDCl_3)



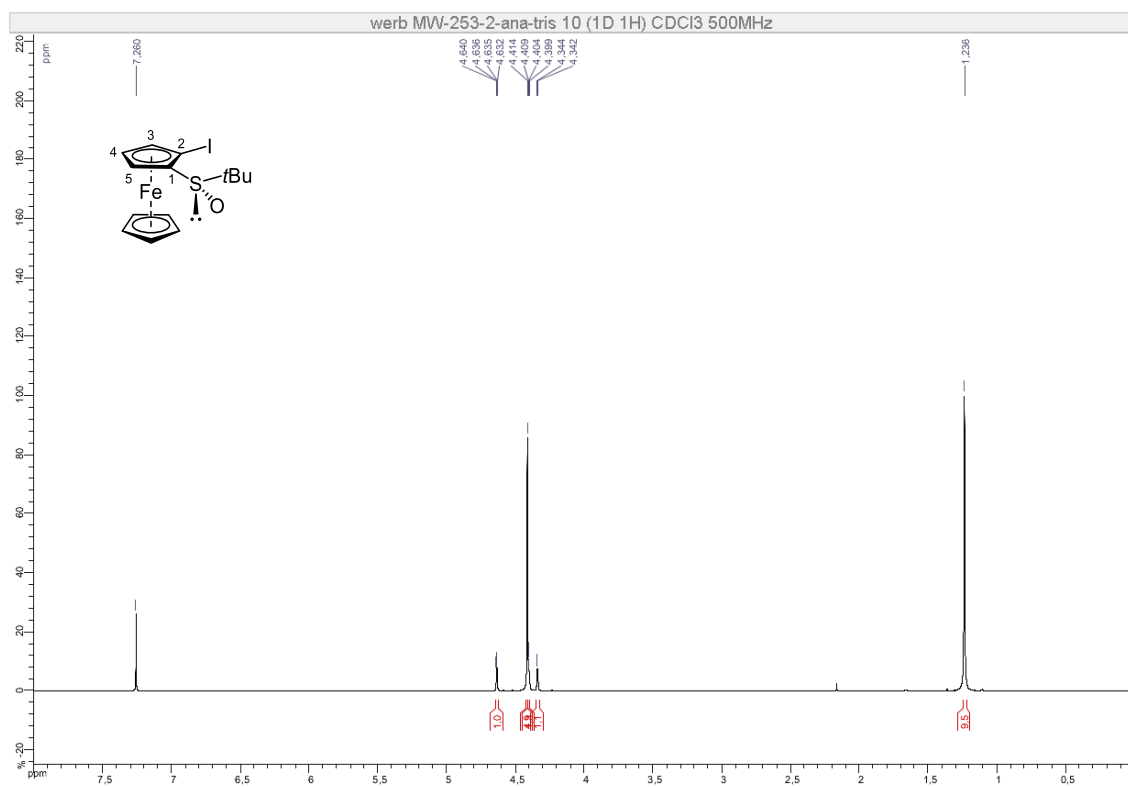
(*R,R*)- and (*S,S*)-*S*-tert-Butyl-2-(trimethylsilyl)ferrocenesulfoxide (*R,R*/*S,S*-1a)

^1H NMR (300 MHz, CDCl_3)

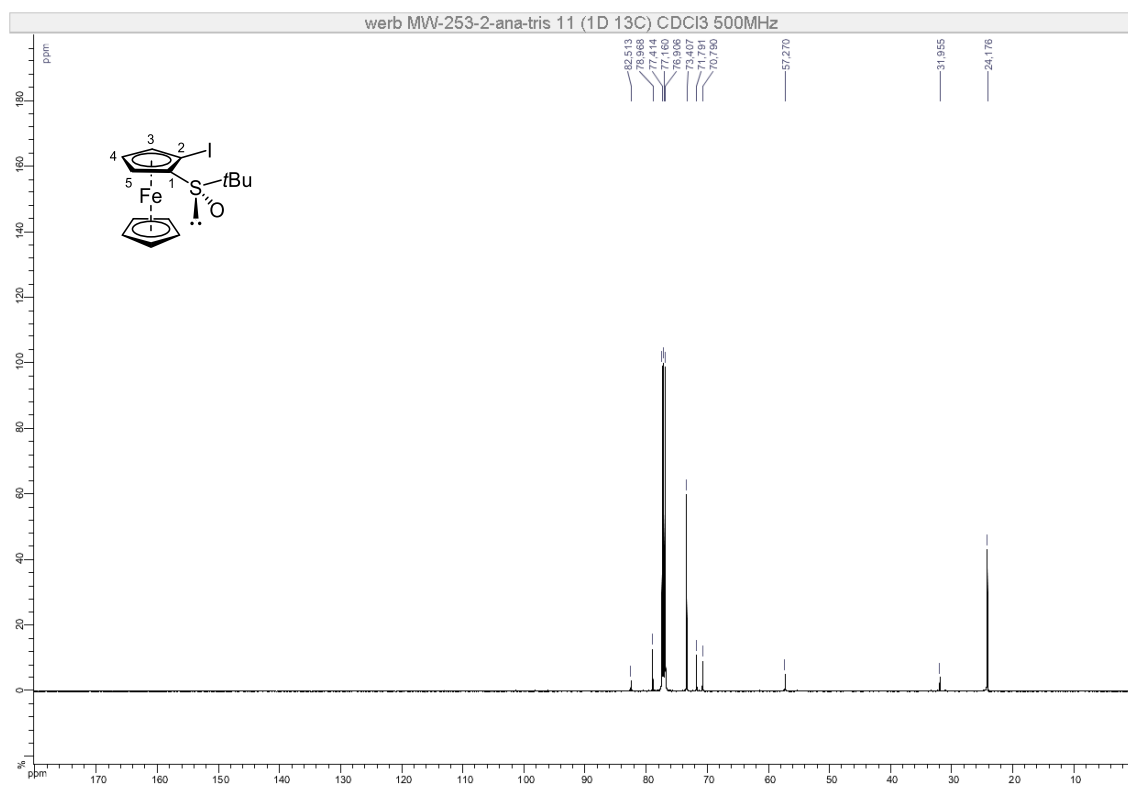


(*S,R_P*)-*S*-tert-Butyl-2-iodoferrocenesulfoxide (*S,R_P*-1b)

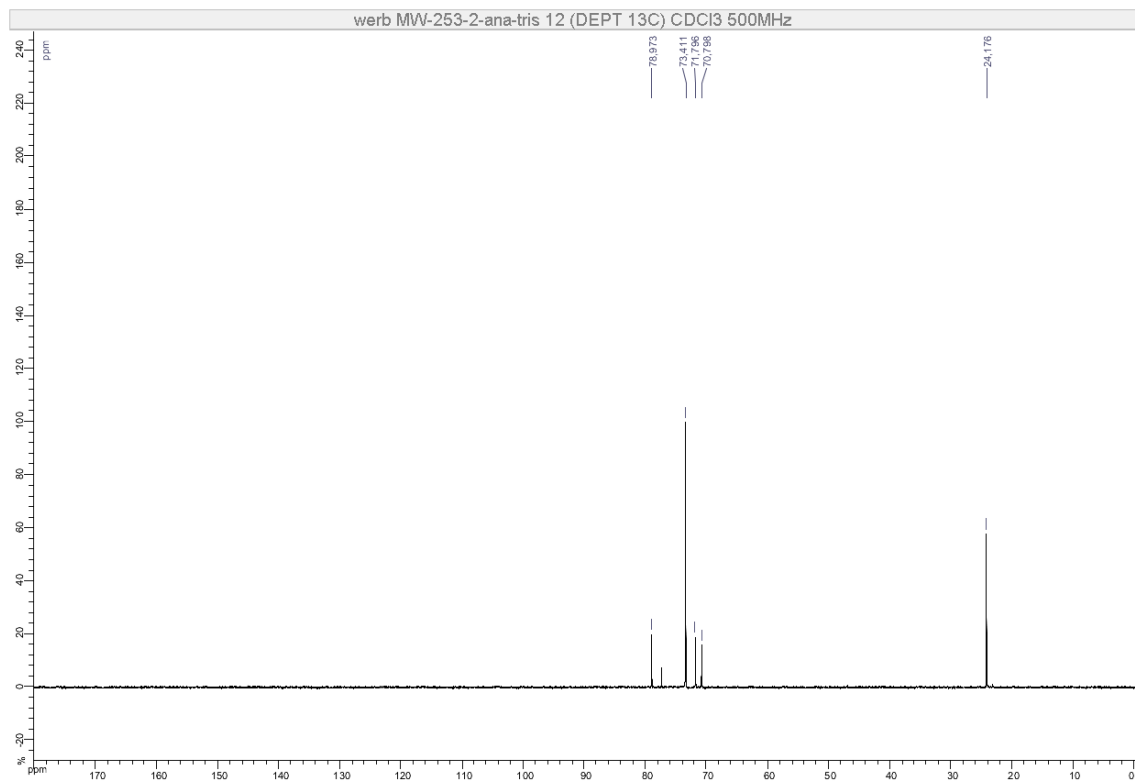
^1H NMR (500 MHz, CDCl_3)



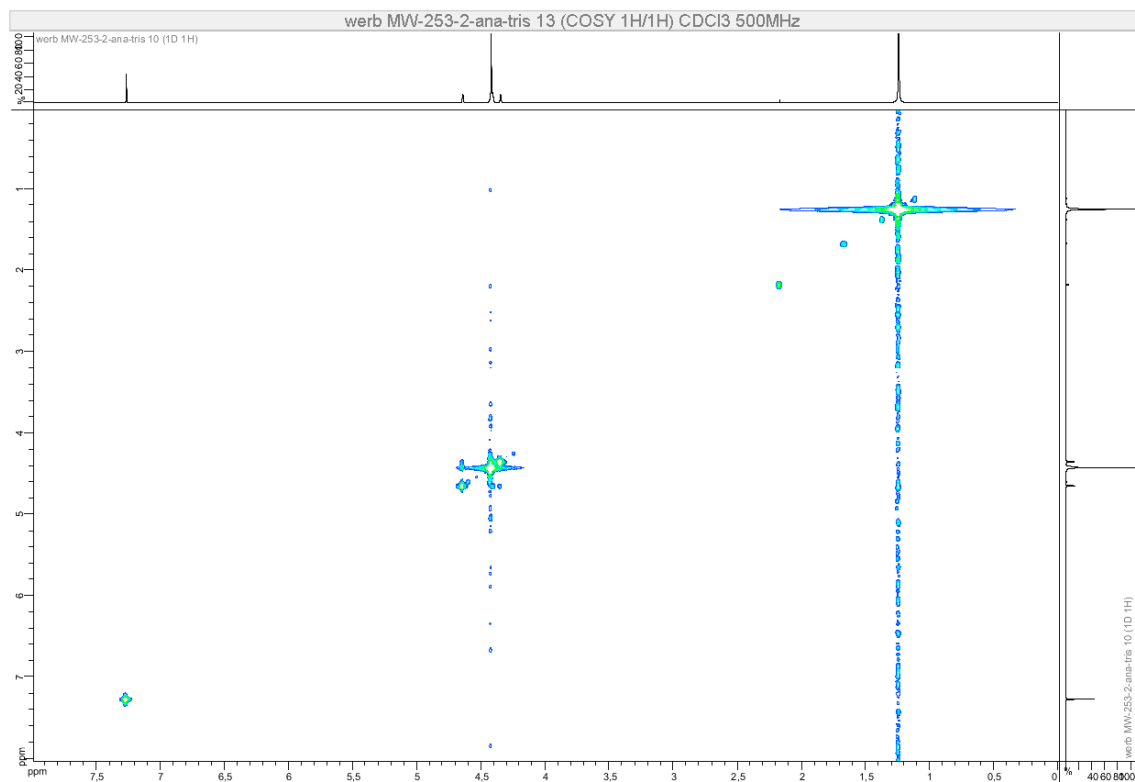
^{13}C NMR (126 MHz, CDCl_3)



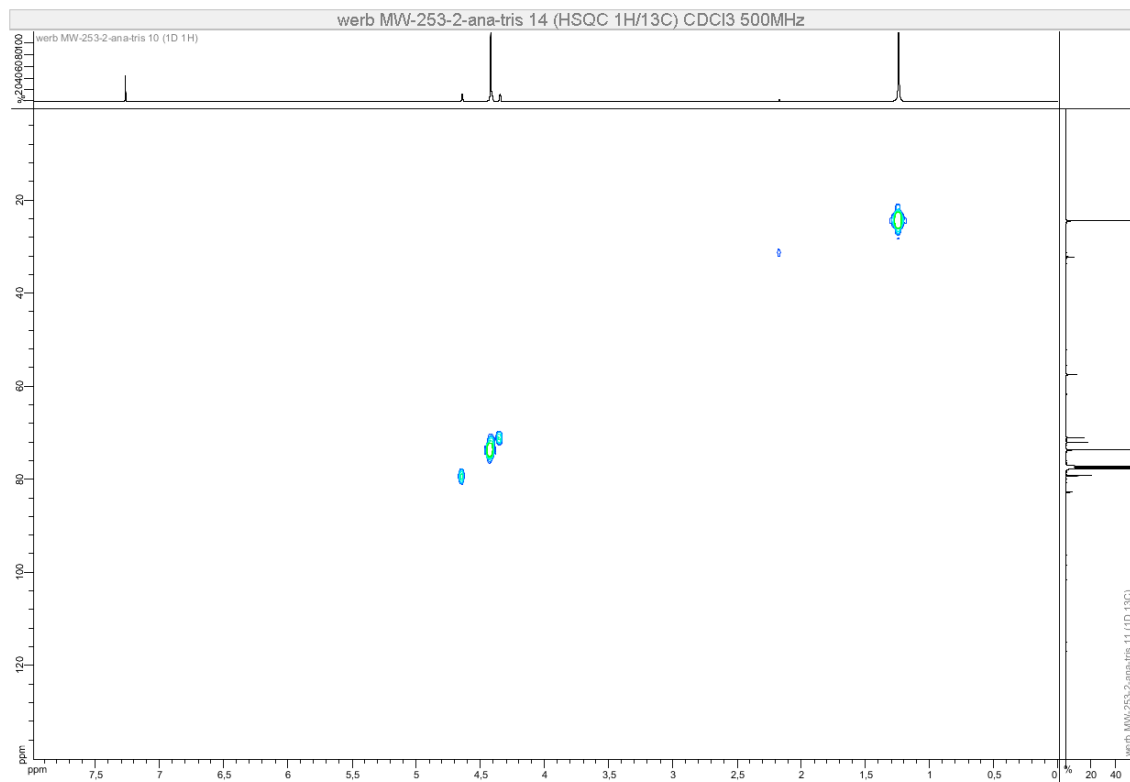
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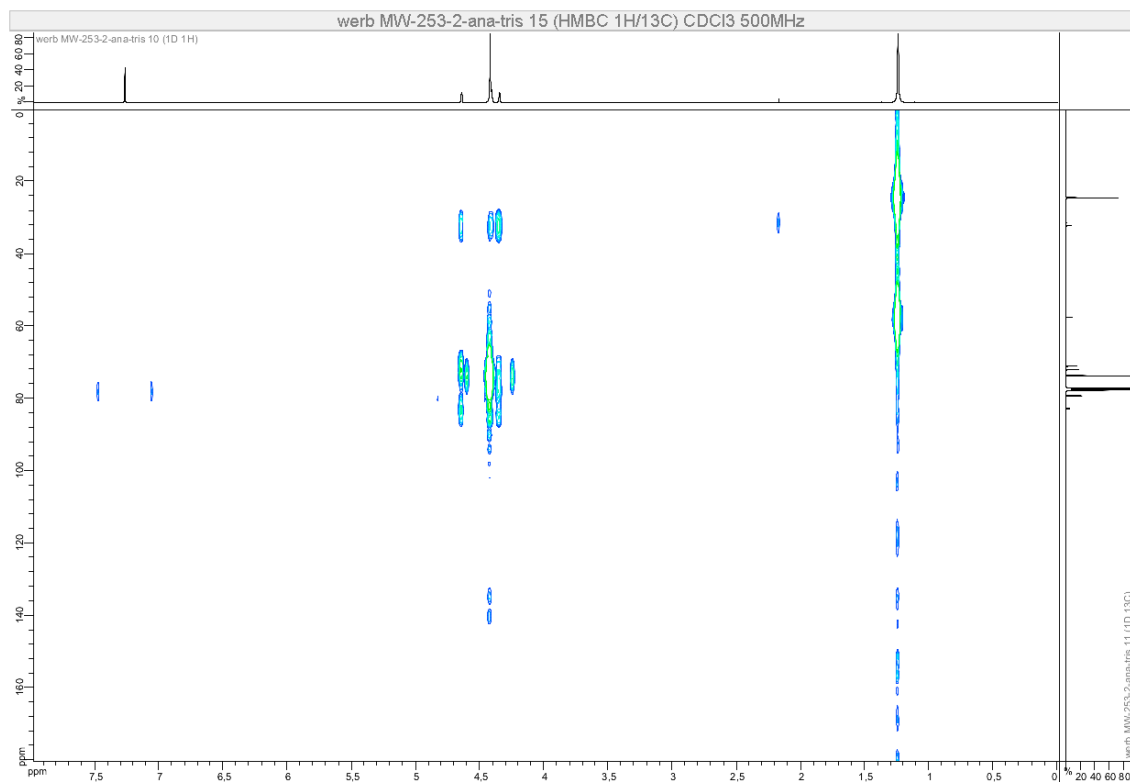
COSY (500 MHz, CDCl₃)



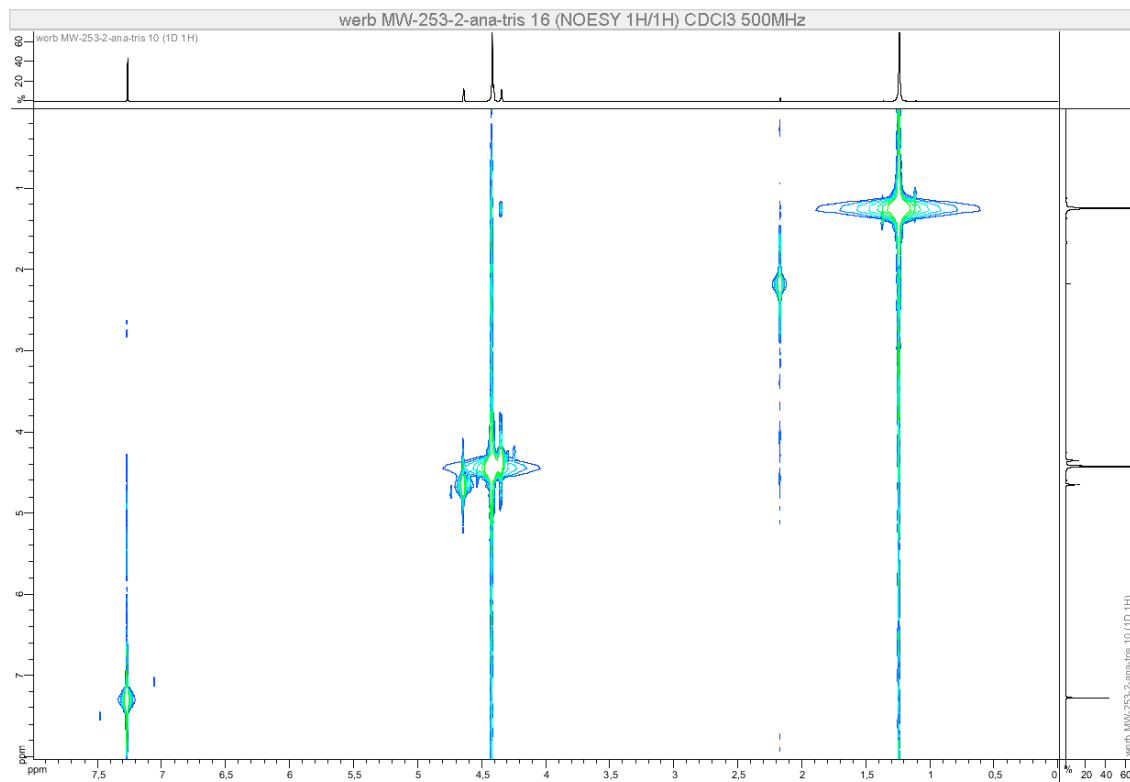
HSQC (500 MHz, CDCl₃)



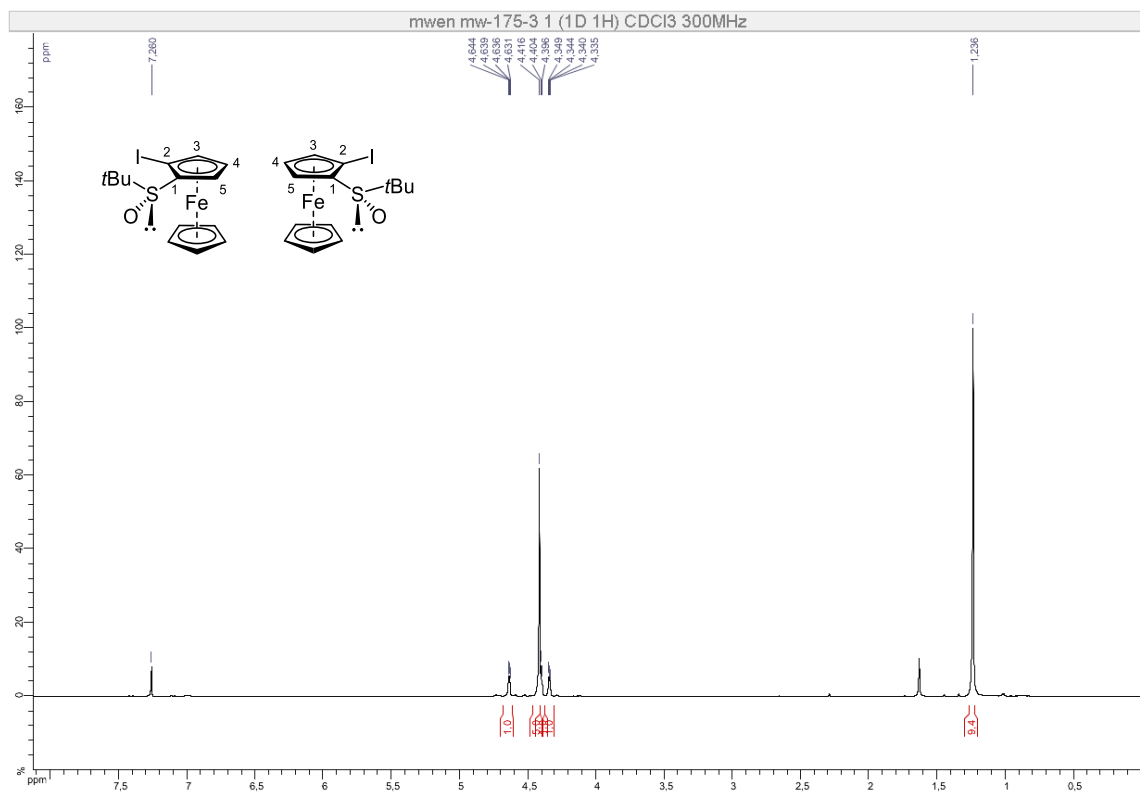
HMBC (500 MHz, CDCl₃)



NOESY (500 MHz, CDCl₃)

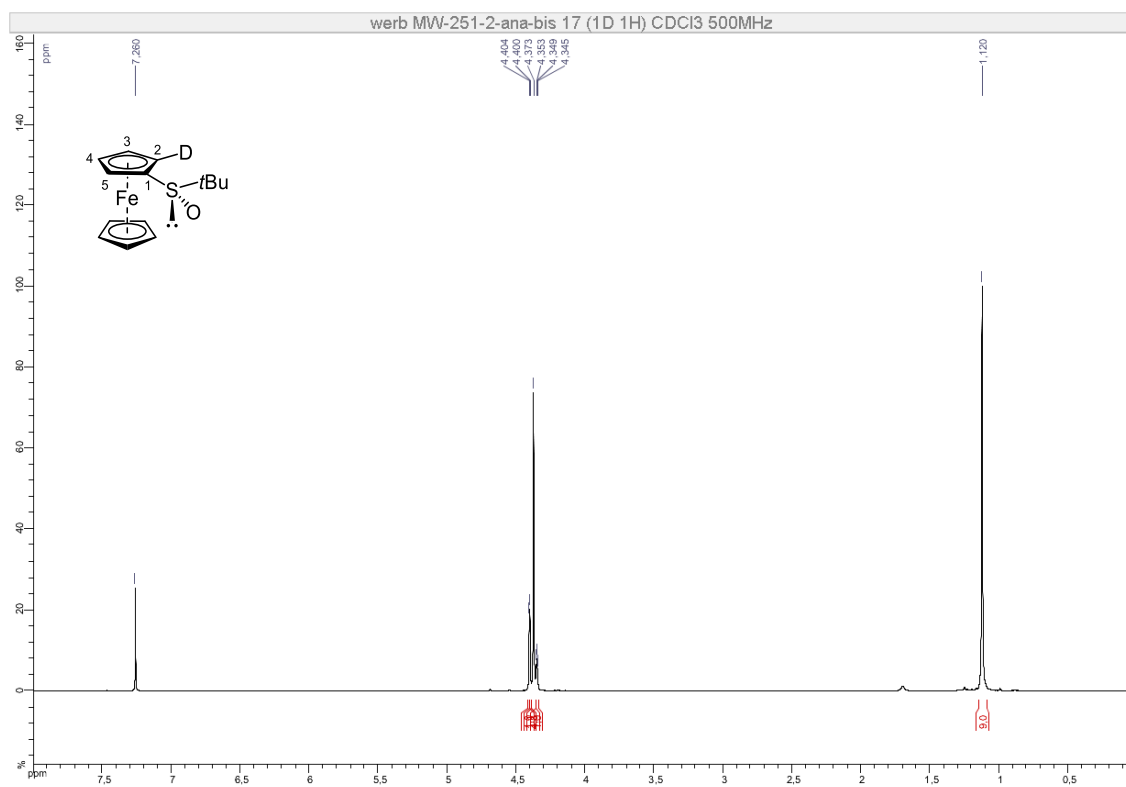


(*S,R_P*)- and (*R,S_P*)-*S*-*tert*-Butyl-2-iodoferrocenesulfoxide (*S,R_P*/*R,S_P*-1b)

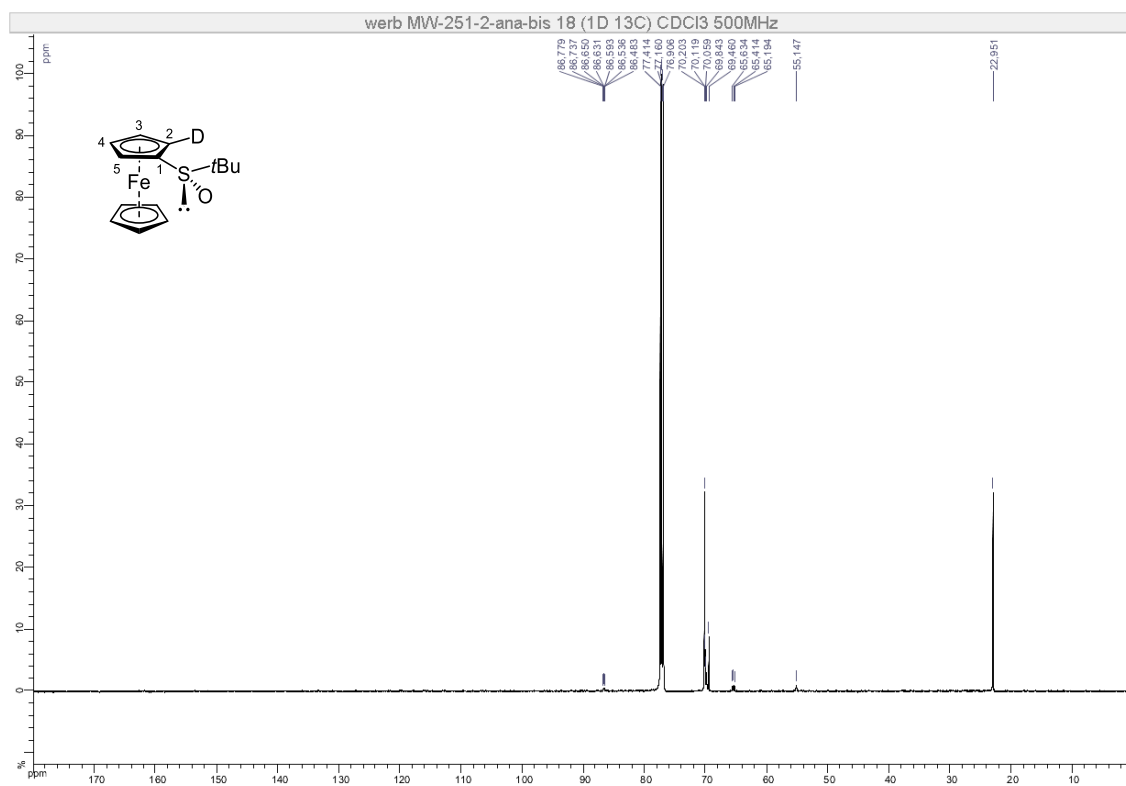


(*S,S*_P)-*S*-*tert*-Butyl-2-deuterioferrocenesulfoxide (*S,S*_P-1c)

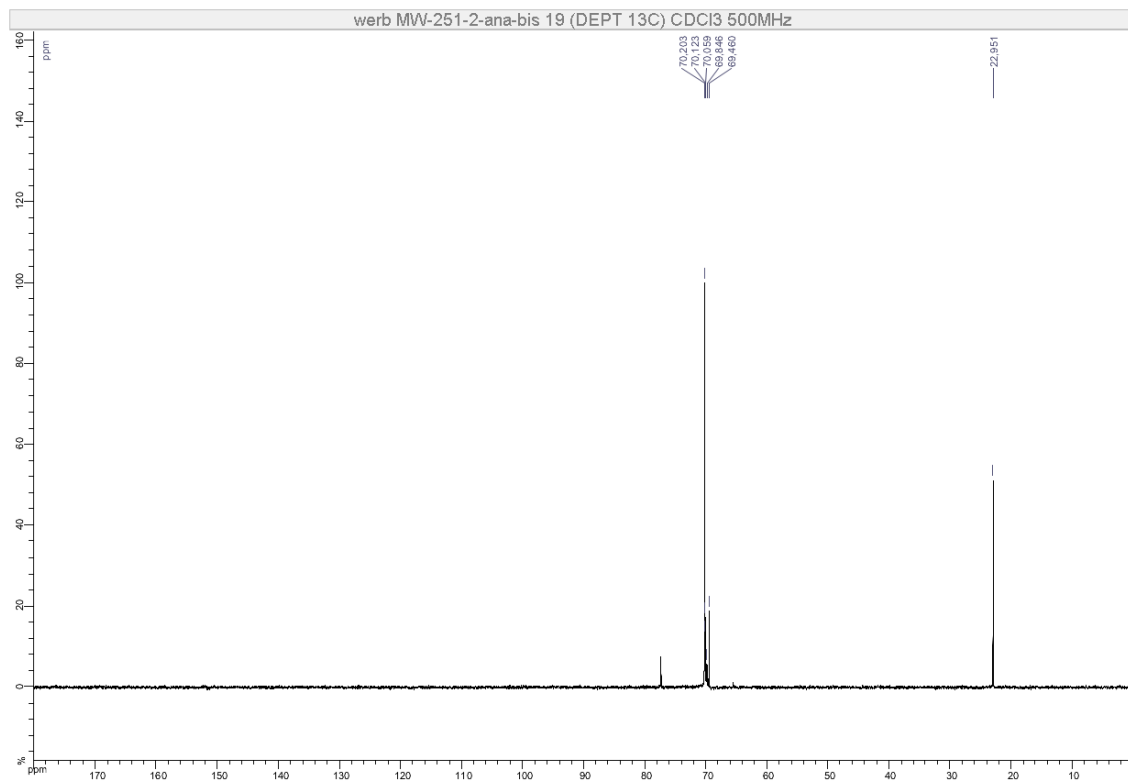
¹H NMR (500 MHz, CDCl₃)



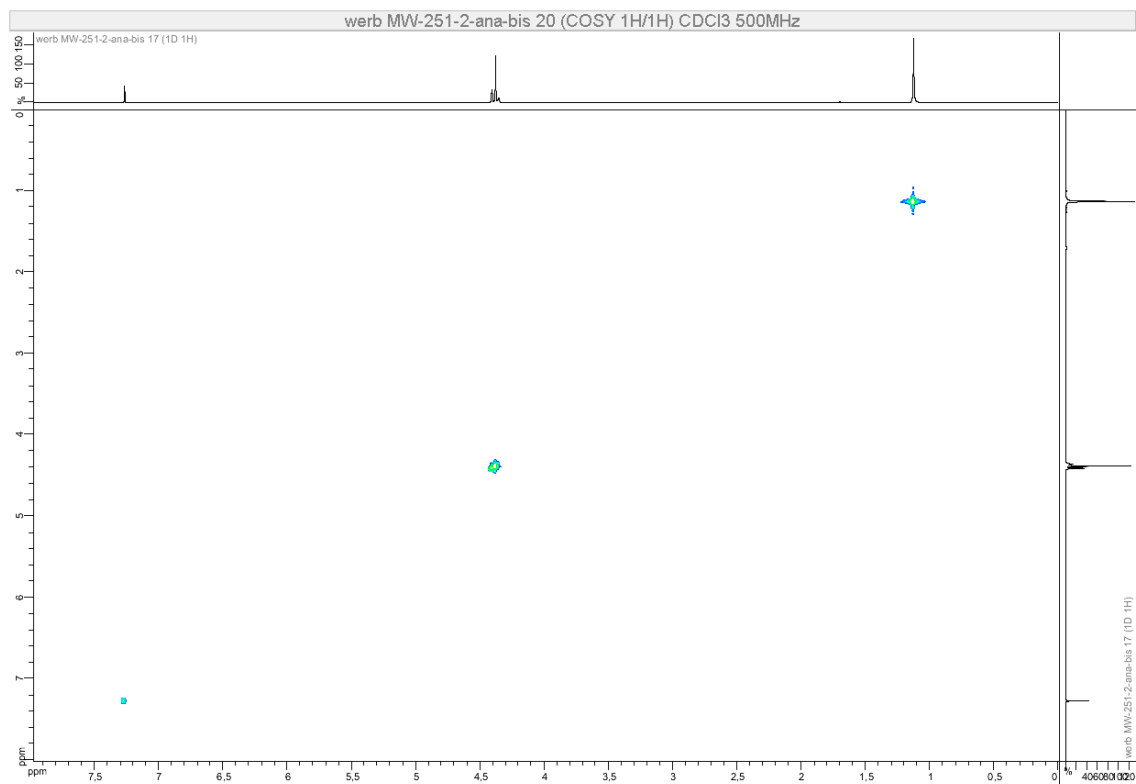
¹³C NMR (126 MHz, CDCl₃)



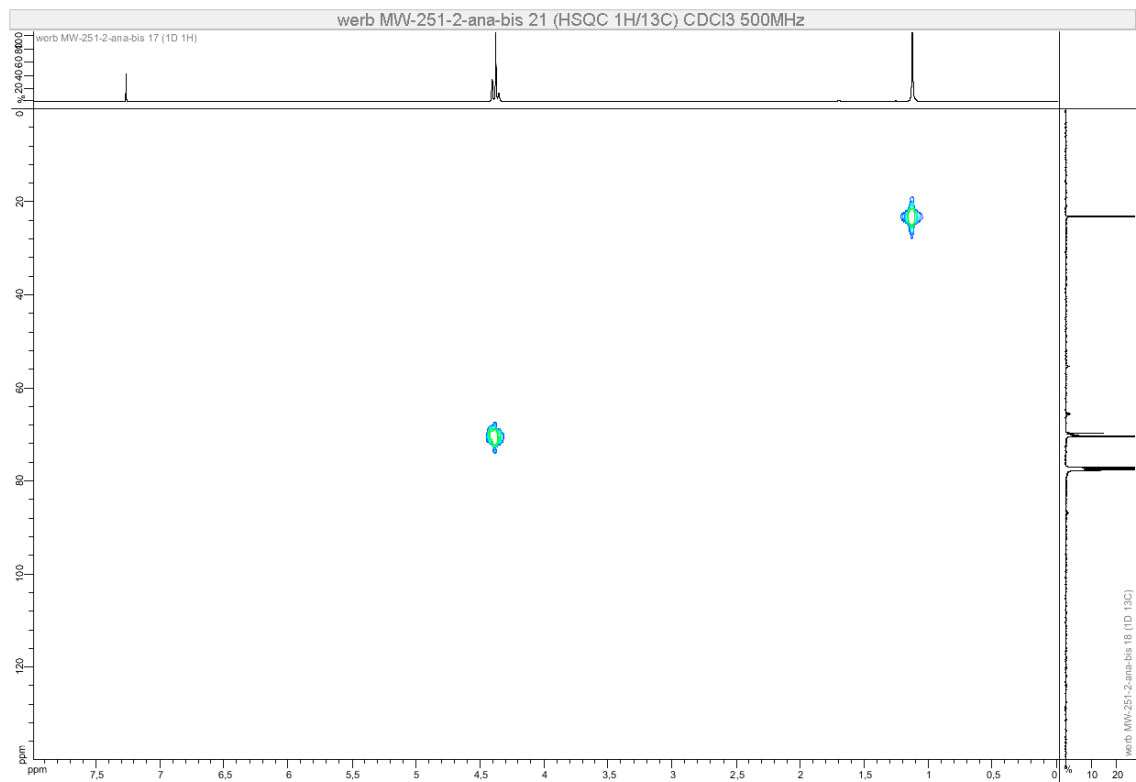
DEPT 135 (126 MHz, CDCl₃)



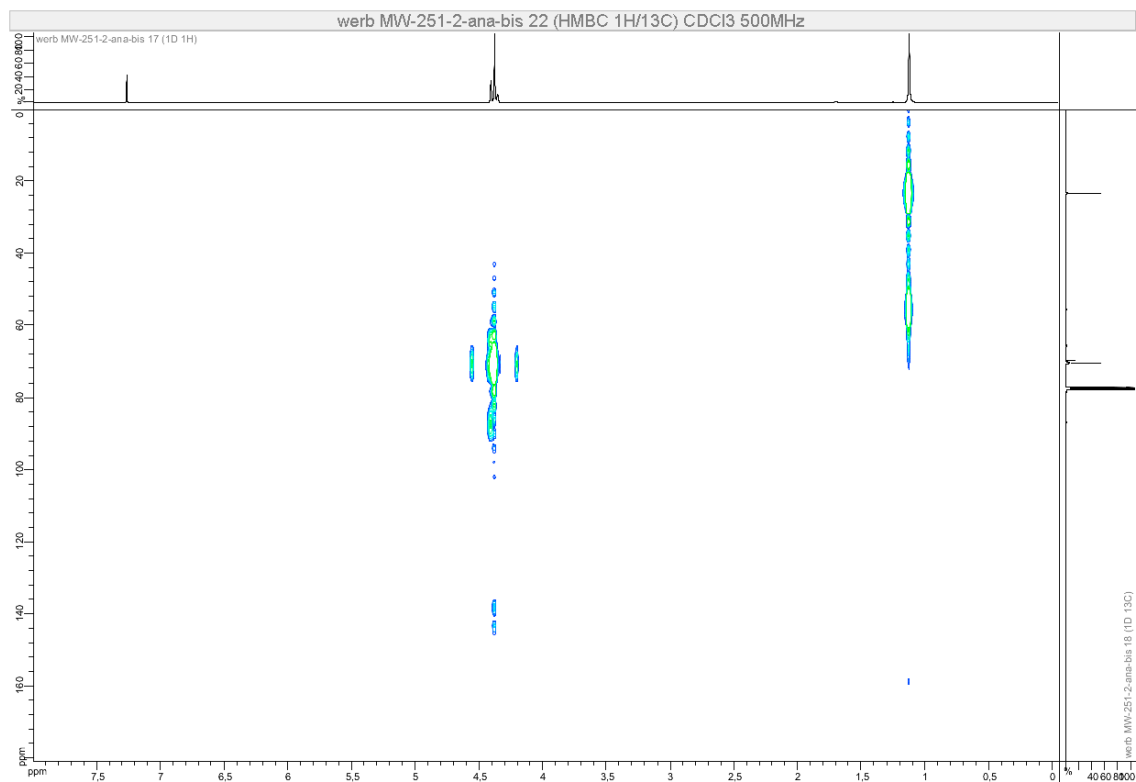
COSY (500 MHz, CDCl₃)



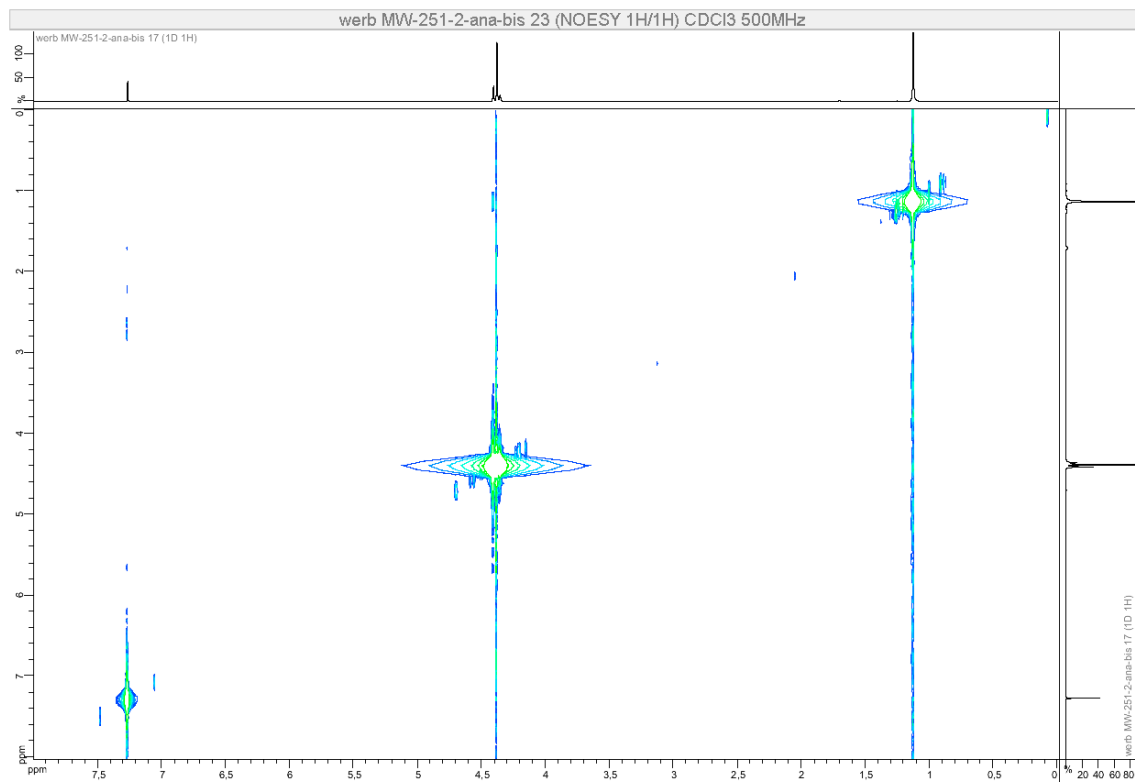
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

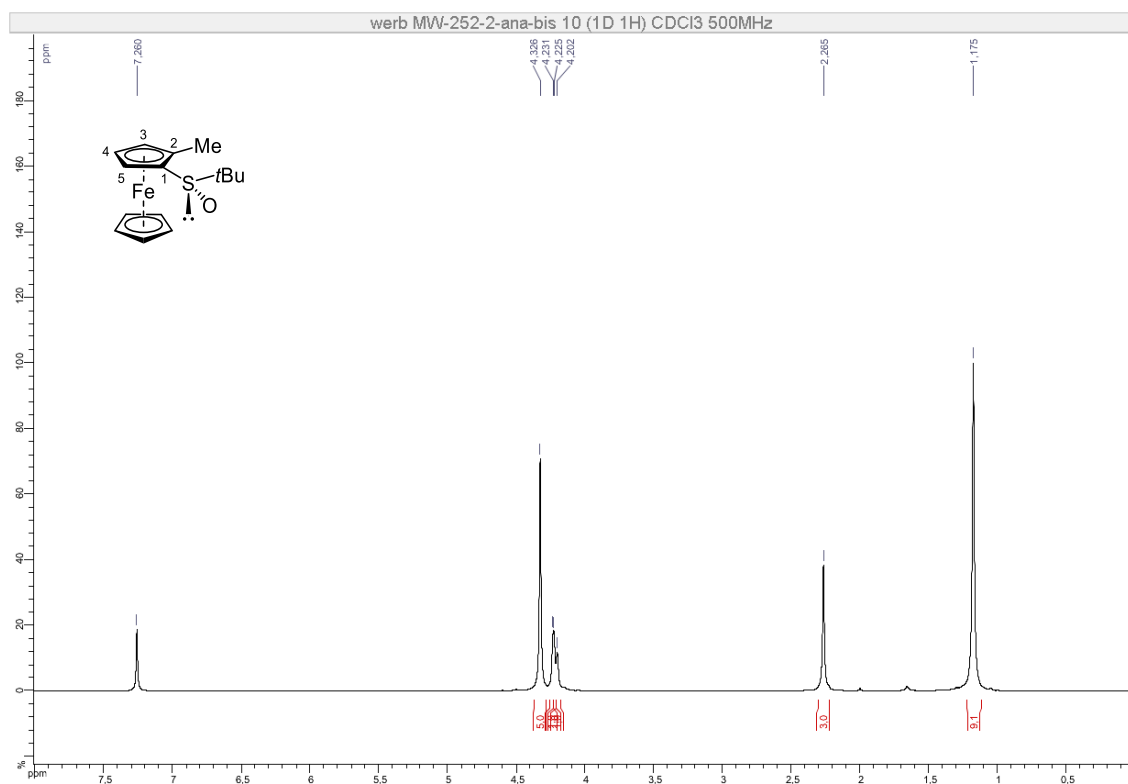


NOESY (500 MHz, CDCl₃)

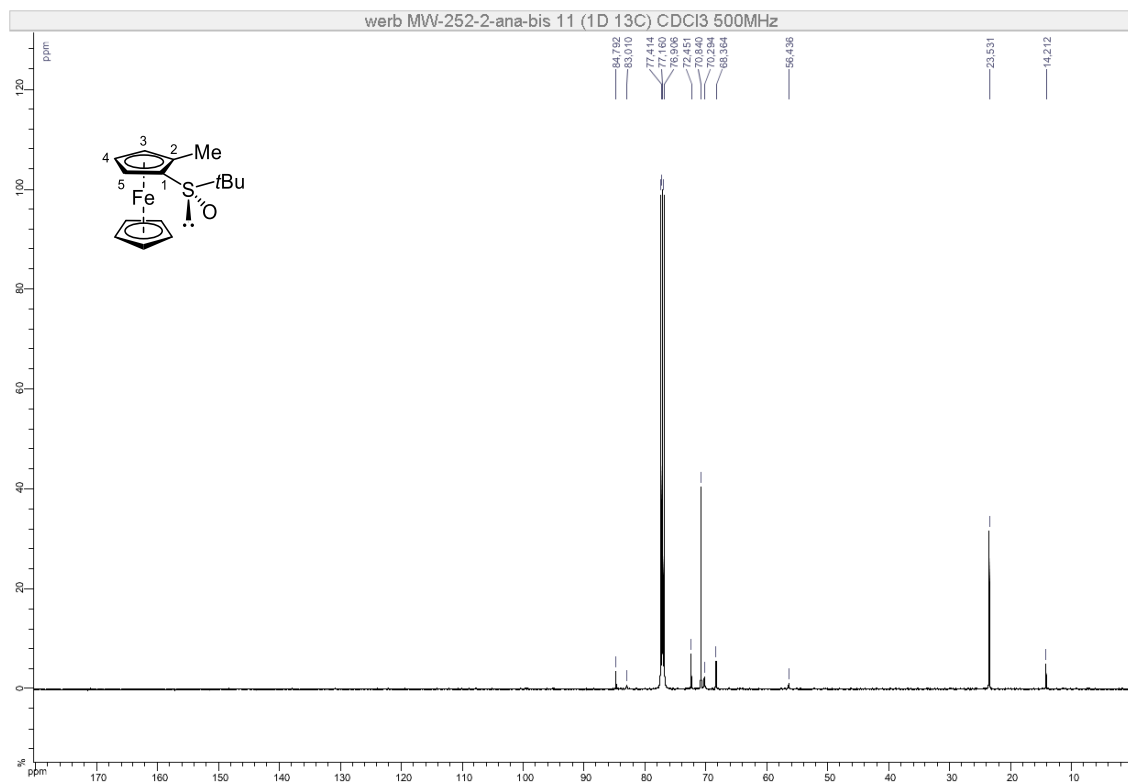


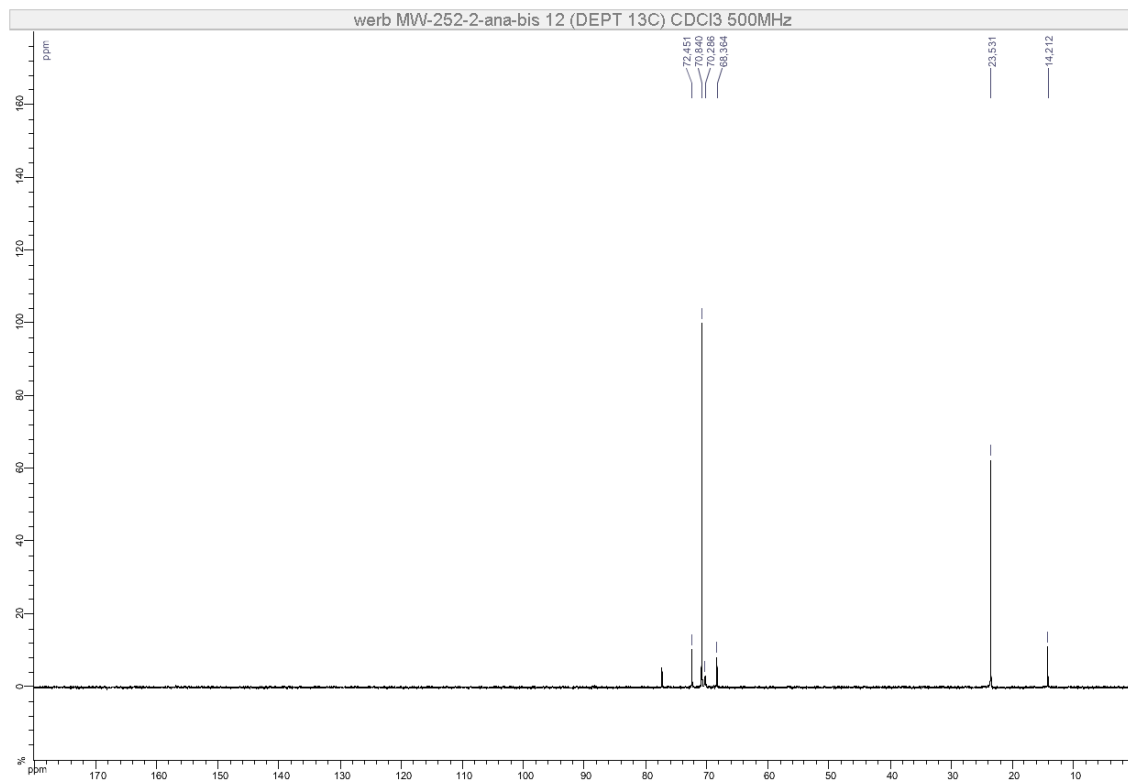
(*S,S*)-*S*-tert-Butyl-2-methylferrocenesulfoxide (*S,S*-1d)

^1H NMR (500 MHz, CDCl_3)

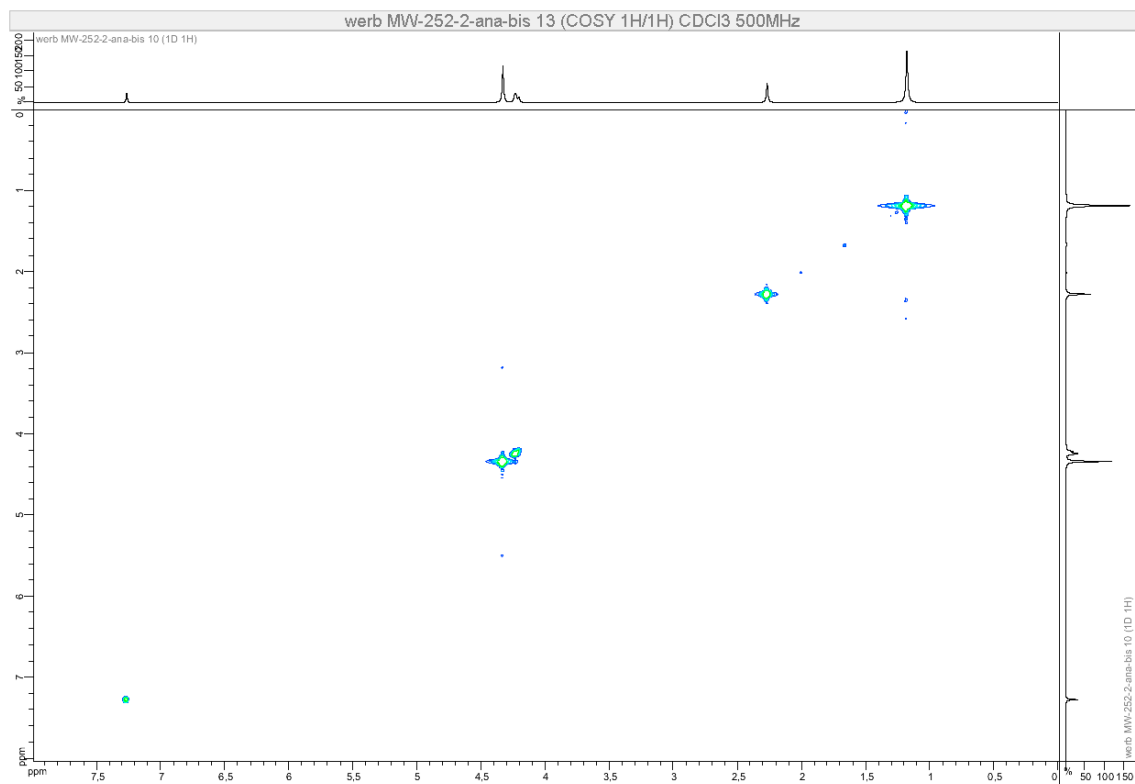


^{13}C NMR (126 MHz, CDCl_3)

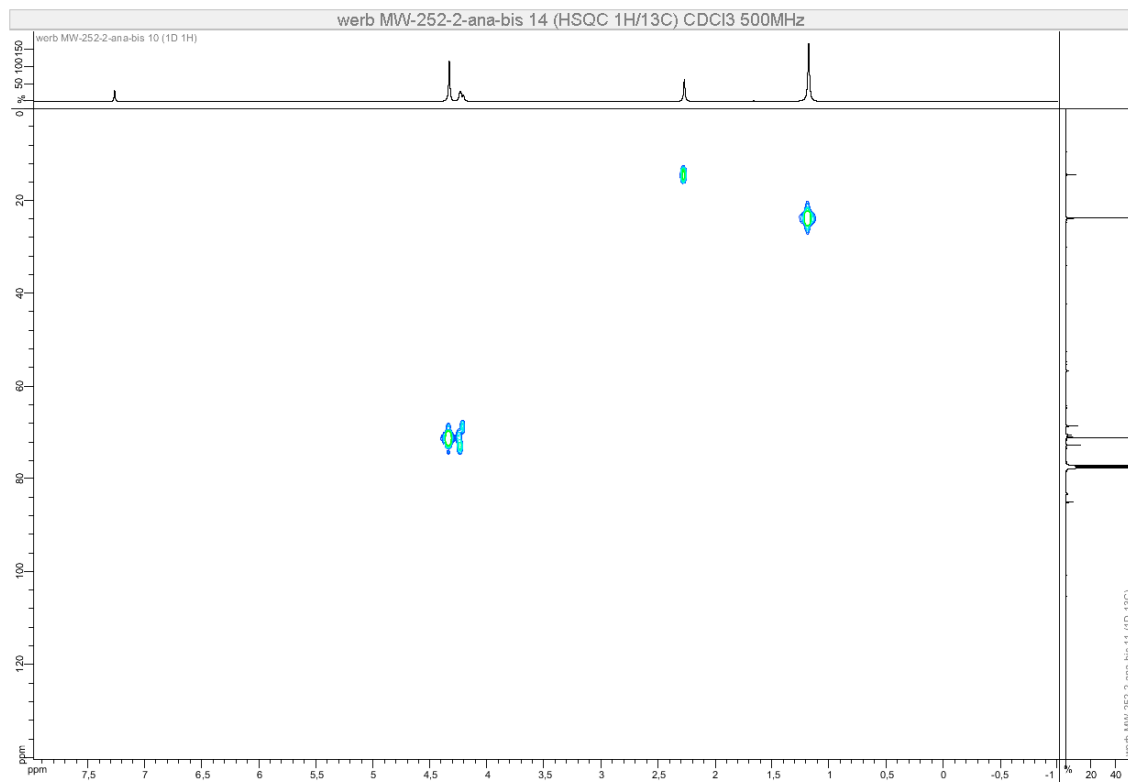


DEPT 135 (126 MHz, CDCl₃)

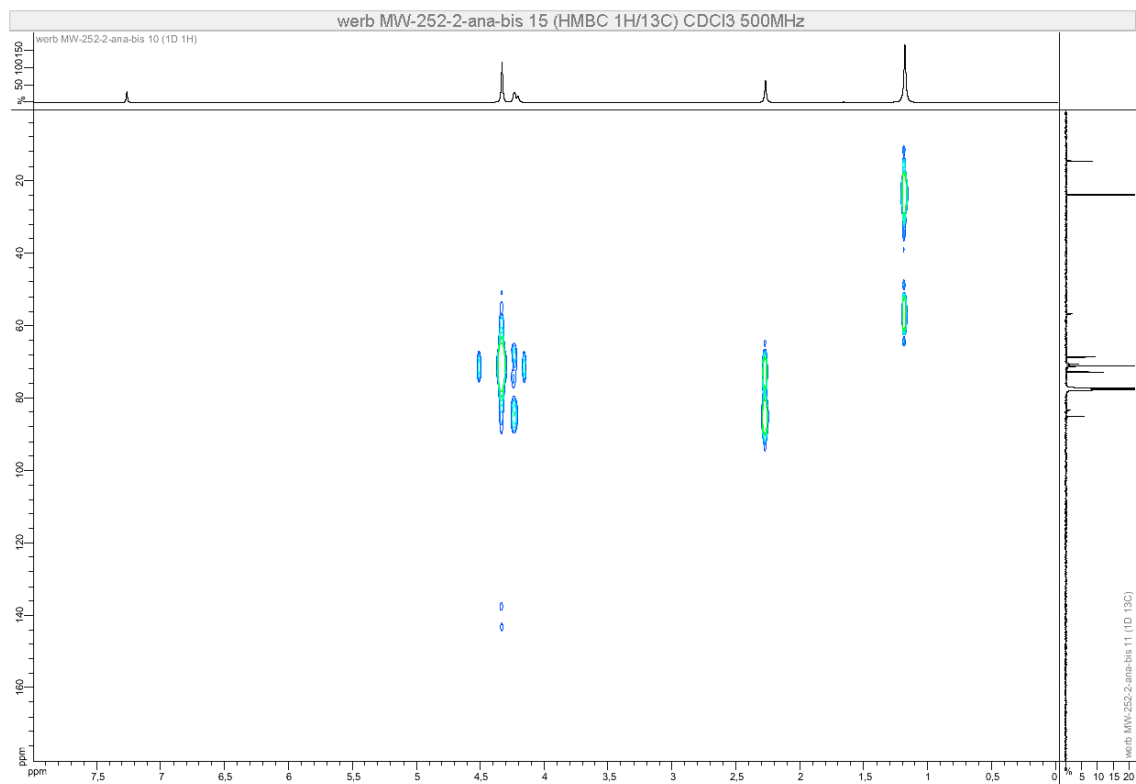
COSY (500 MHz, CDCl₃)



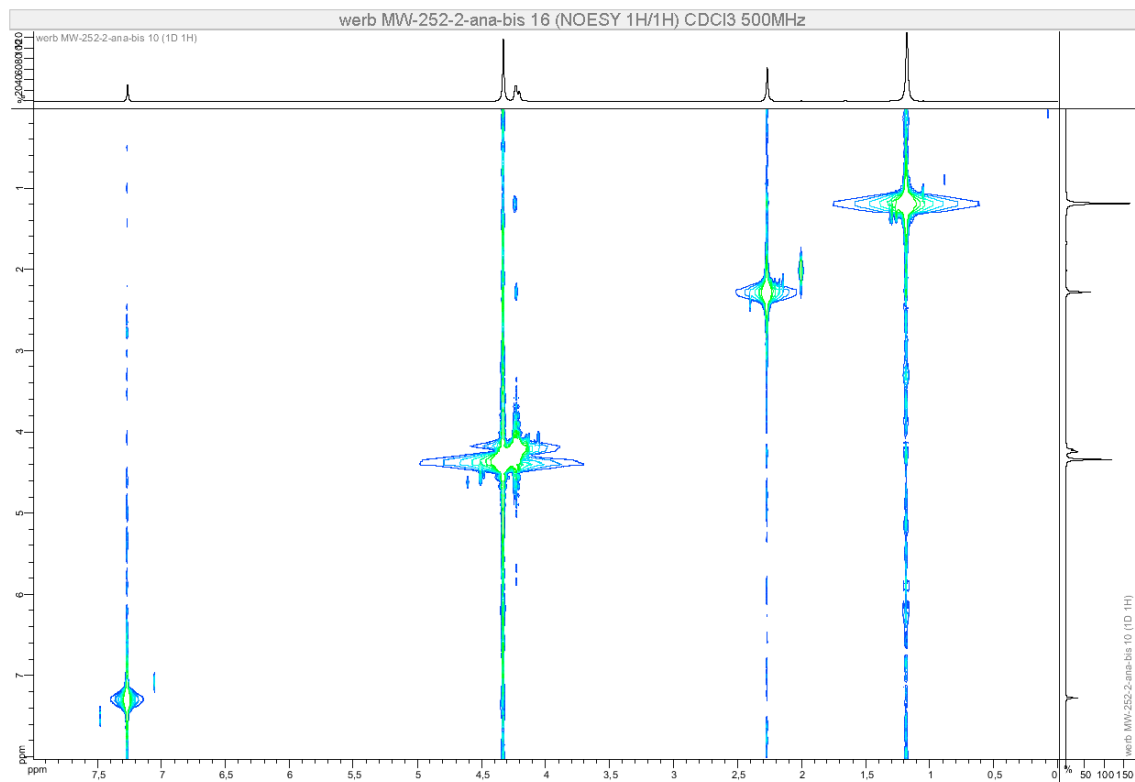
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

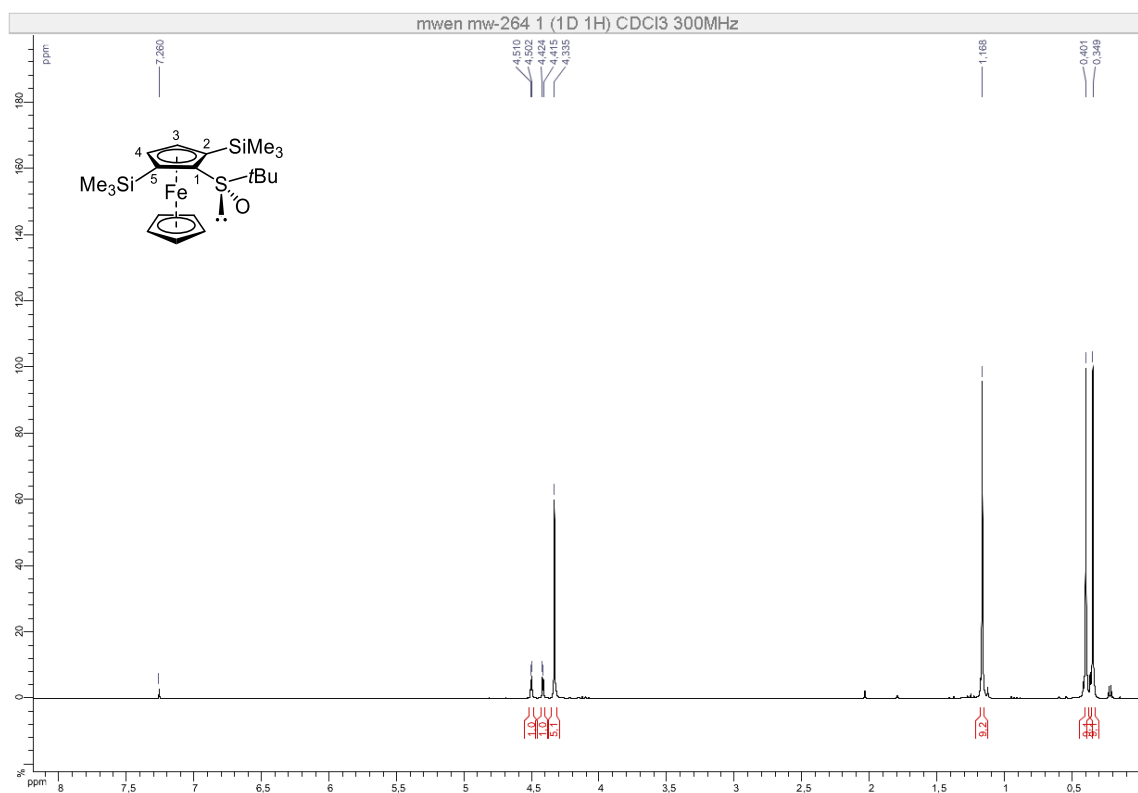


NOESY (500 MHz, CDCl₃)



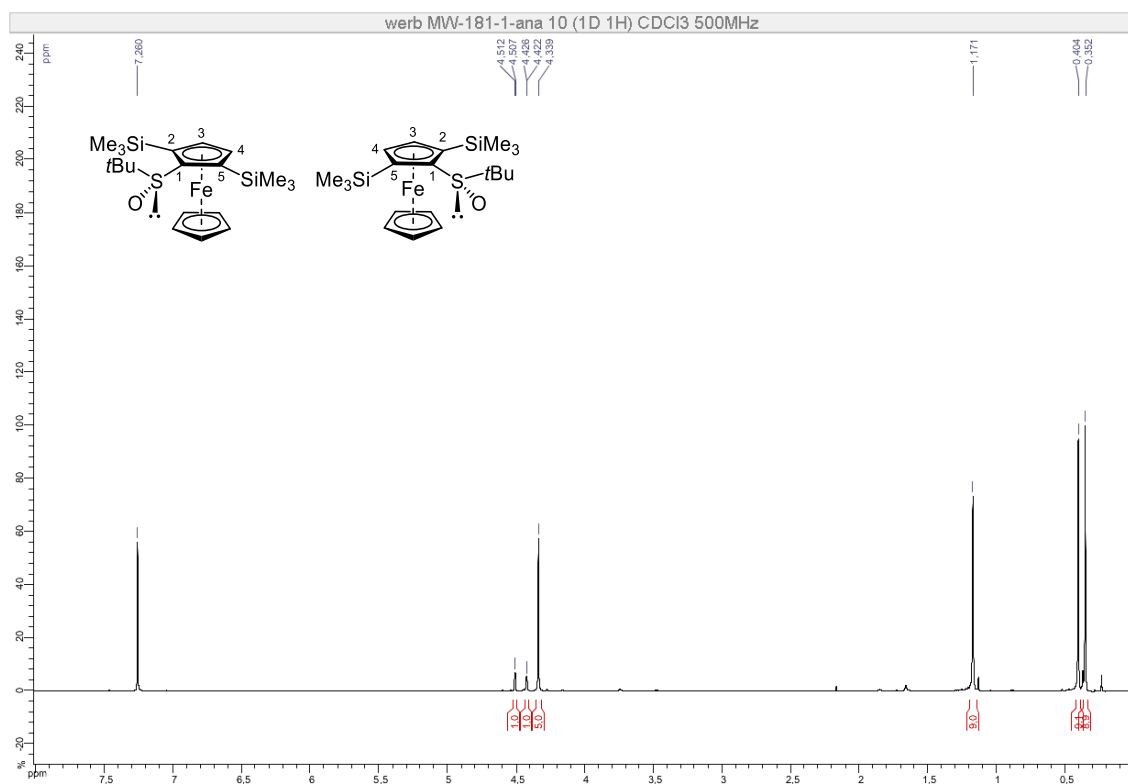
(*S*)-*S*-tert-Butyl-2,5-bis(trimethylsilyl)ferrocenesulfoxide (*S*-2aa)

^1H NMR (300 MHz, CDCl_3)

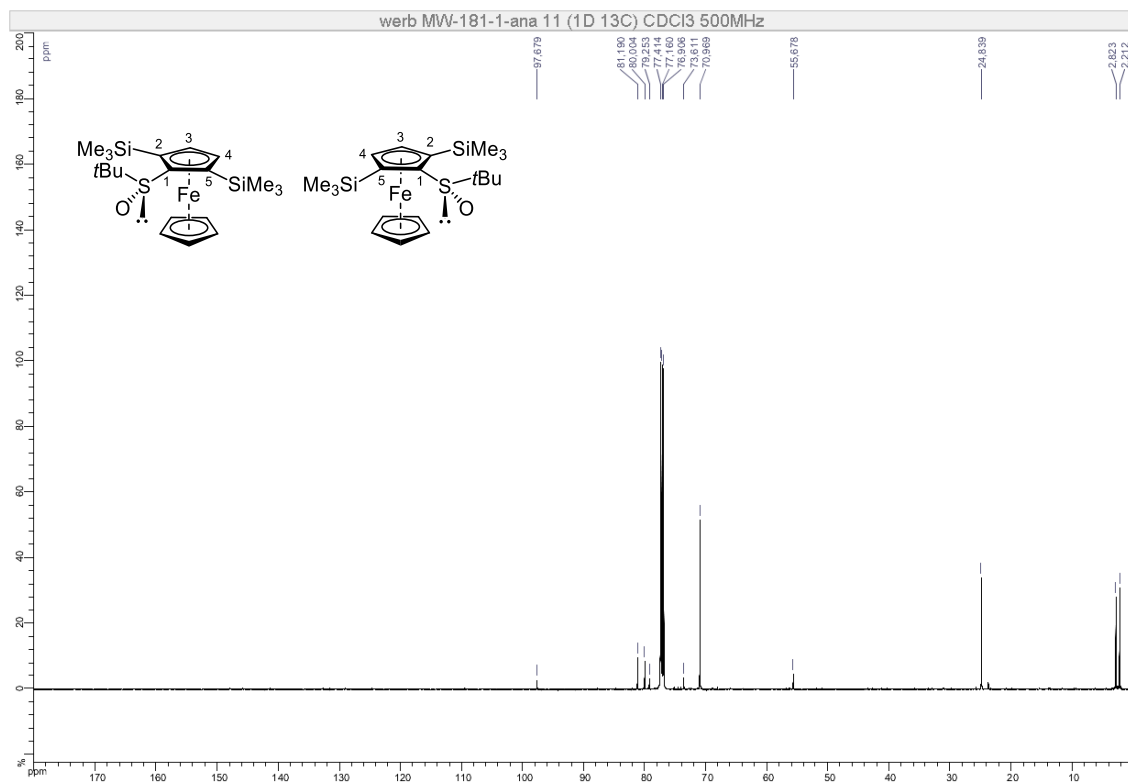


(R)- and (S)-*tert*-Butyl-2,5-bis(trimethylsilyl)ferrocenesulfoxide (*rac*-2aa)

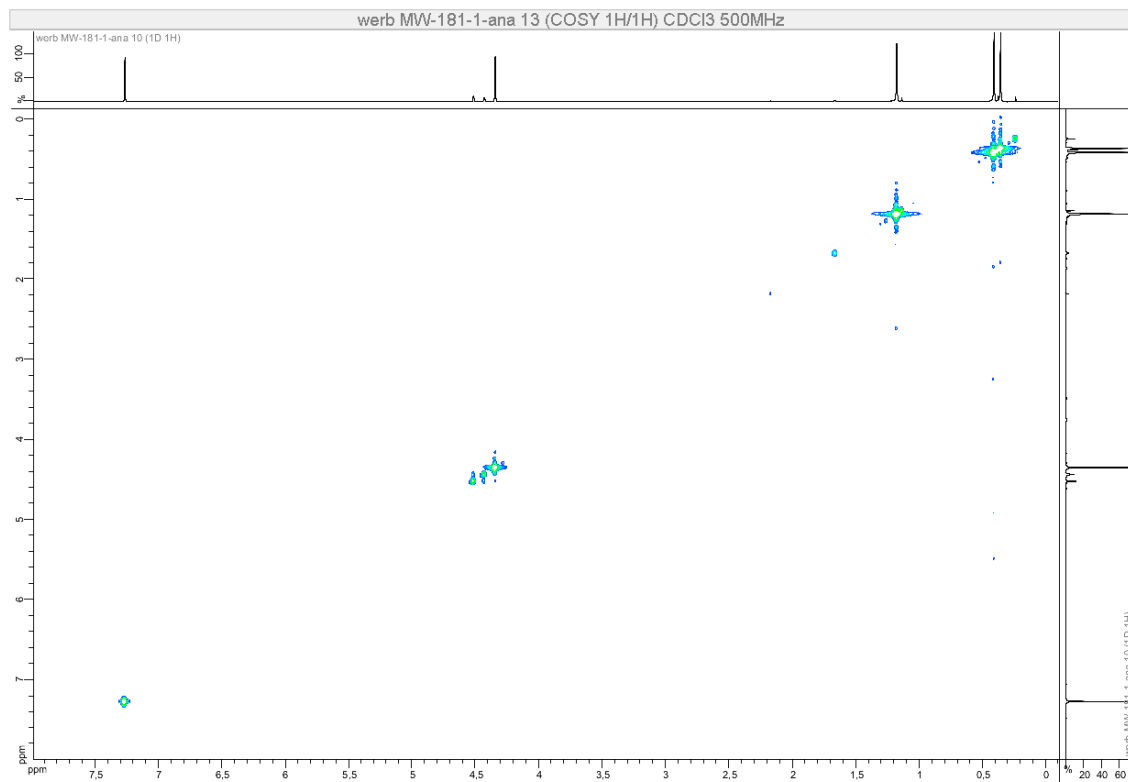
^1H NMR (500 MHz, CDCl_3)



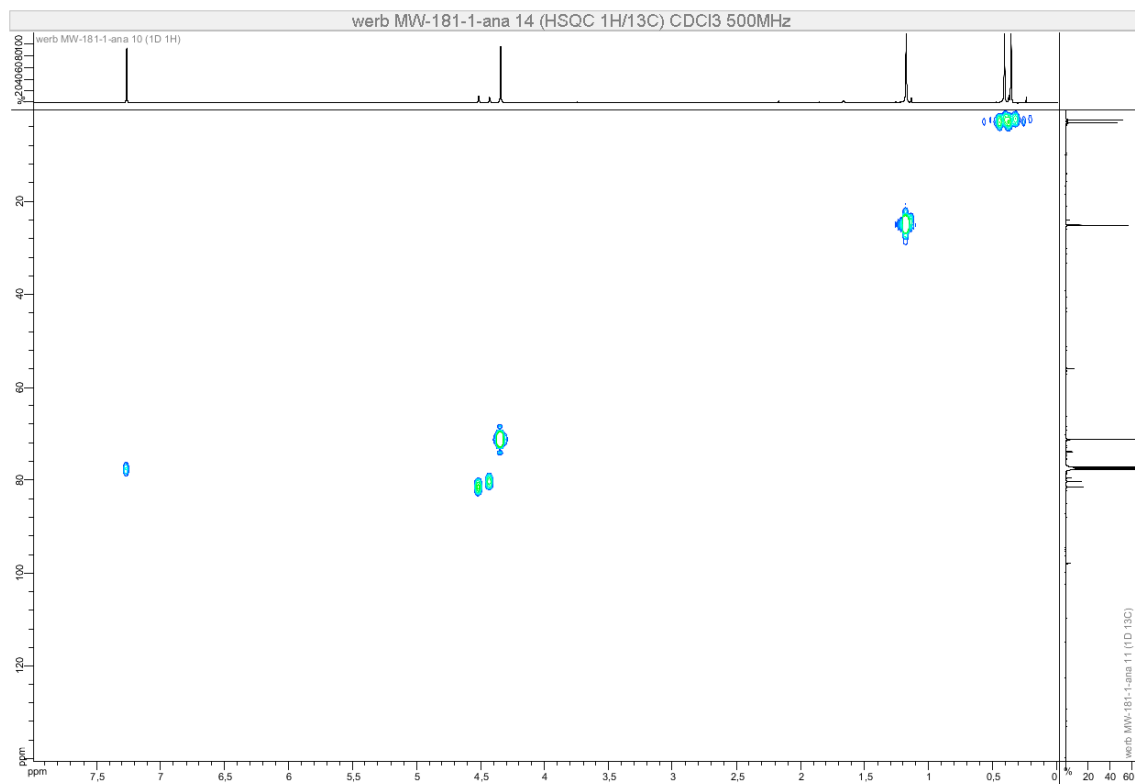
^{13}C NMR (126 MHz, CDCl_3)



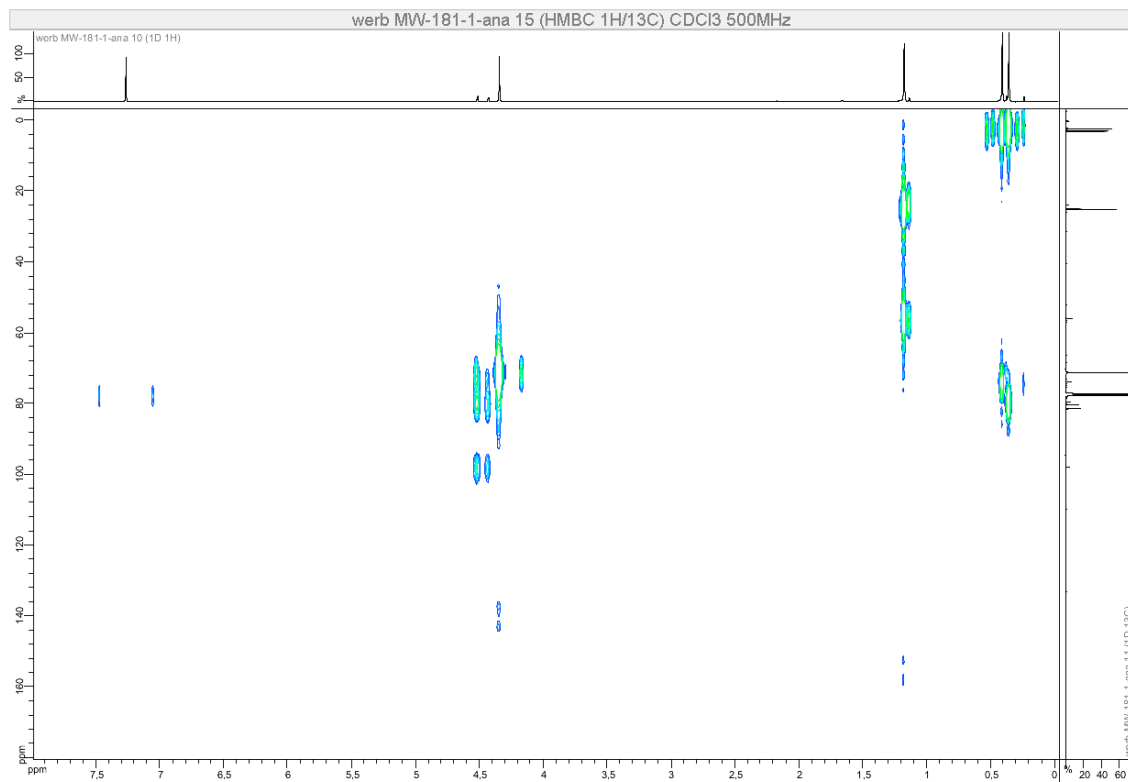
COSY (500 MHz, CDCl₃)



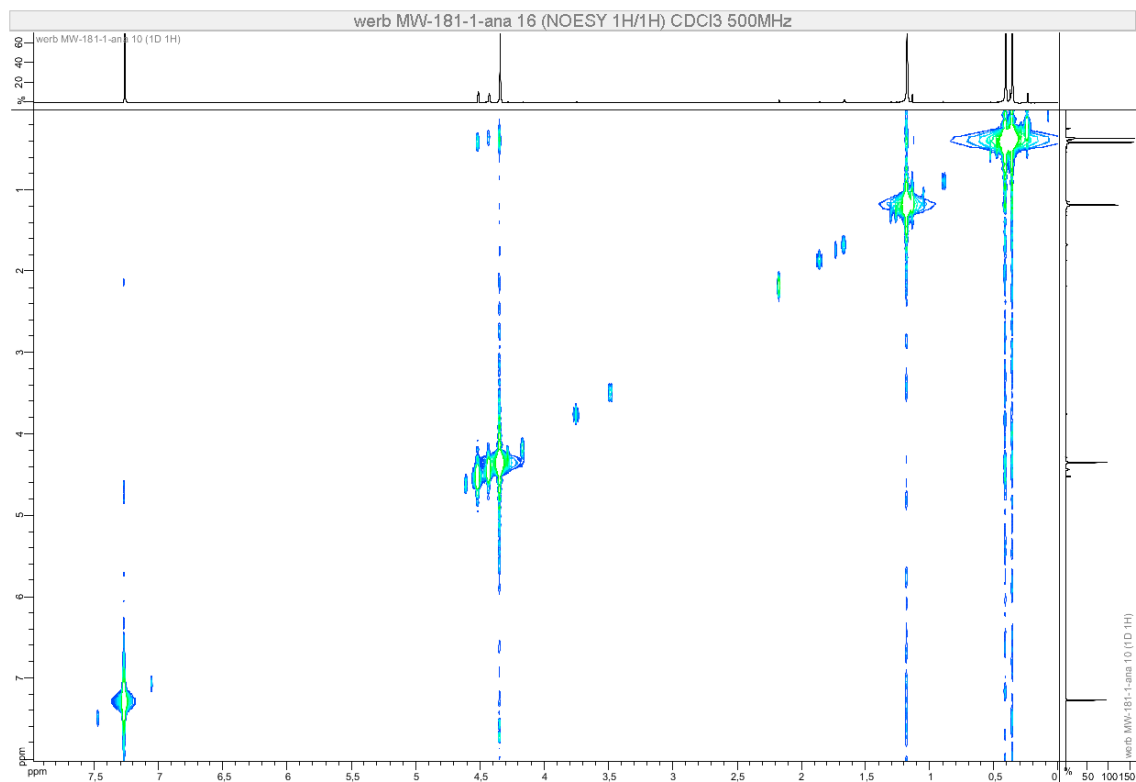
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

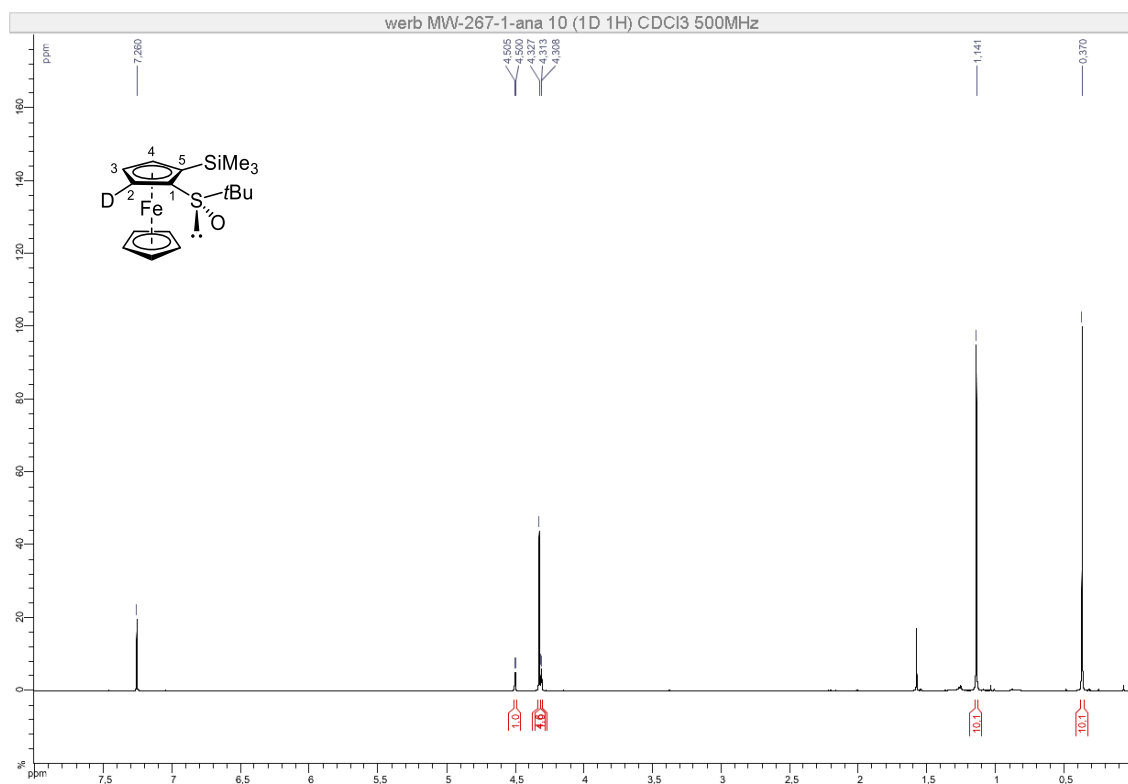


NOESY (500 MHz, CDCl₃)

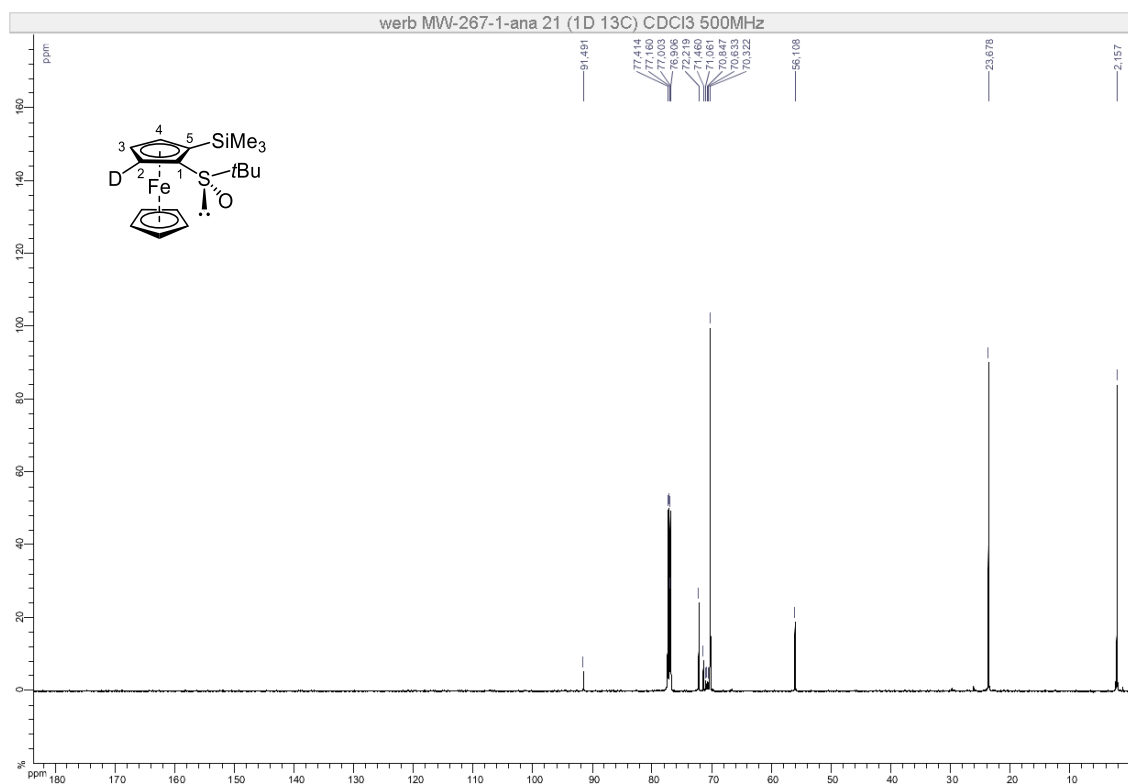


(*S,S*)-*S*-tert-Butyl-2-deuterio-5-(trimethylsilyl)ferrocenesulfoxide (*S,S*-2ac)

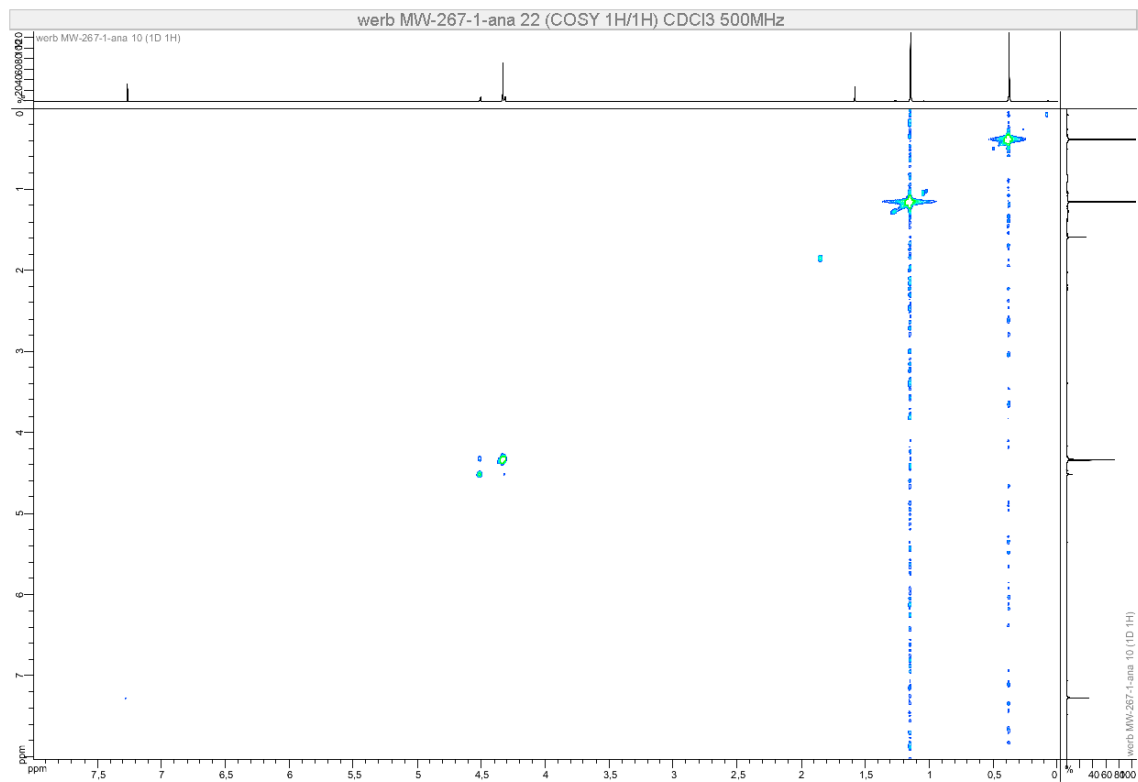
^1H NMR (500 MHz, CDCl_3)



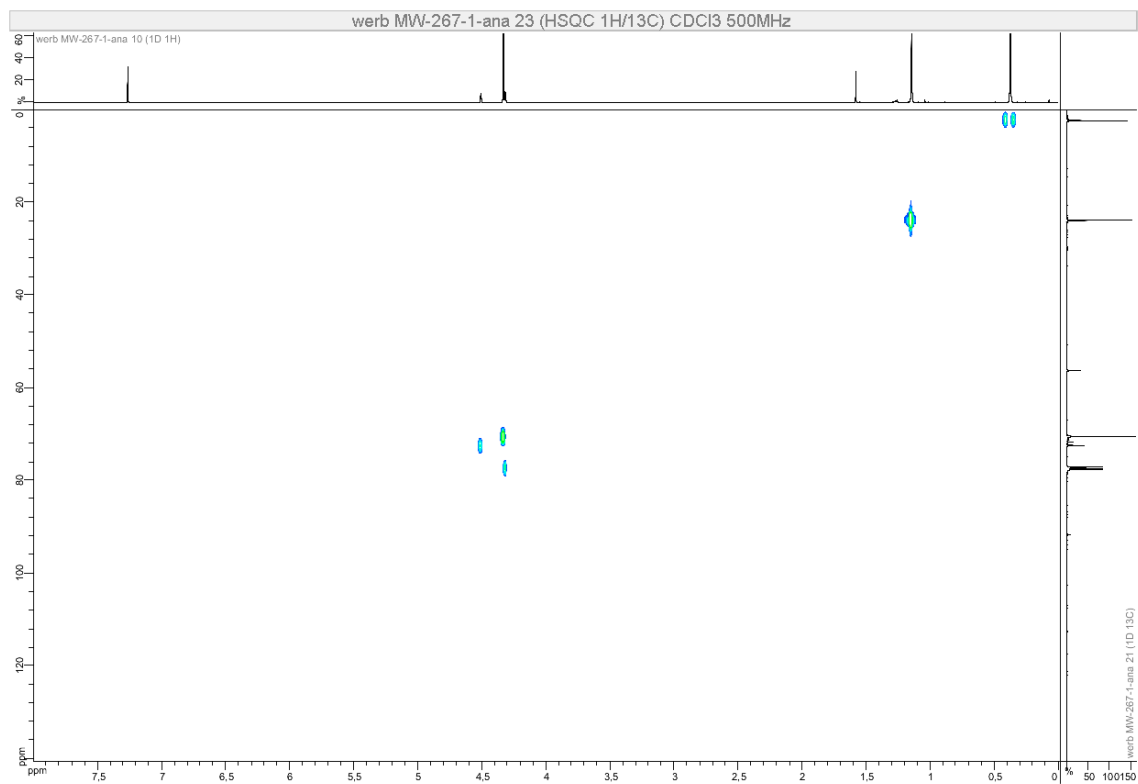
^{13}C NMR (126 MHz, CDCl_3)



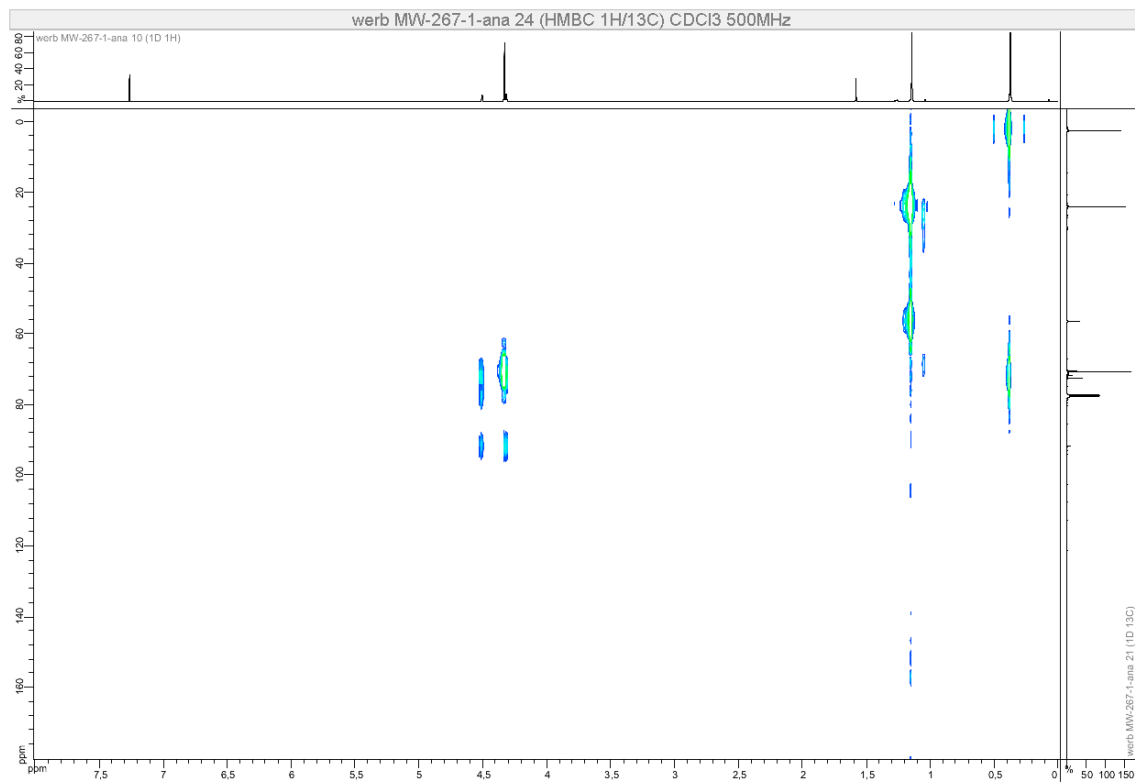
COSY (500 MHz, CDCl₃)



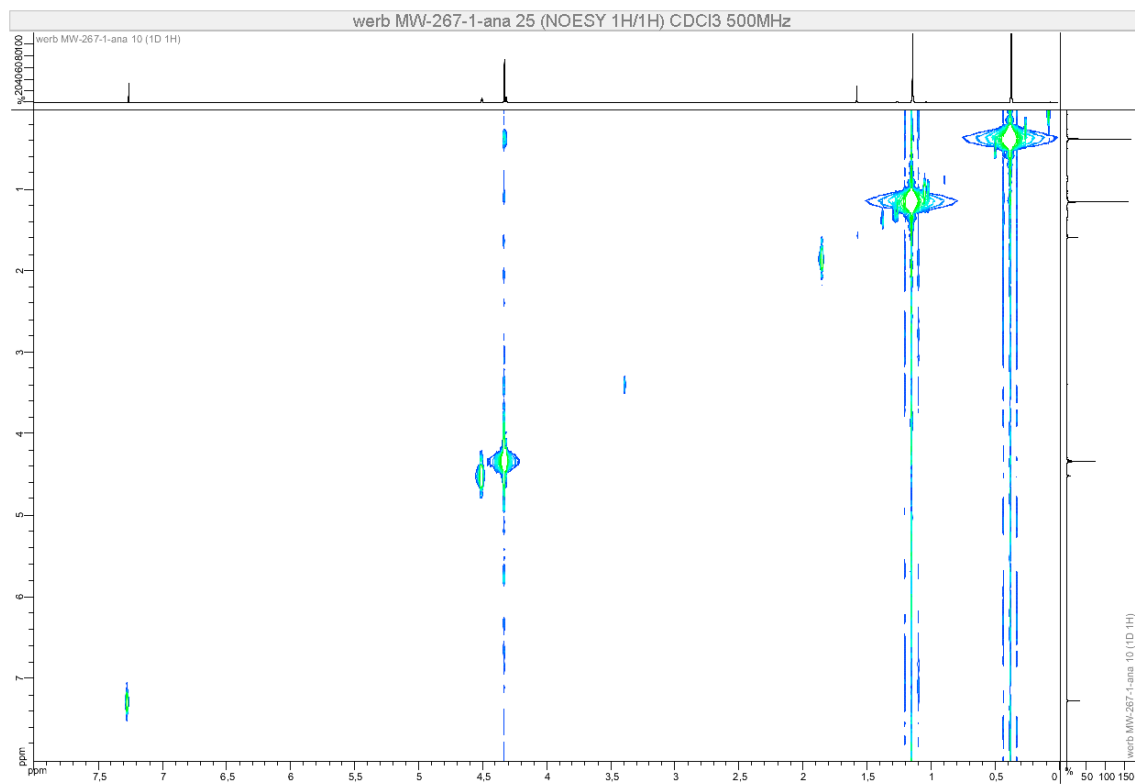
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

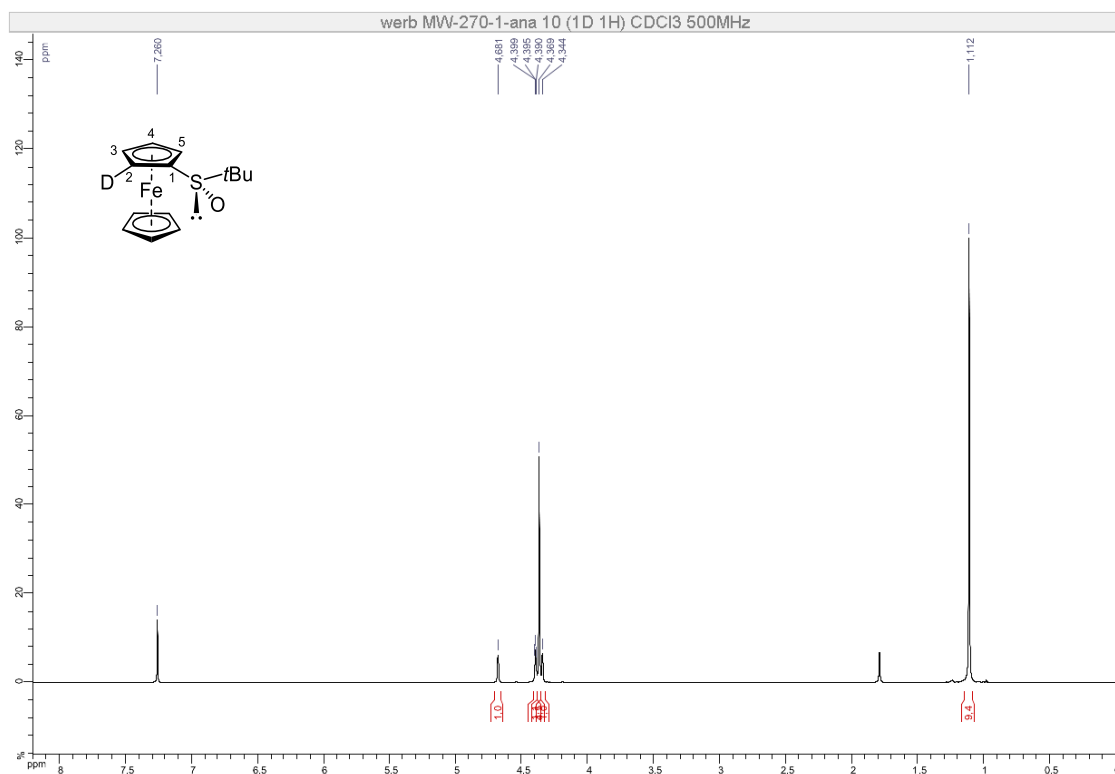


NOESY (500 MHz, CDCl₃)

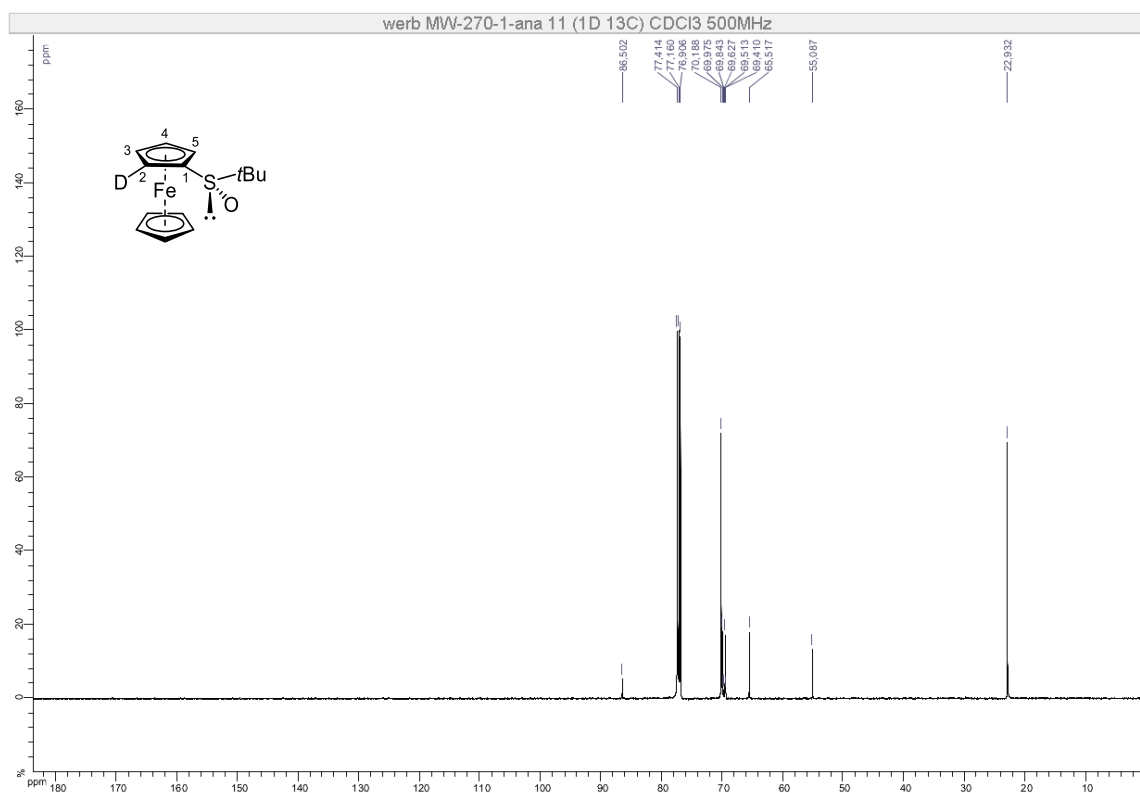


(*S,R_P*)-*S*-tert-Butyl-2-deuterioferrocenesulfoxide (*S,R_P*-1c)

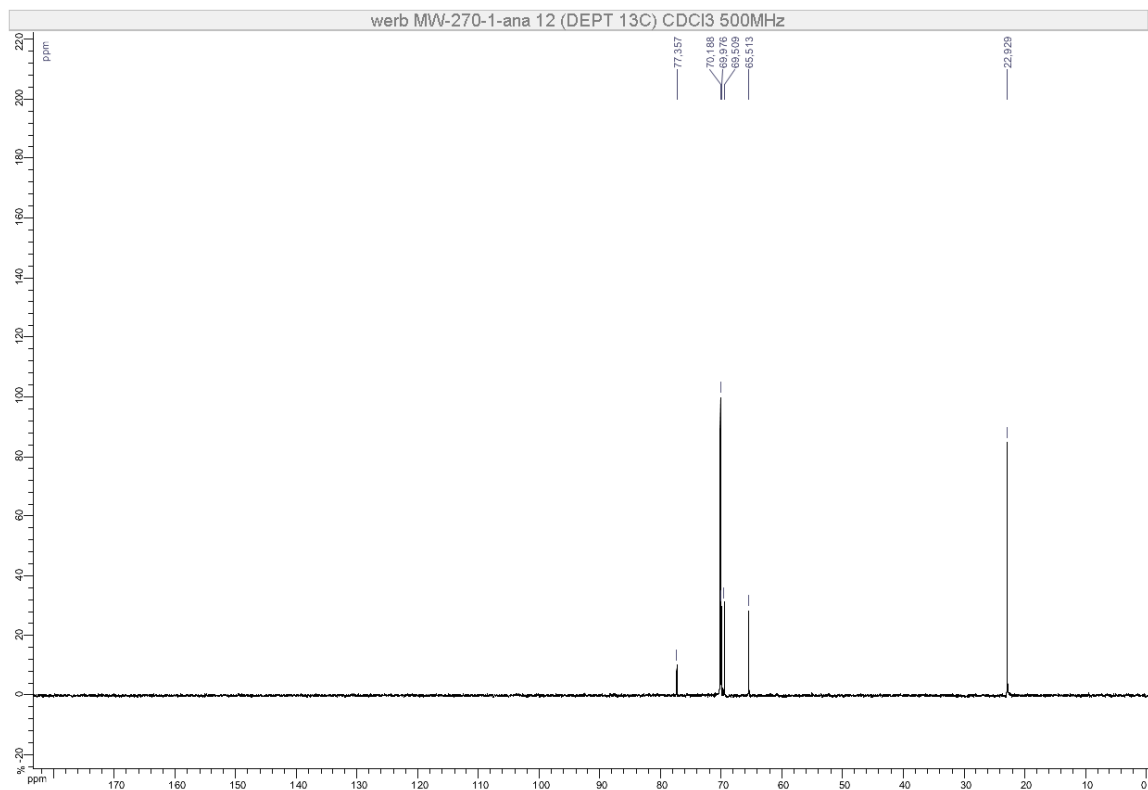
^1H NMR (500 MHz, CDCl_3)



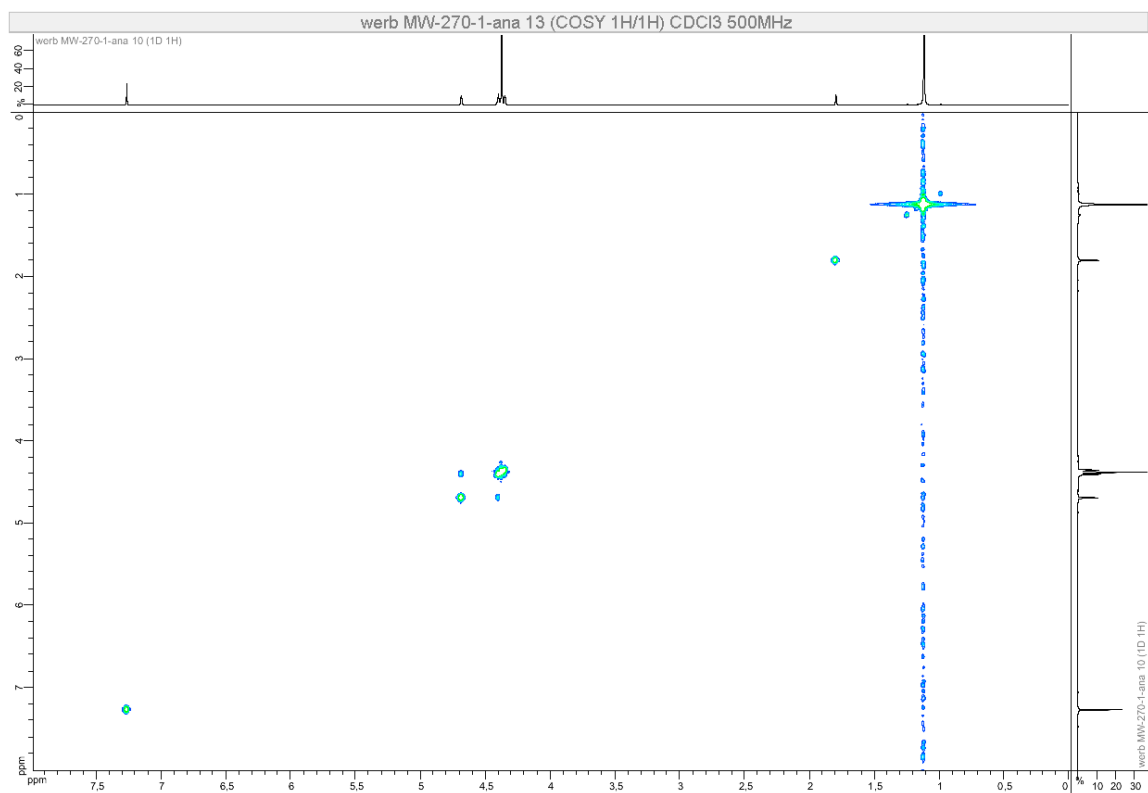
^{13}C NMR (126 MHz, CDCl_3)



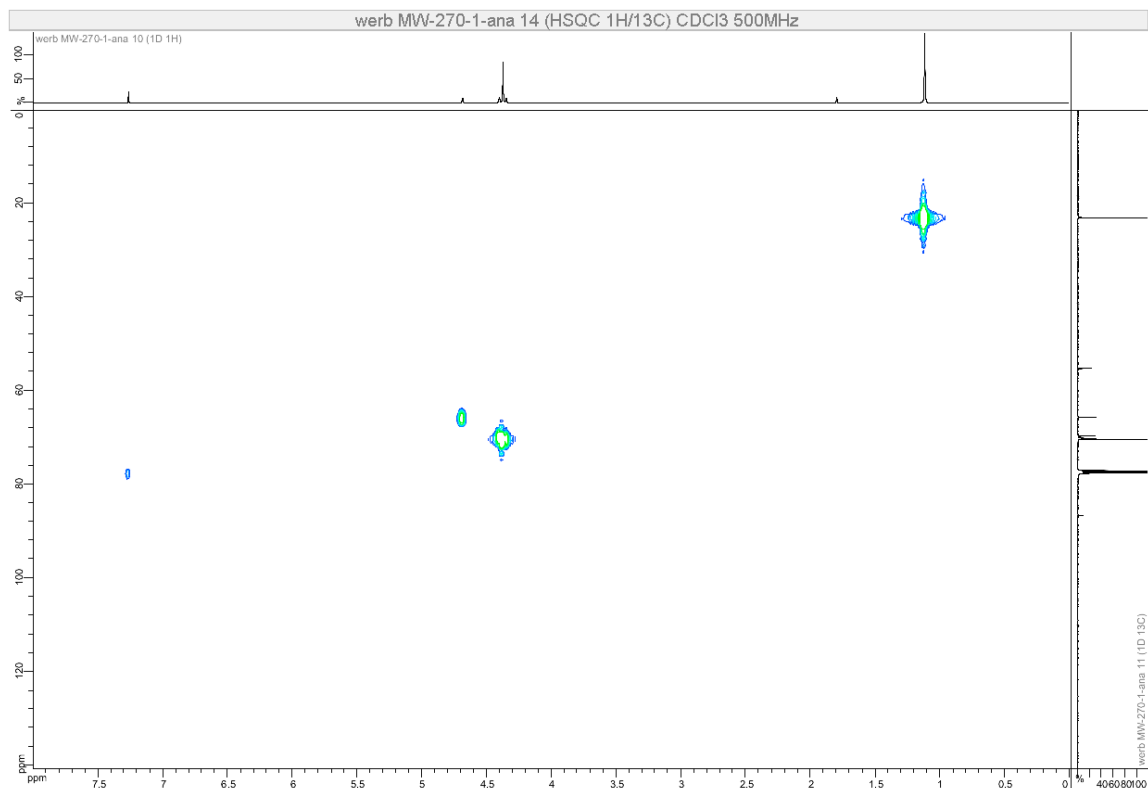
DEPT 135 (126 MHz, CDCl₃)



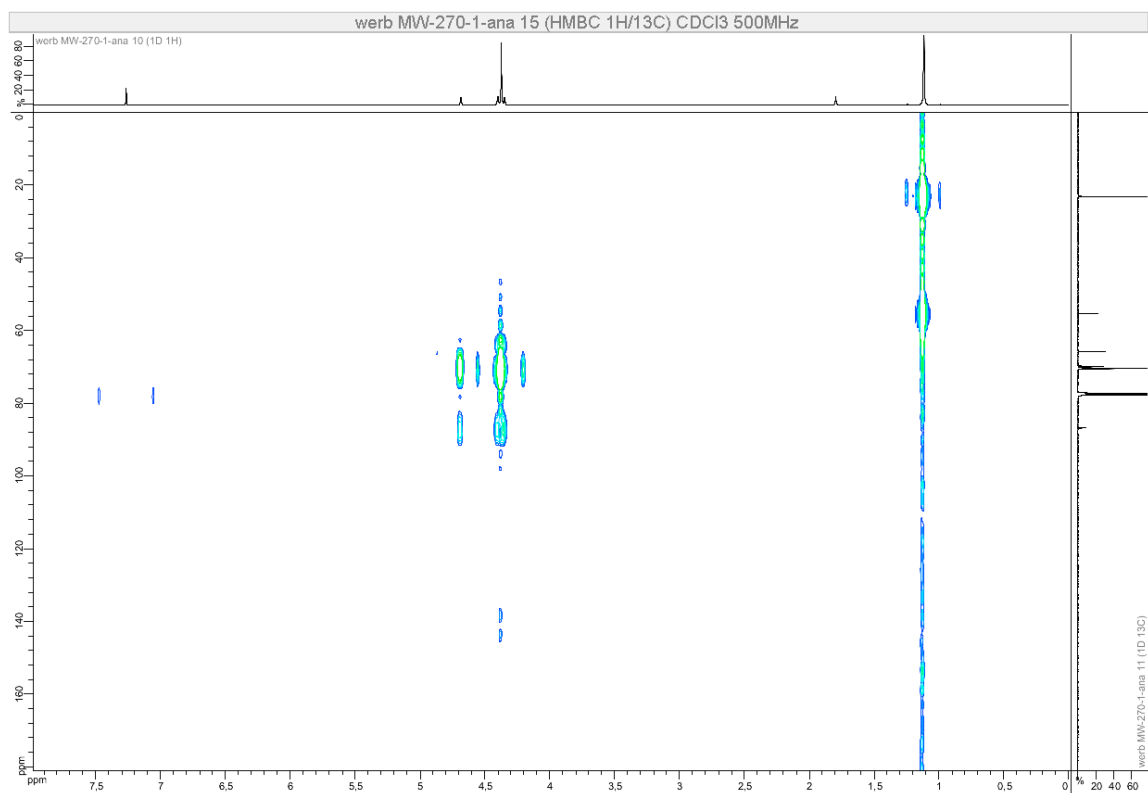
COSY (500 MHz, CDCl₃)



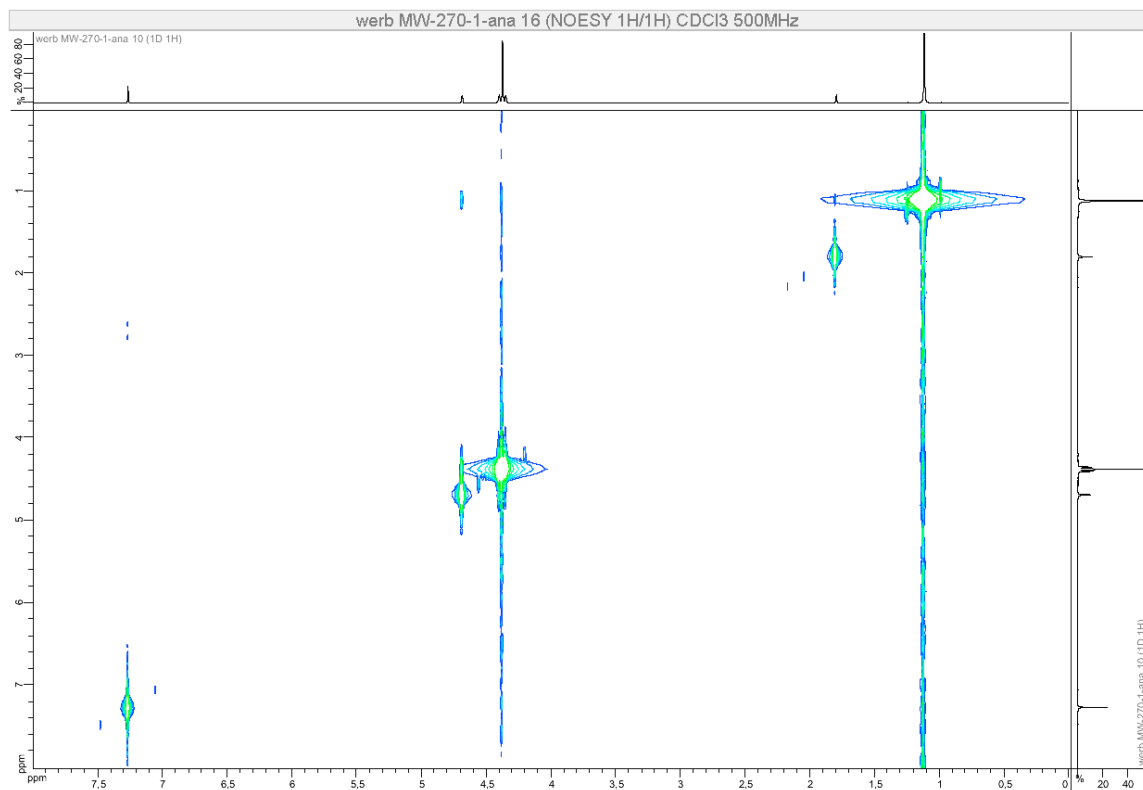
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

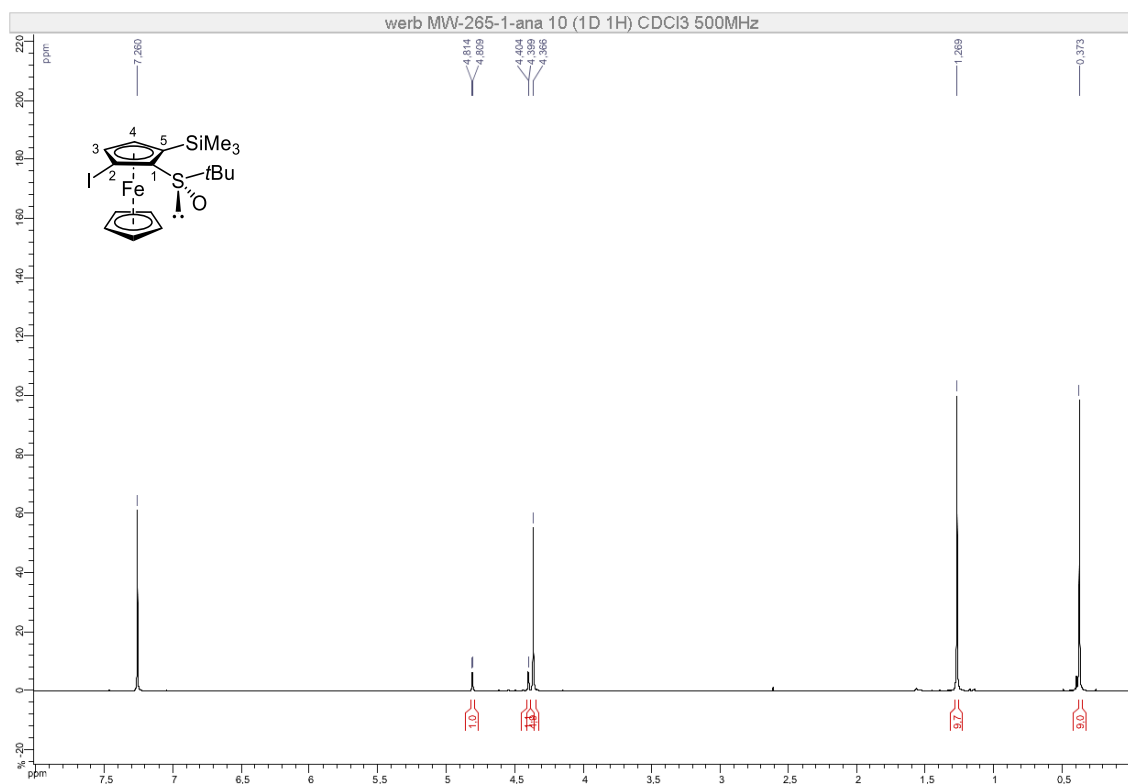


NOESY (500 MHz, CDCl₃)

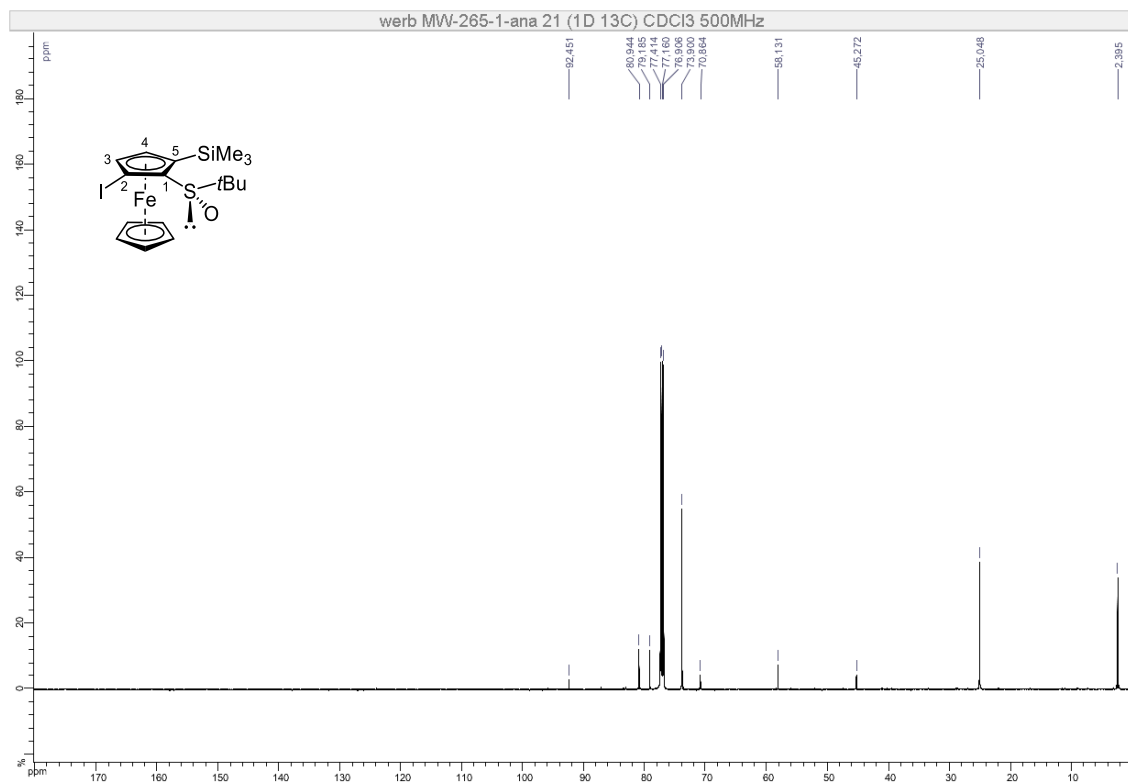


(*S,S*_P)-*S*-tert-Butyl-2-iodo-5-(trimethylsilyl)ferrocenesulfoxide (*S,S*_P-2ab)

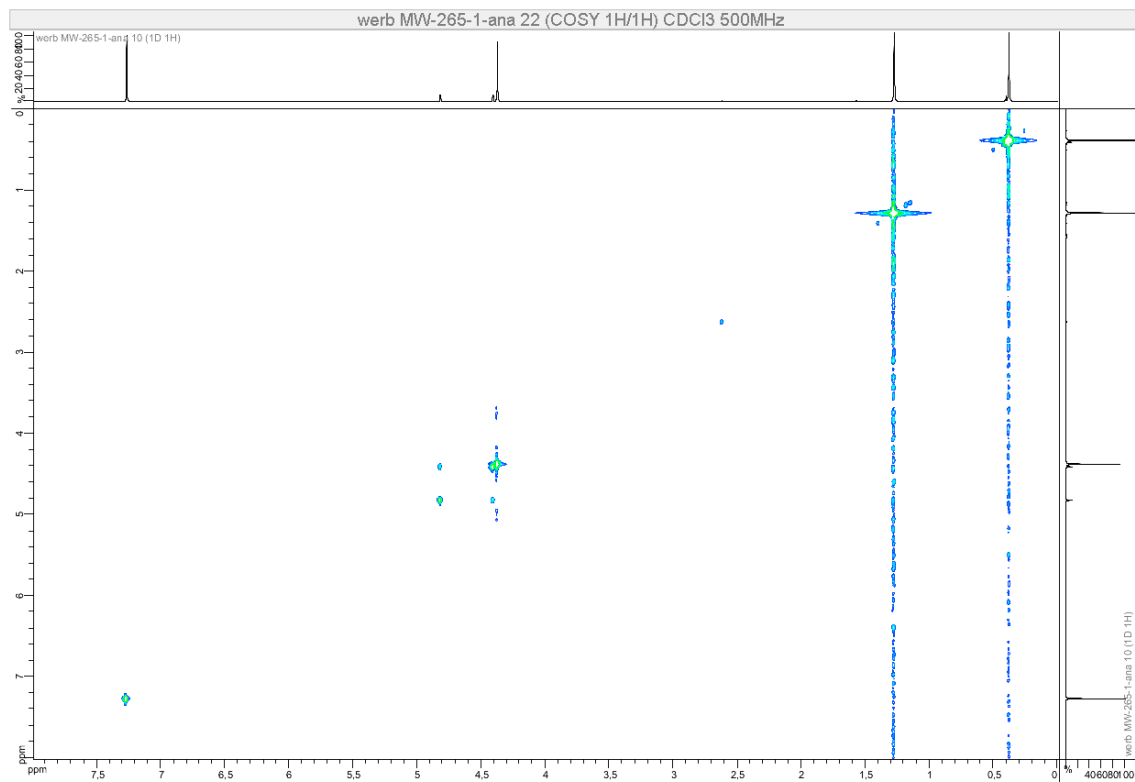
¹H NMR (500 MHz, CDCl₃)



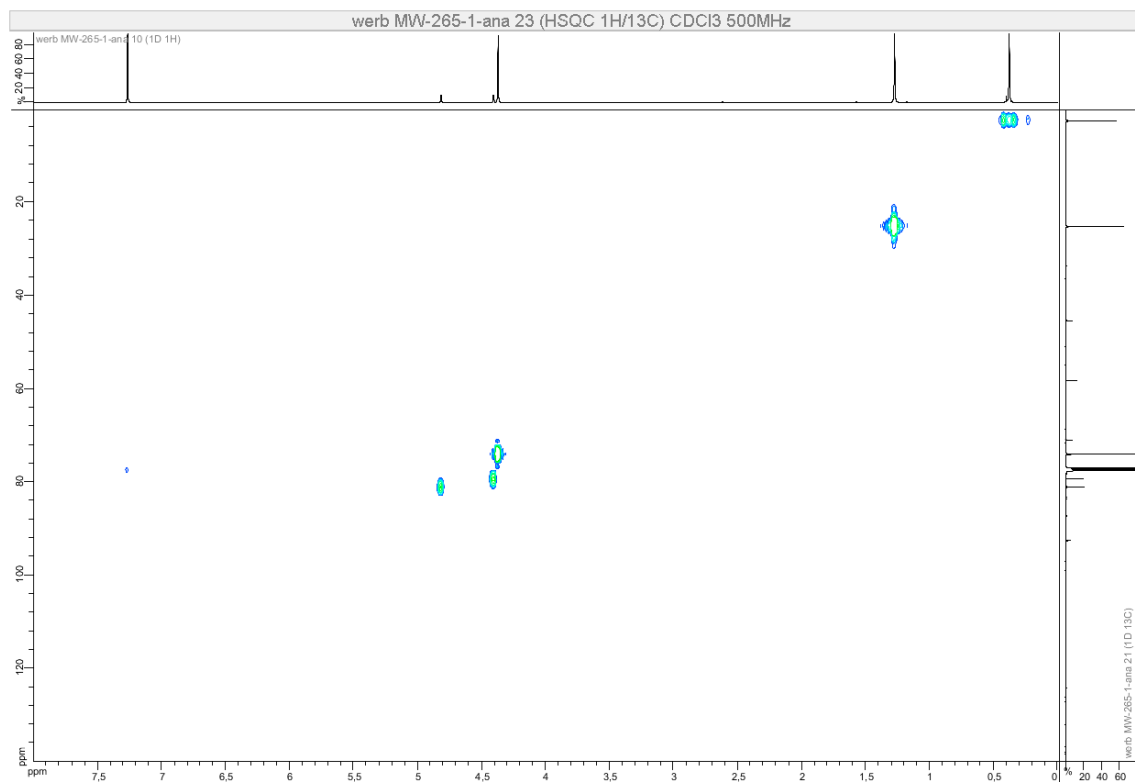
¹³C NMR (126 MHz, CDCl₃)



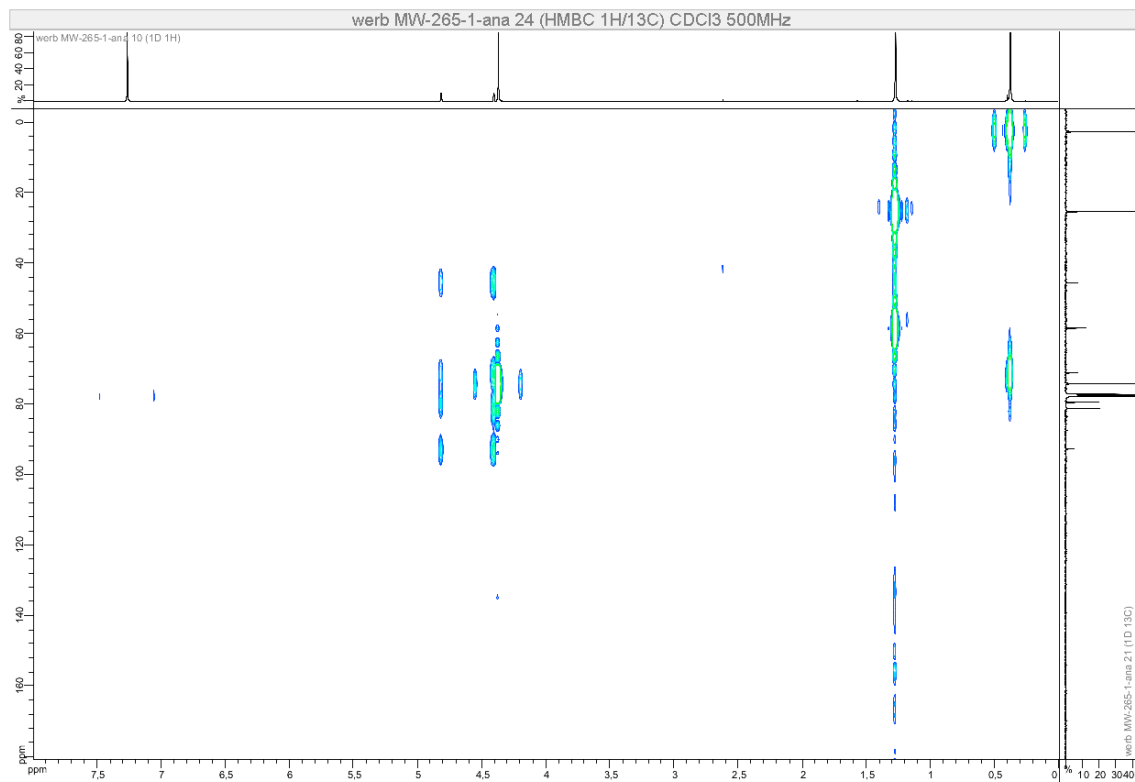
COSY (500 MHz, CDCl₃)



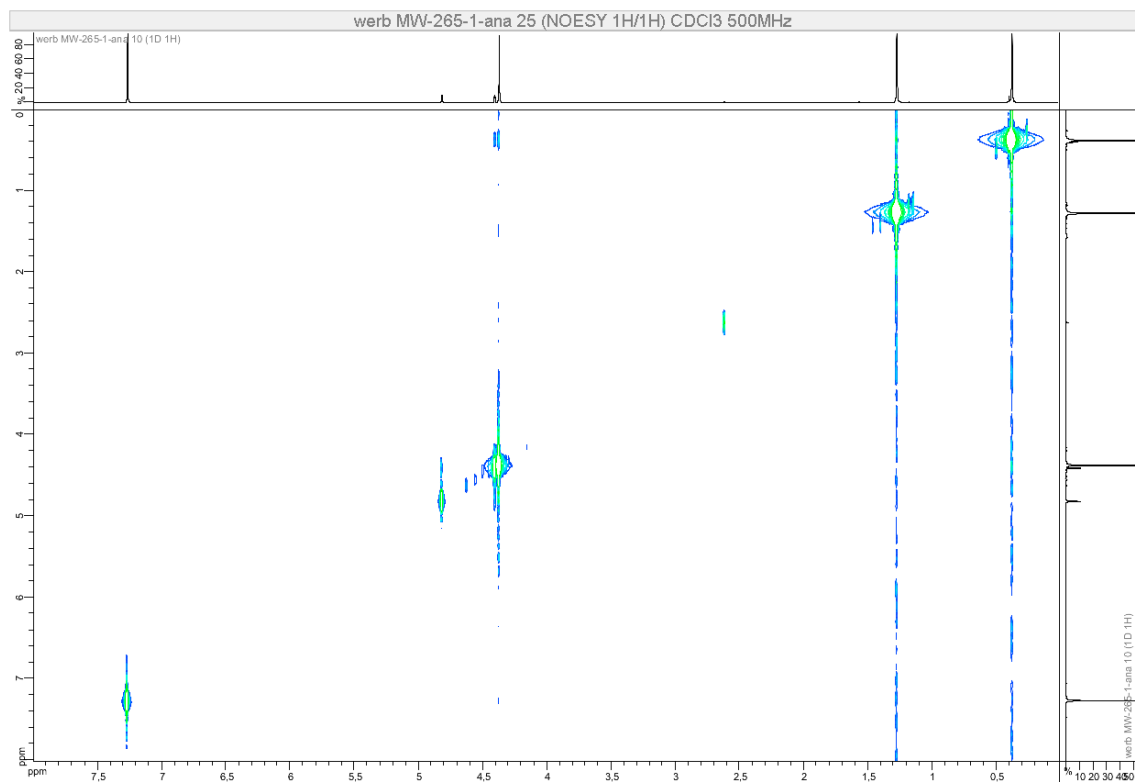
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

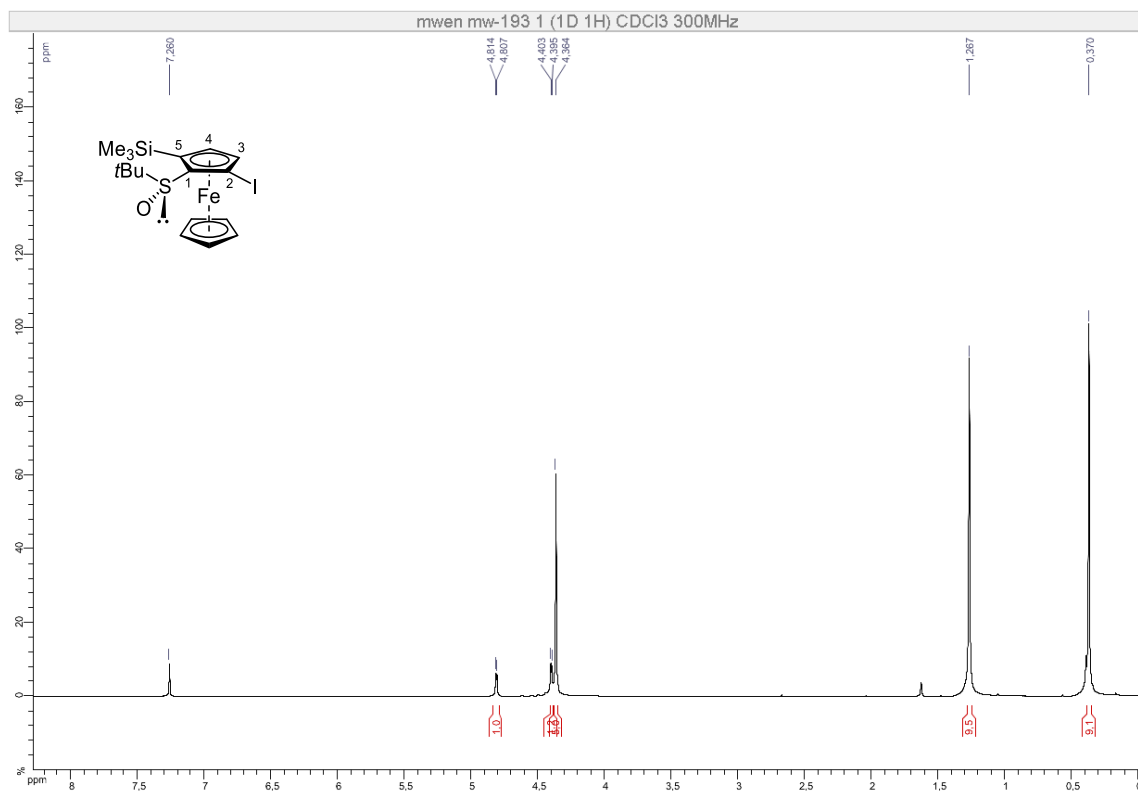


NOESY (500 MHz, CDCl₃)

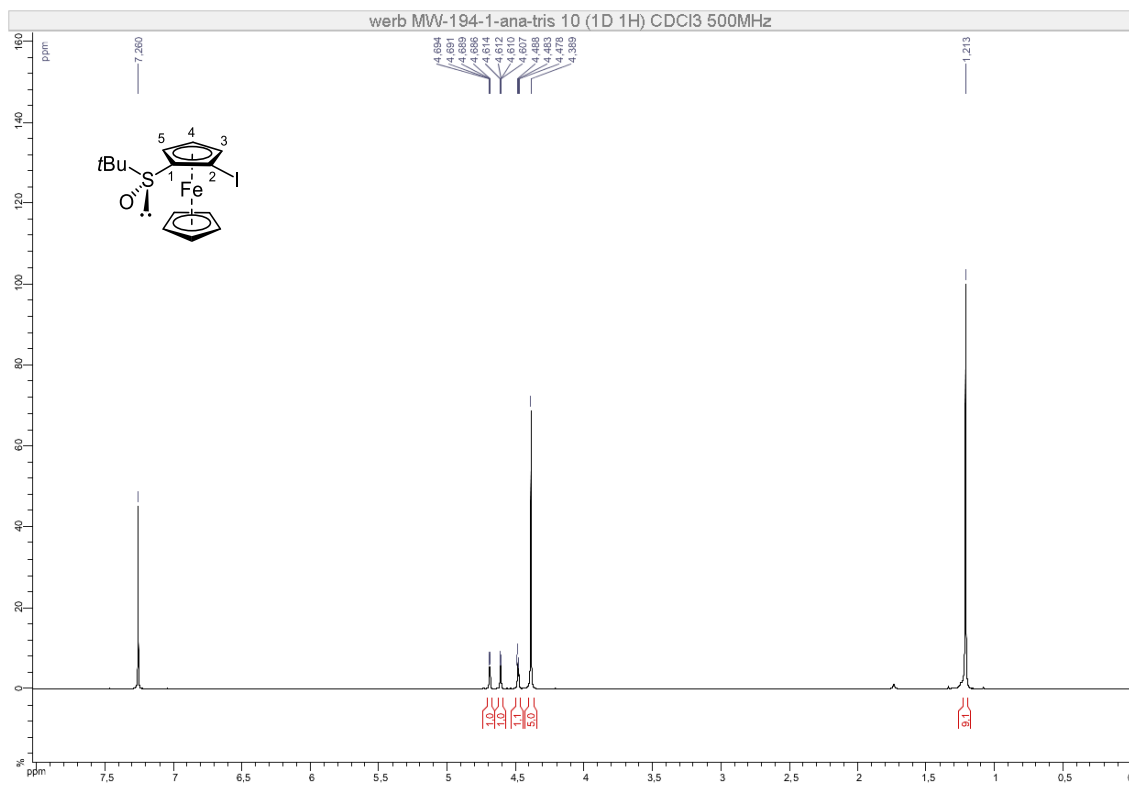
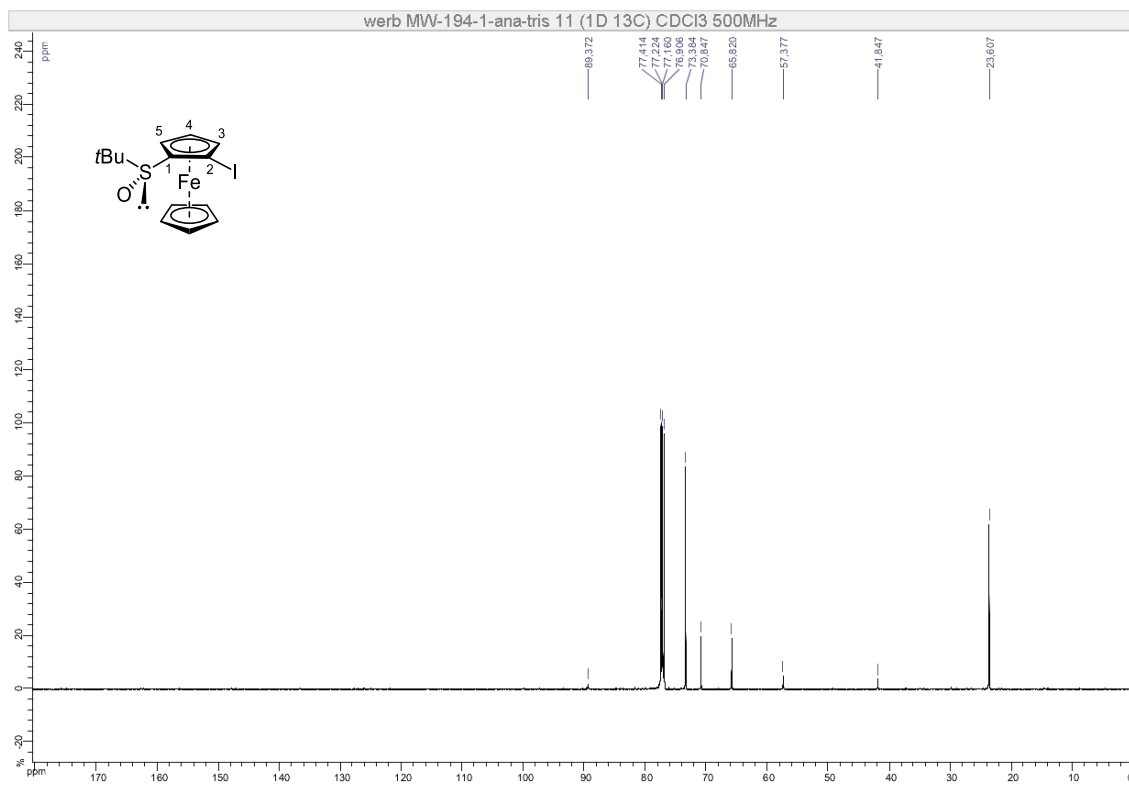


(*R,R*)-*S*-tert-Butyl-2-iodo-5-(trimethylsilyl)ferrocenesulfoxide (*R,R*-2ab)

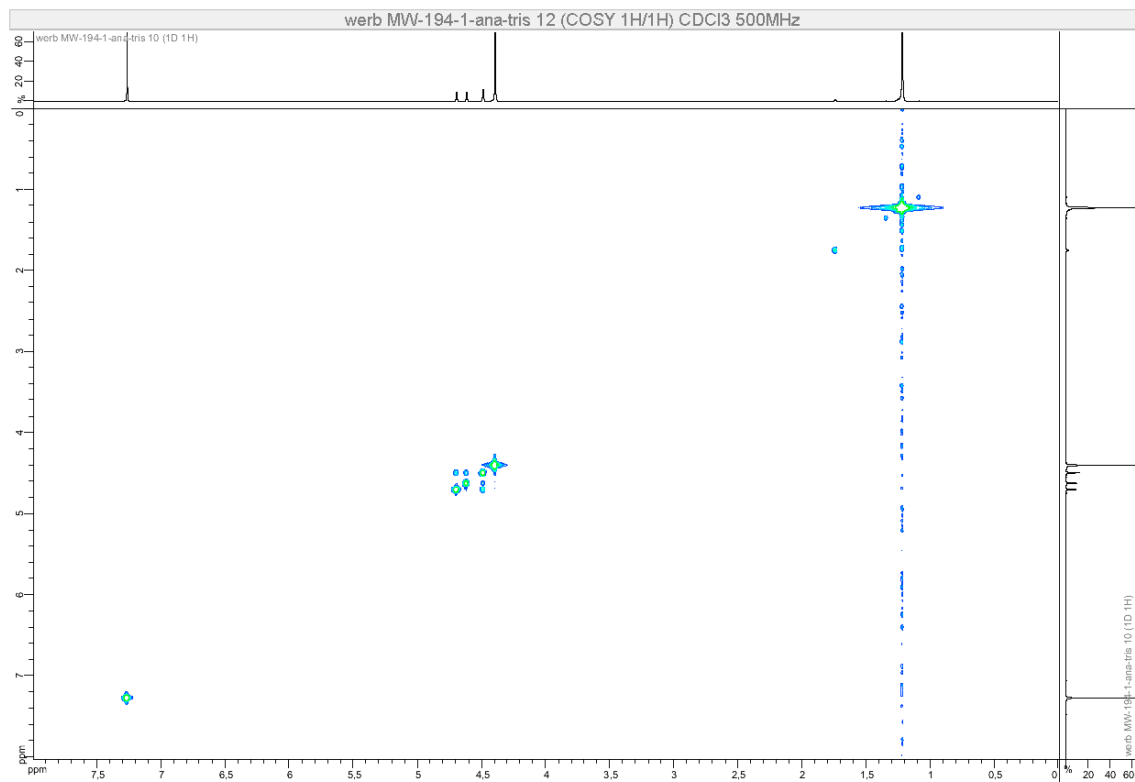
^1H NMR (500 MHz, CDCl_3)



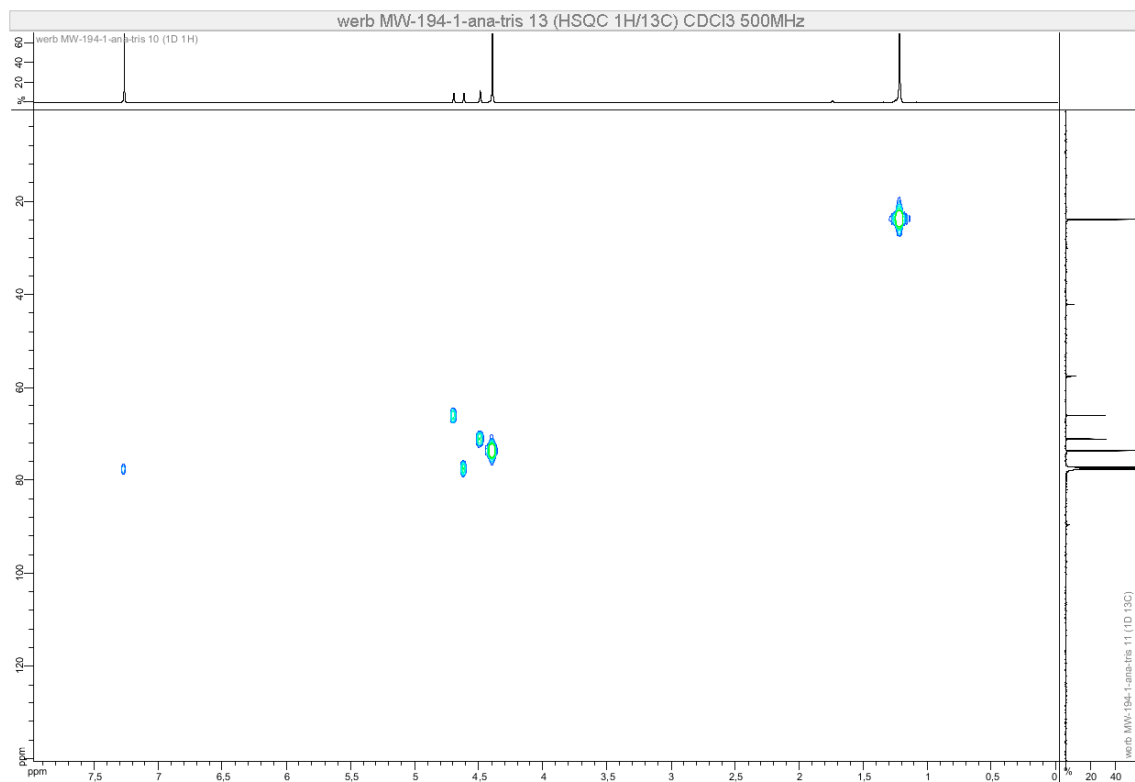
(*R,R*_P)-*S*-tert-Butyl-2-iodoferrocenesulfoxide (*R,R*_P-1b)

¹H NMR (500 MHz, CDCl₃) ^{13}C NMR (126 MHz, CDCl_3)

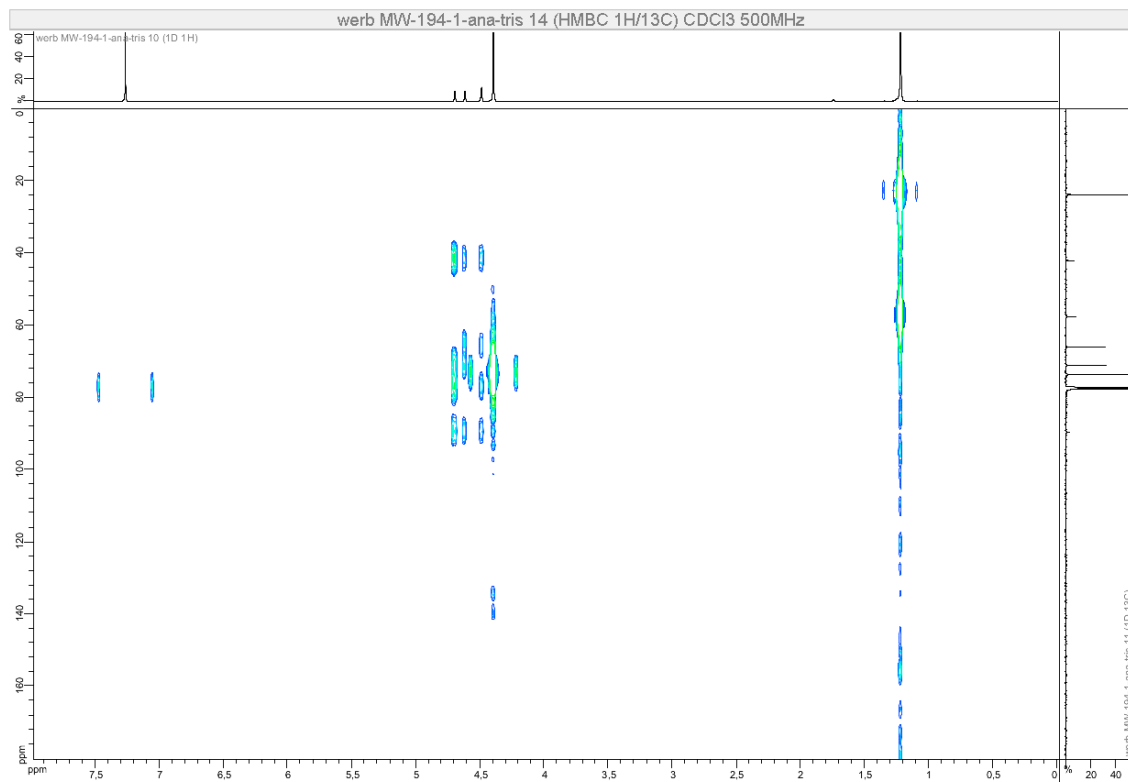
COSY (500 MHz, CDCl₃)



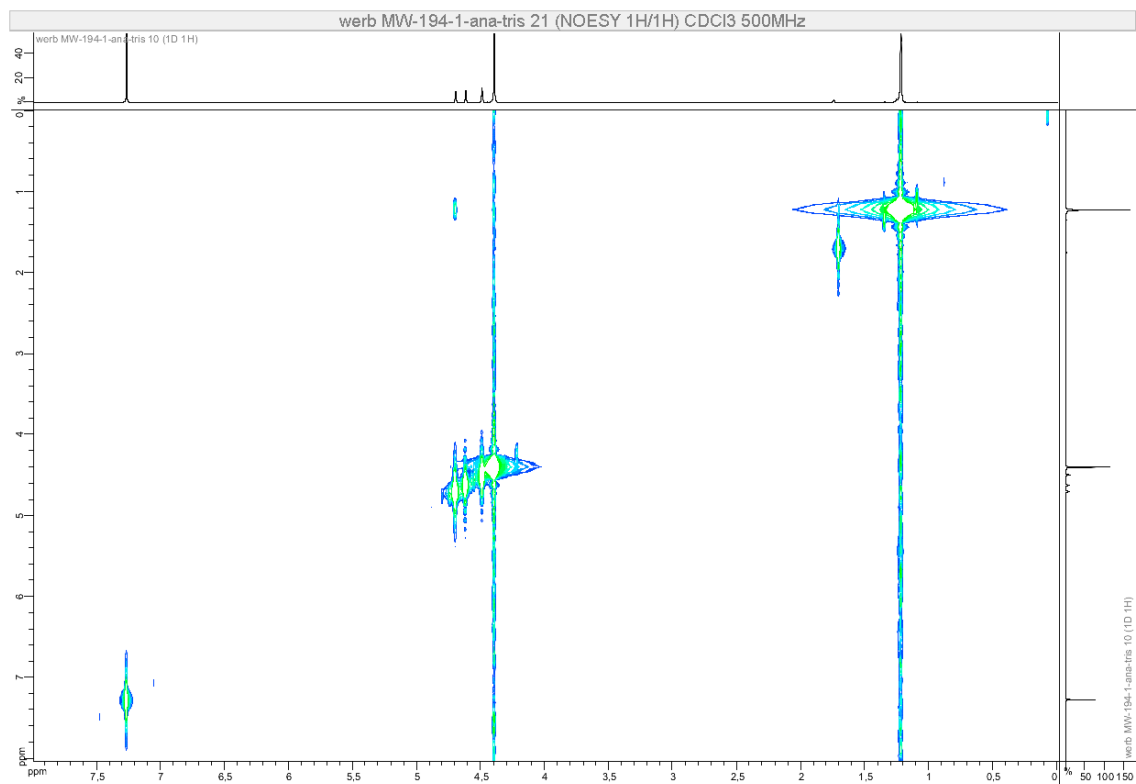
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

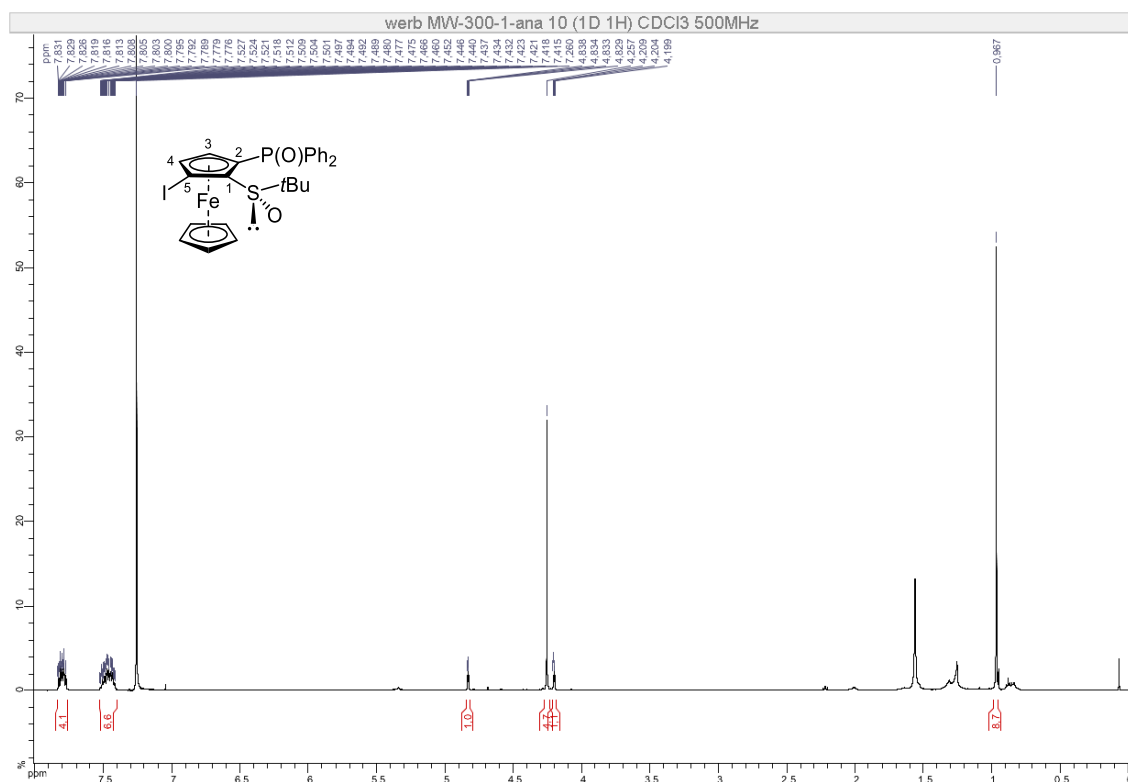


NOESY (500 MHz, CDCl₃)

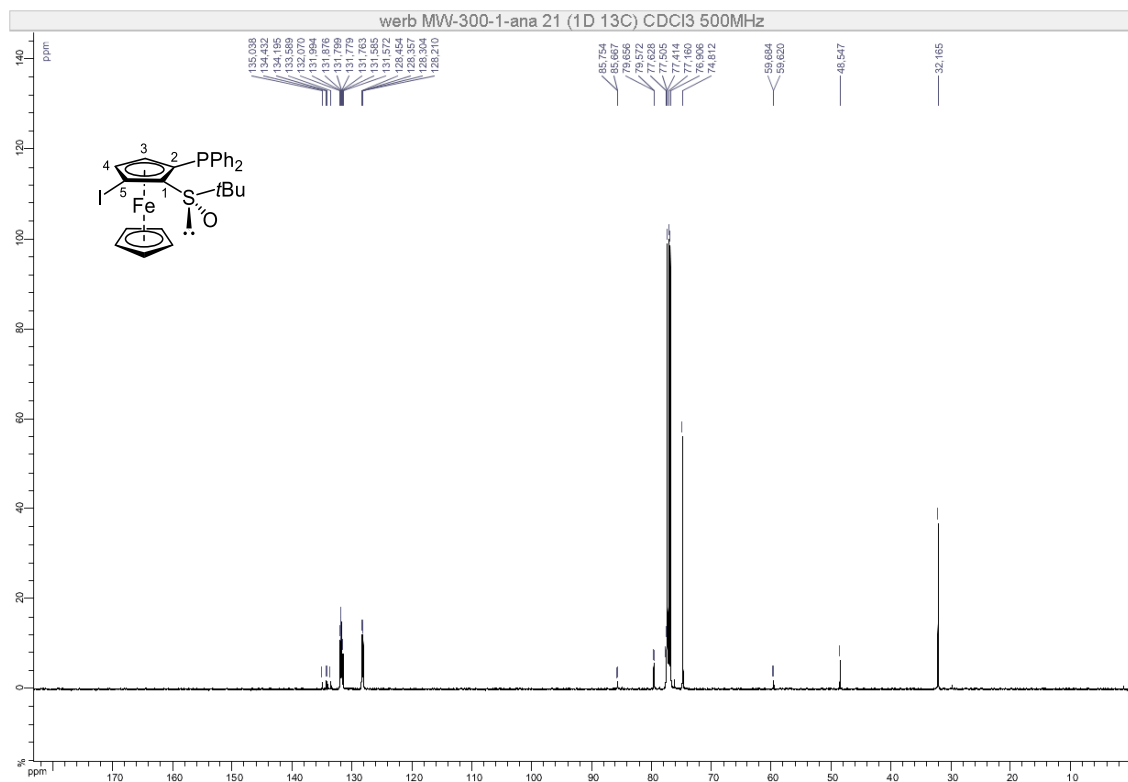


(*S,S*_P)-*S*-*tert*-Butyl-2-(diphenylphosphinyl)-5-iodoferrocenesulfoxide (*S,S*_P-2eb)

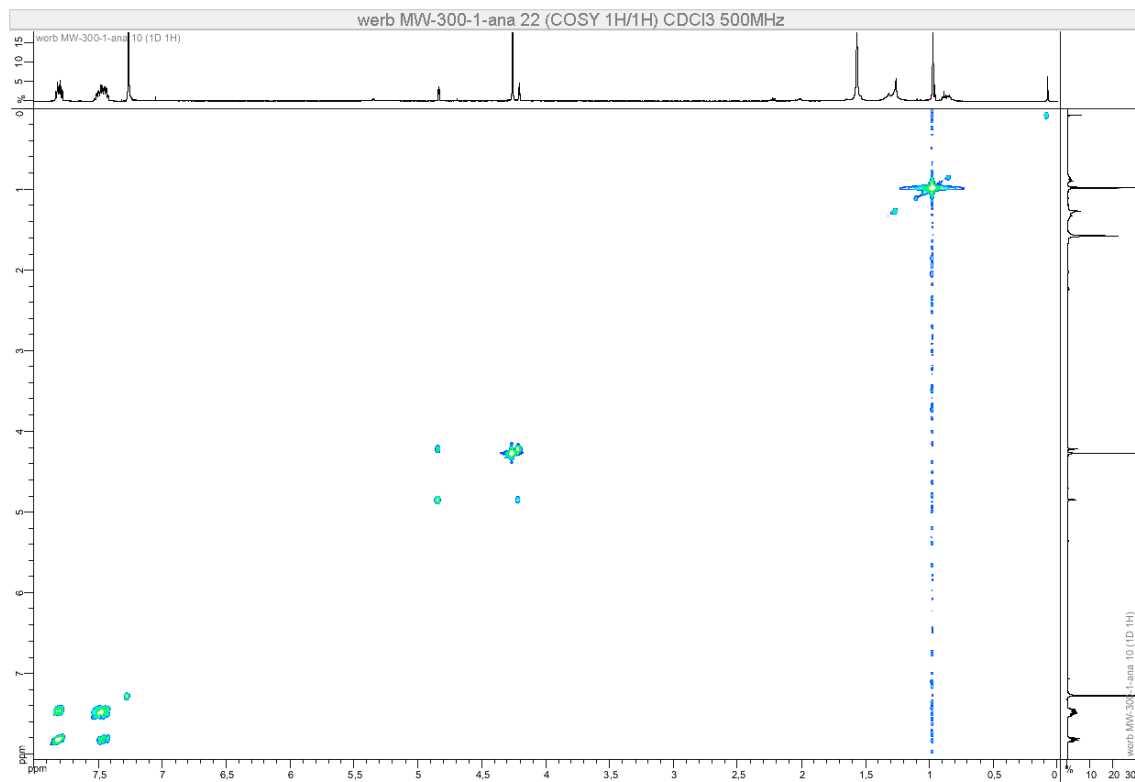
¹H NMR (500 MHz, CDCl₃)



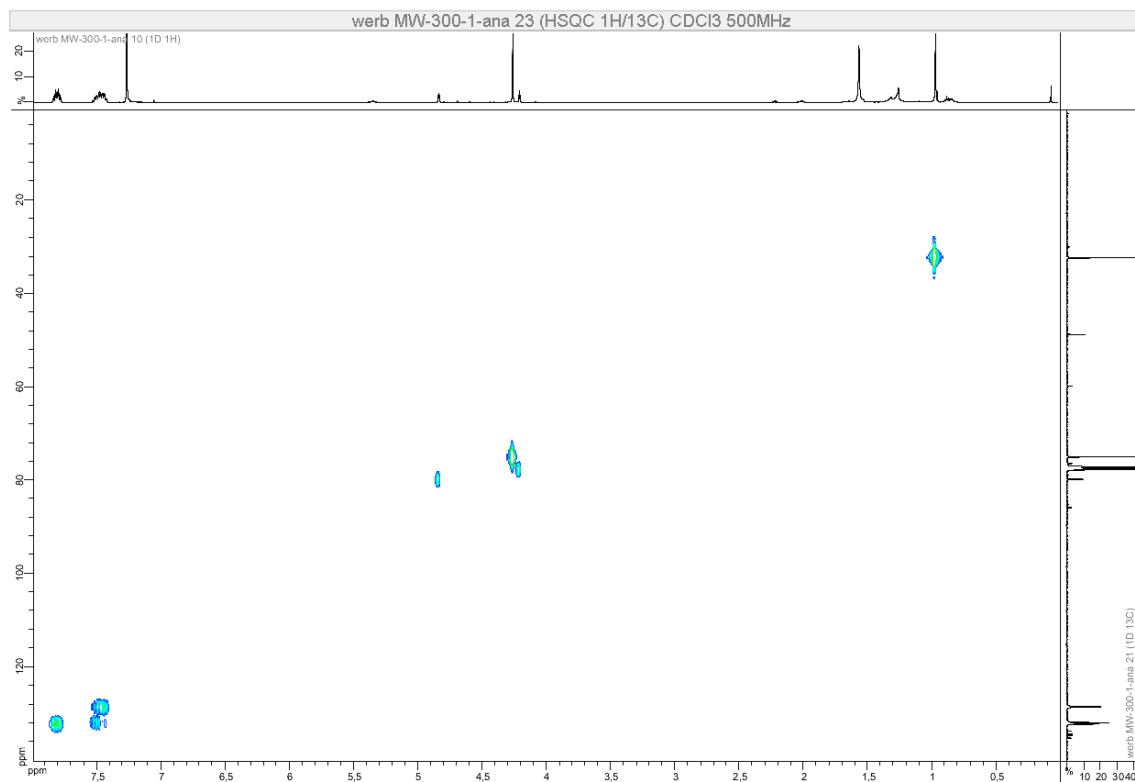
¹³C NMR (126 MHz, CDCl₃)



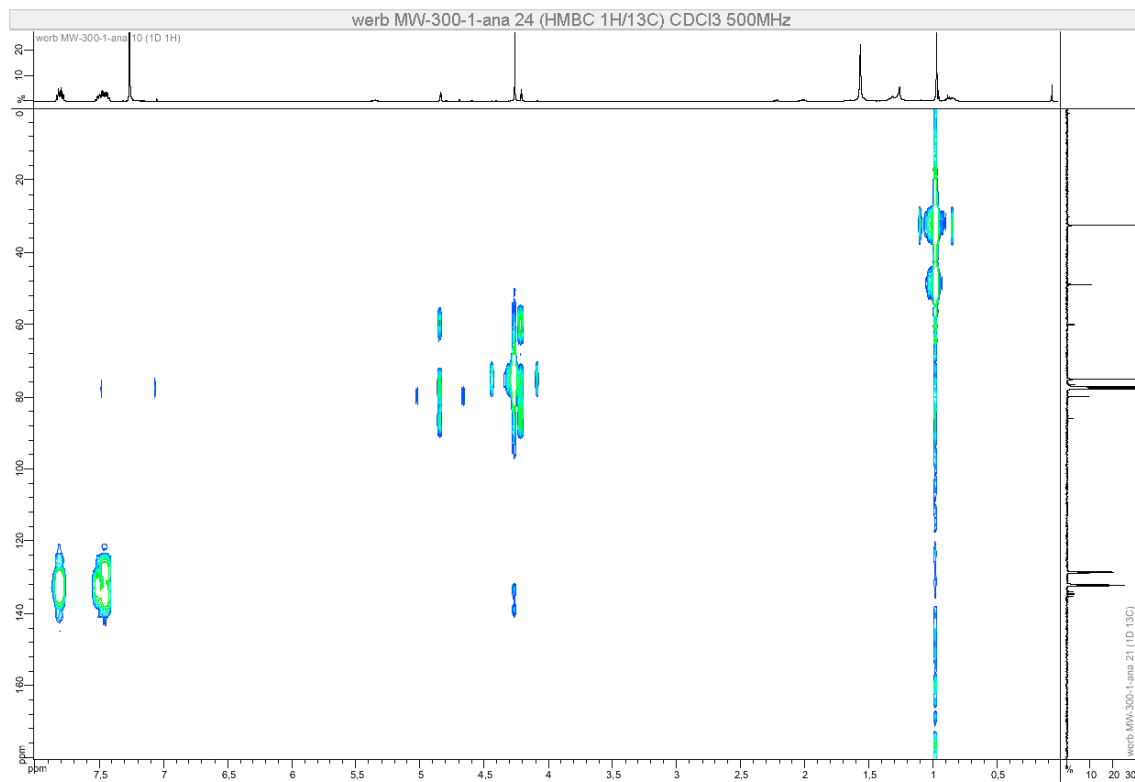
COSY (500 MHz, CDCl₃)



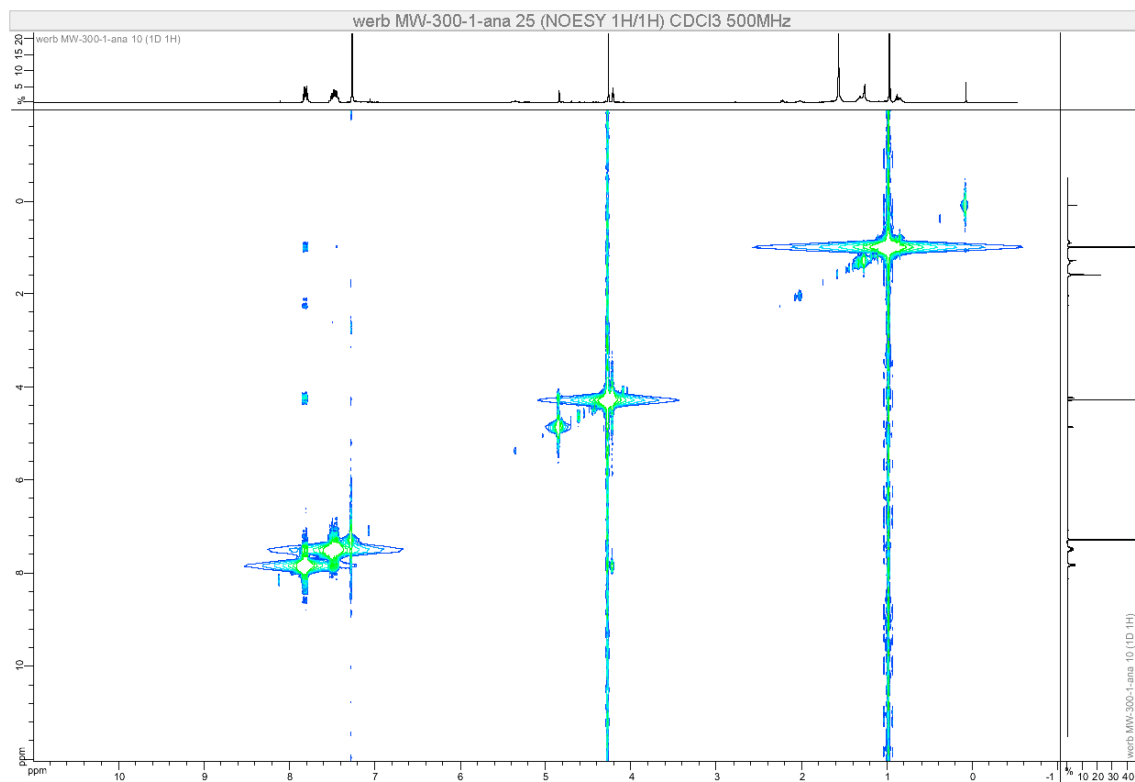
HSQC (500 MHz, CDCl₃)



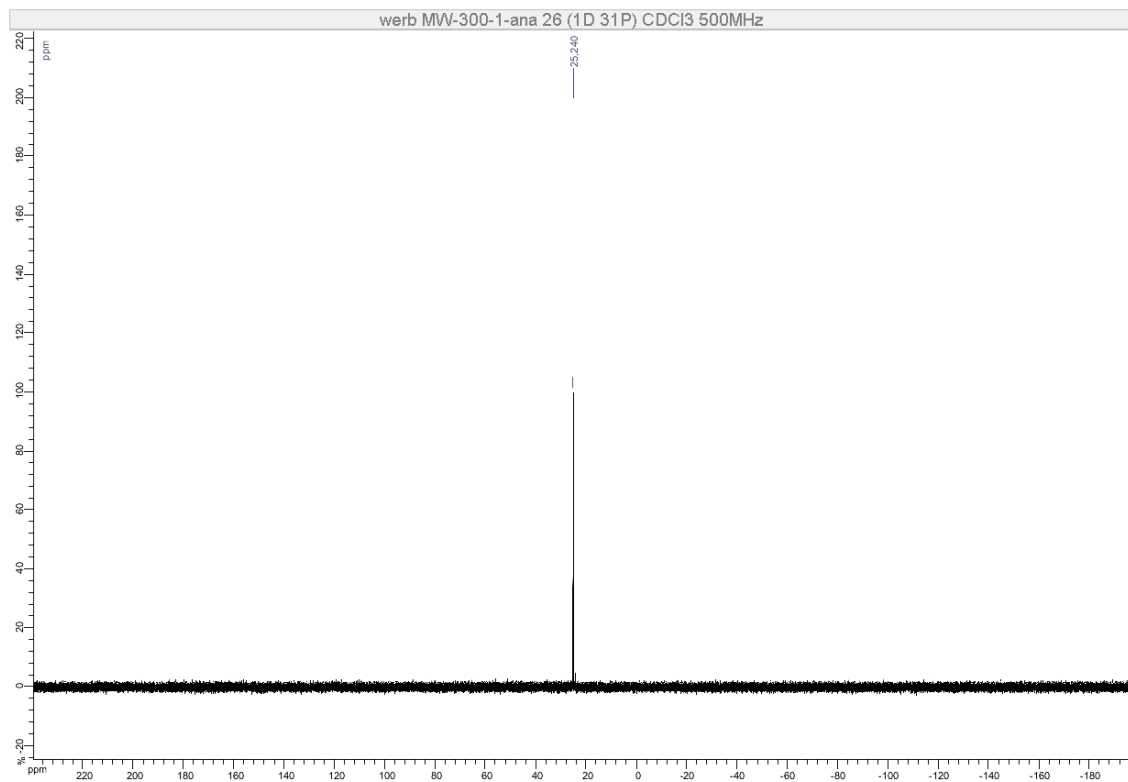
HMBC (500 MHz, CDCl₃)



NOESY (500 MHz, CDCl₃)

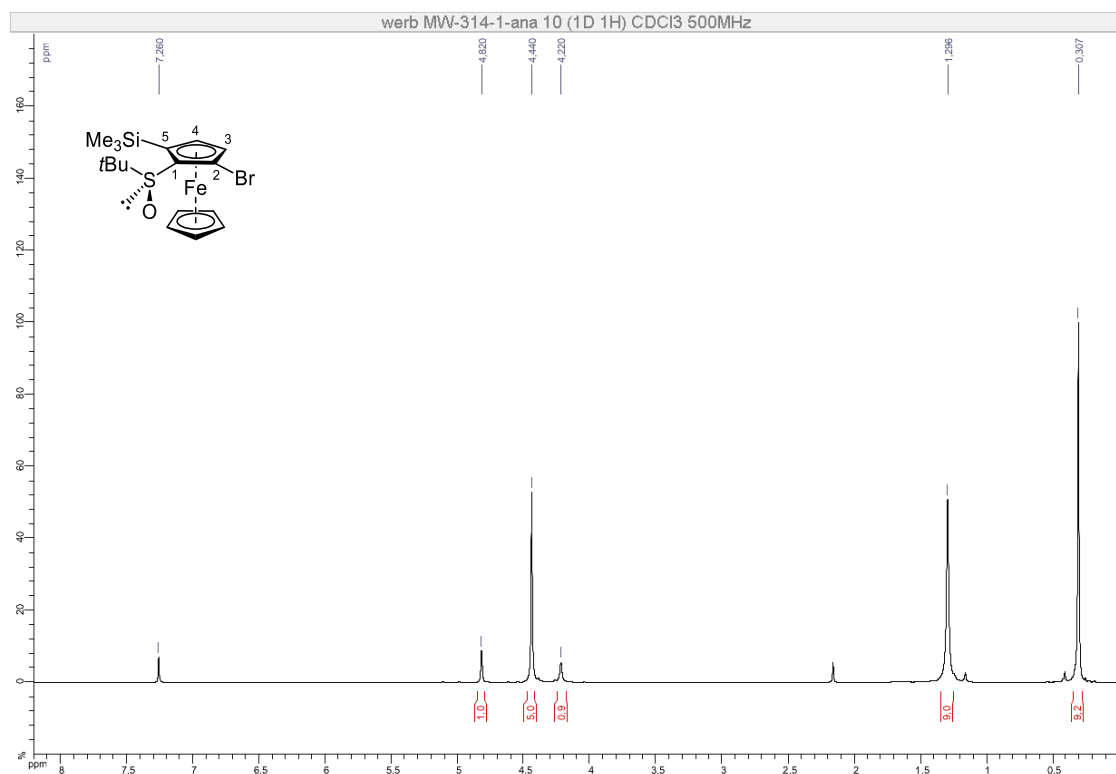


^{31}P NMR (202 MHz, CDCl_3)

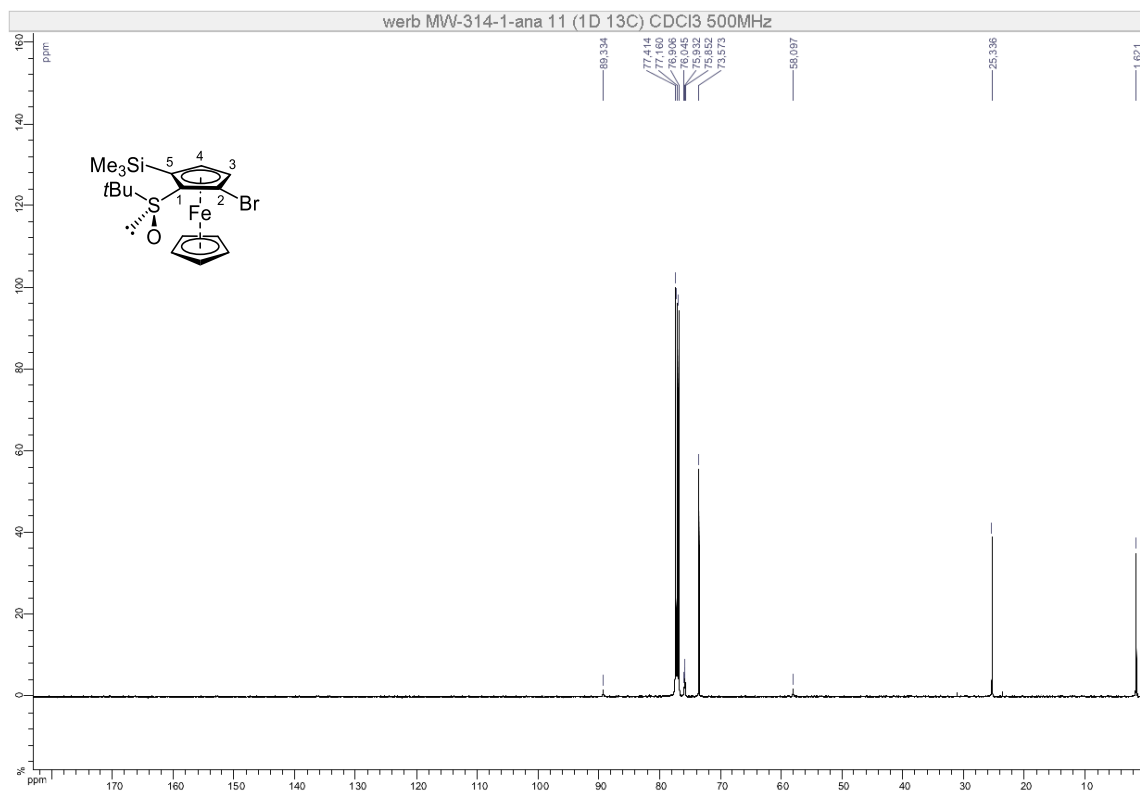


(*S,R_P*)-2-Bromo-*S*-*tert*-butyl-5-(trimethylsilyl)ferrocenesulfoxide (*S,R_P*-2ja)

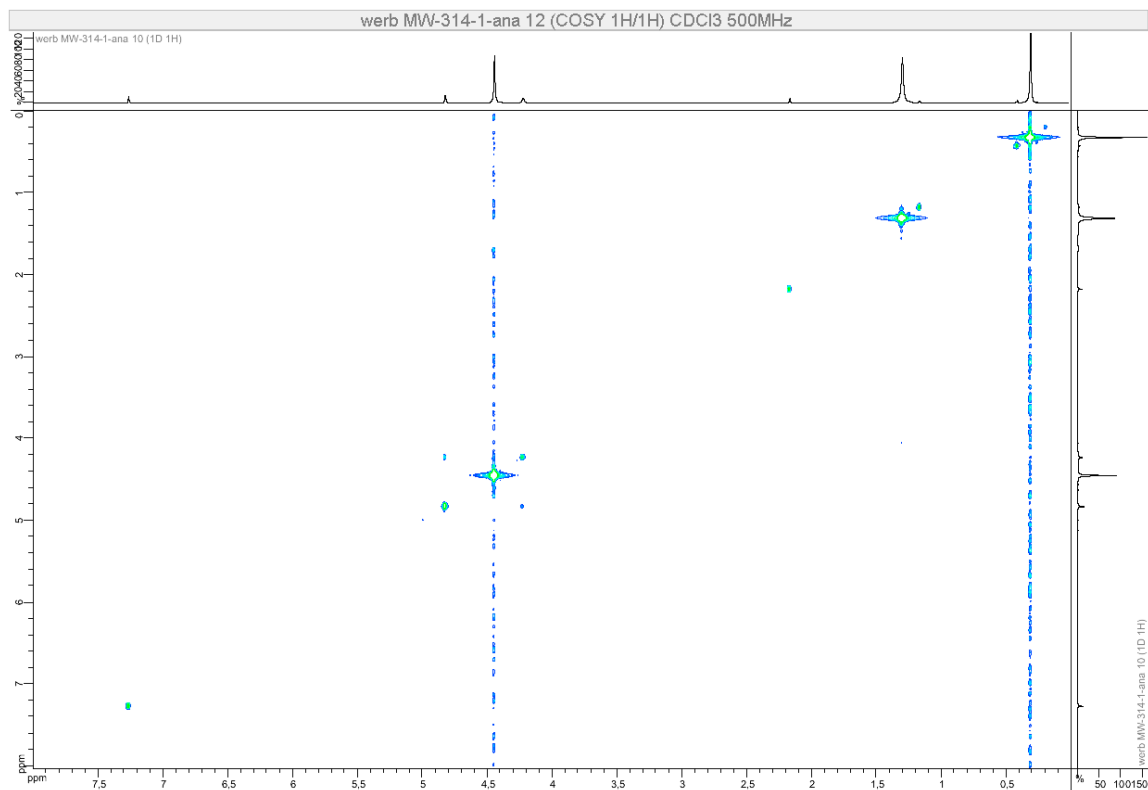
^1H NMR (500 MHz, CDCl_3)



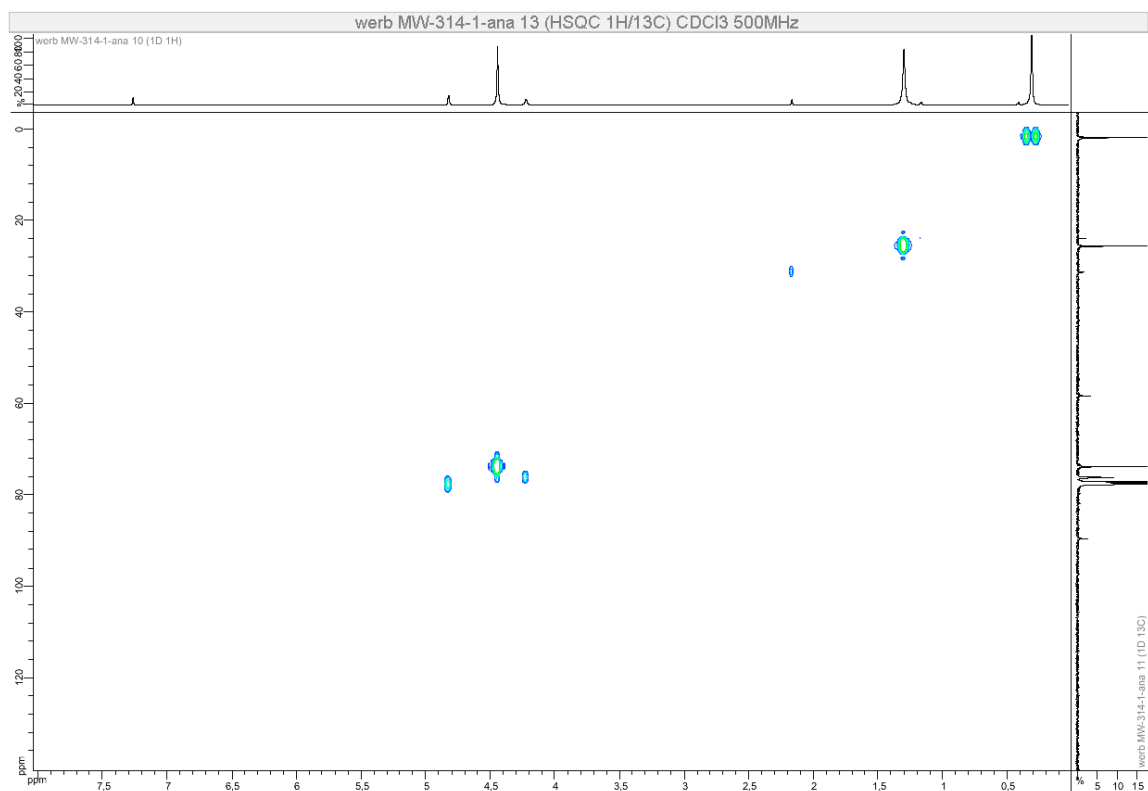
^{13}C NMR (126 MHz, CDCl_3)



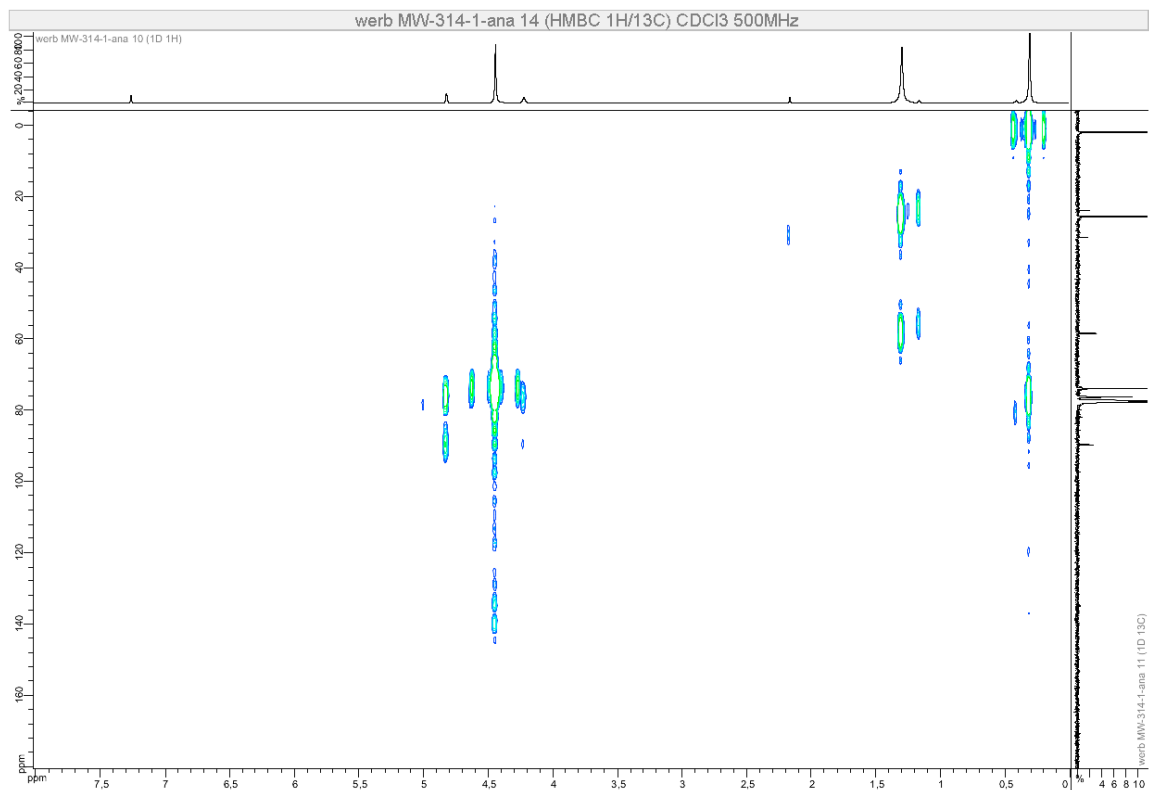
COSY (500 MHz, CDCl₃)



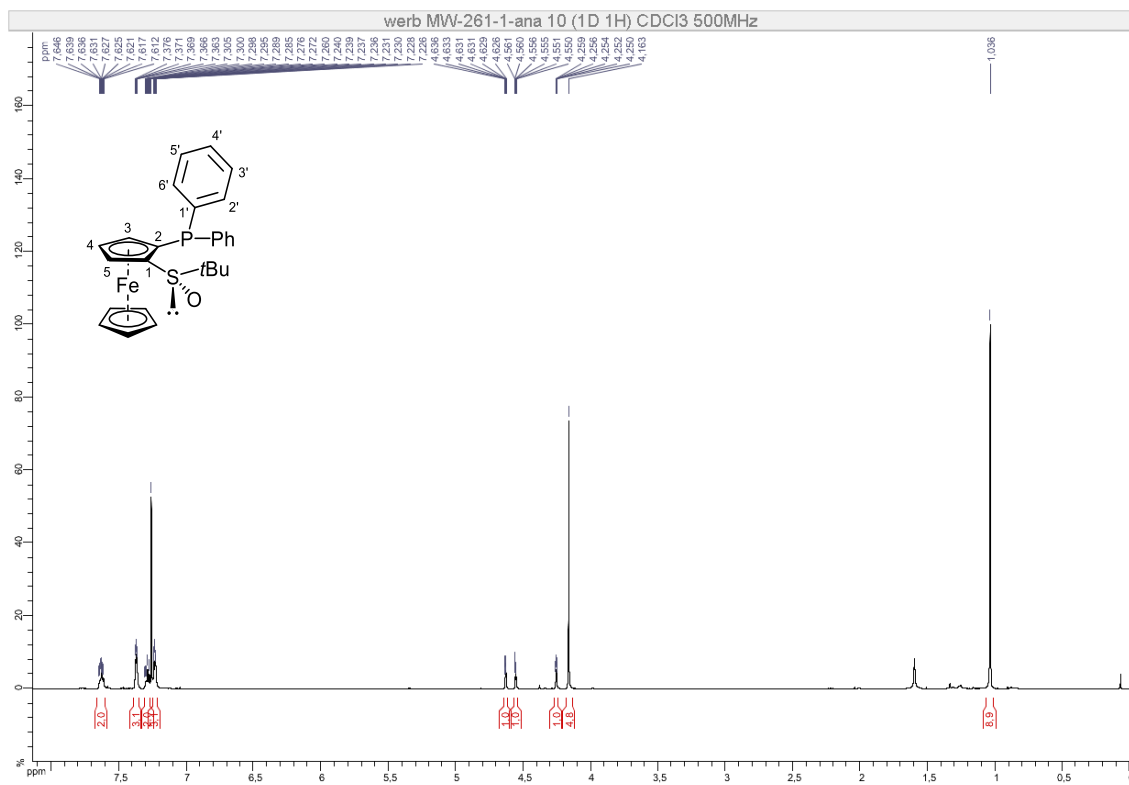
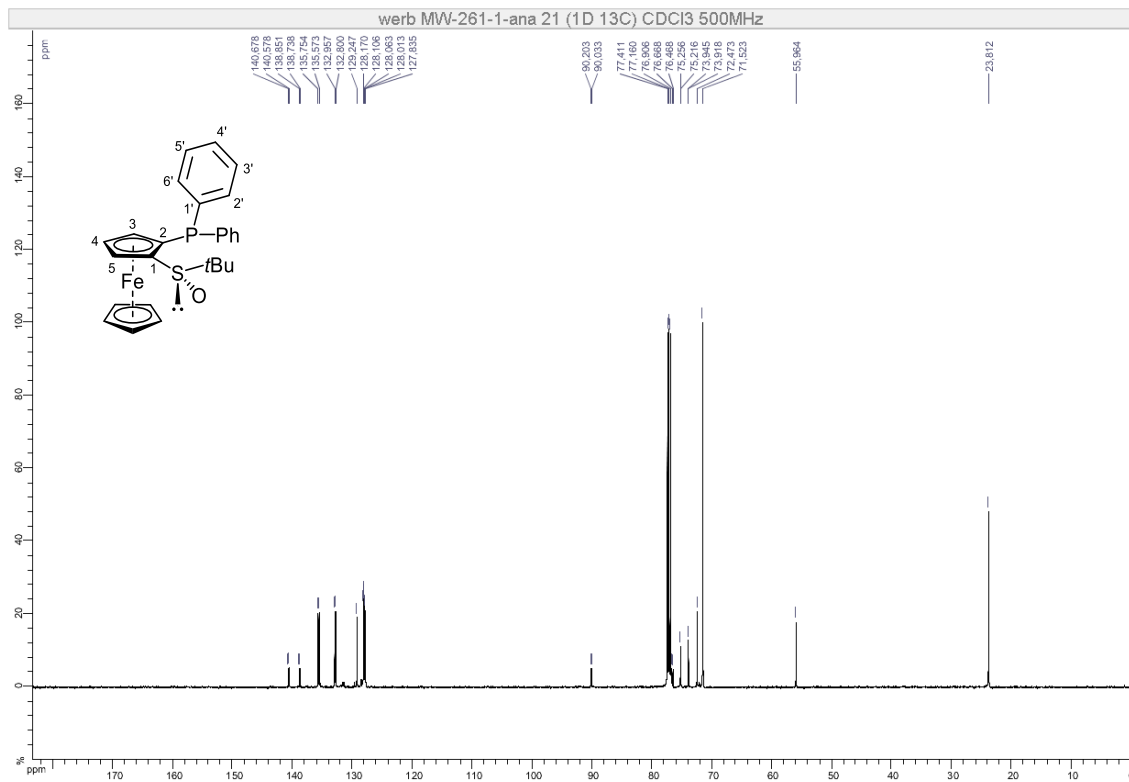
HSQC (500 MHz, CDCl₃)



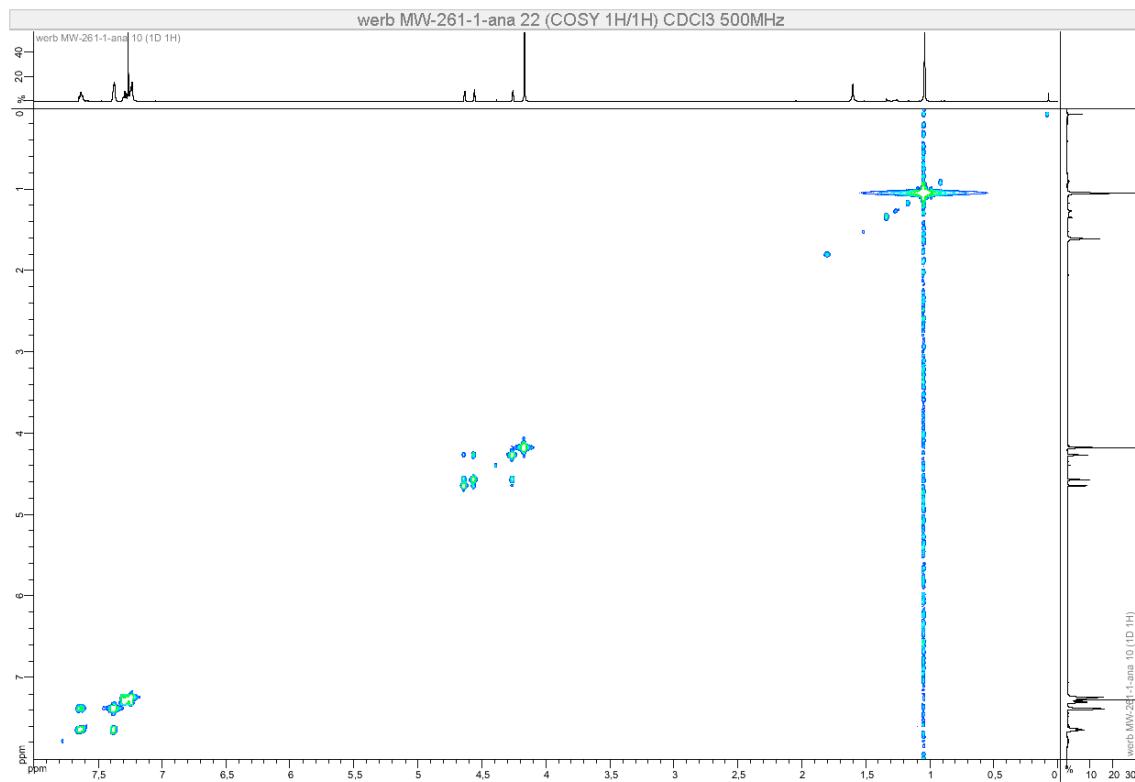
HMBC (500 MHz, CDCl₃)



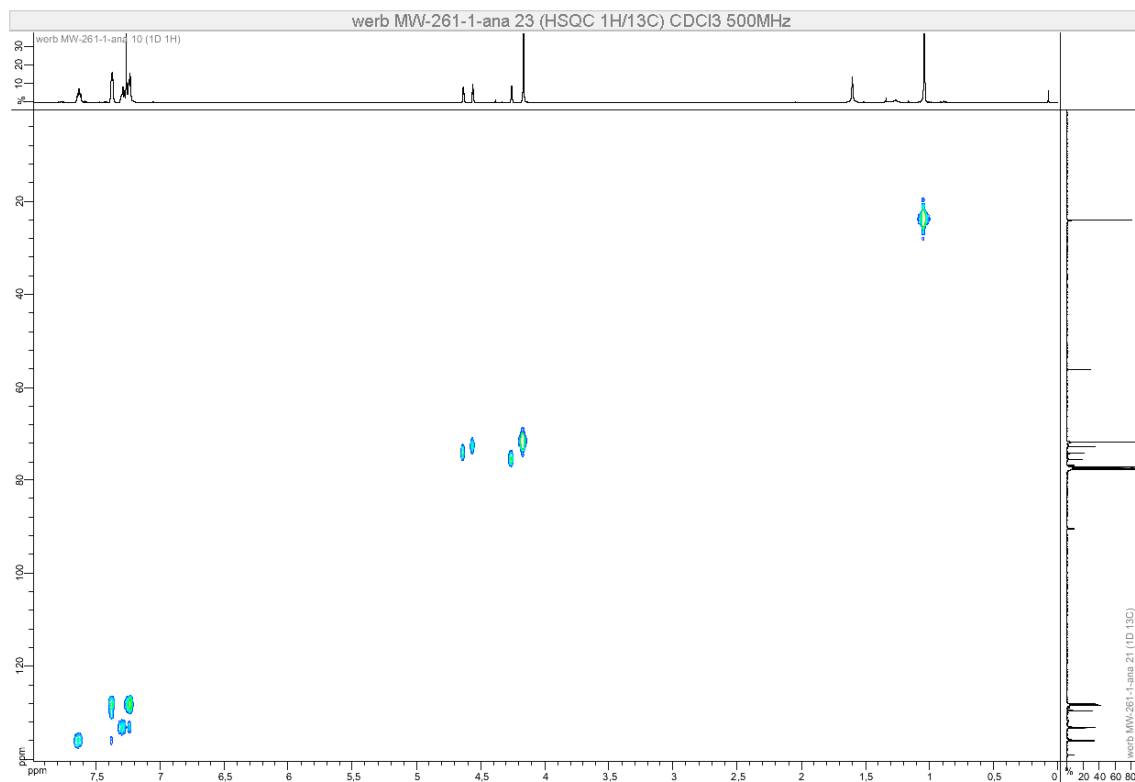
(*S,S*_P)-*S*-tert-Butyl-2-(diphenylphosphino)ferrocenesulfoxide (*S,S*_P-1e)

¹H NMR (500 MHz, CDCl₃) ^{13}C NMR (126 MHz, CDCl_3)

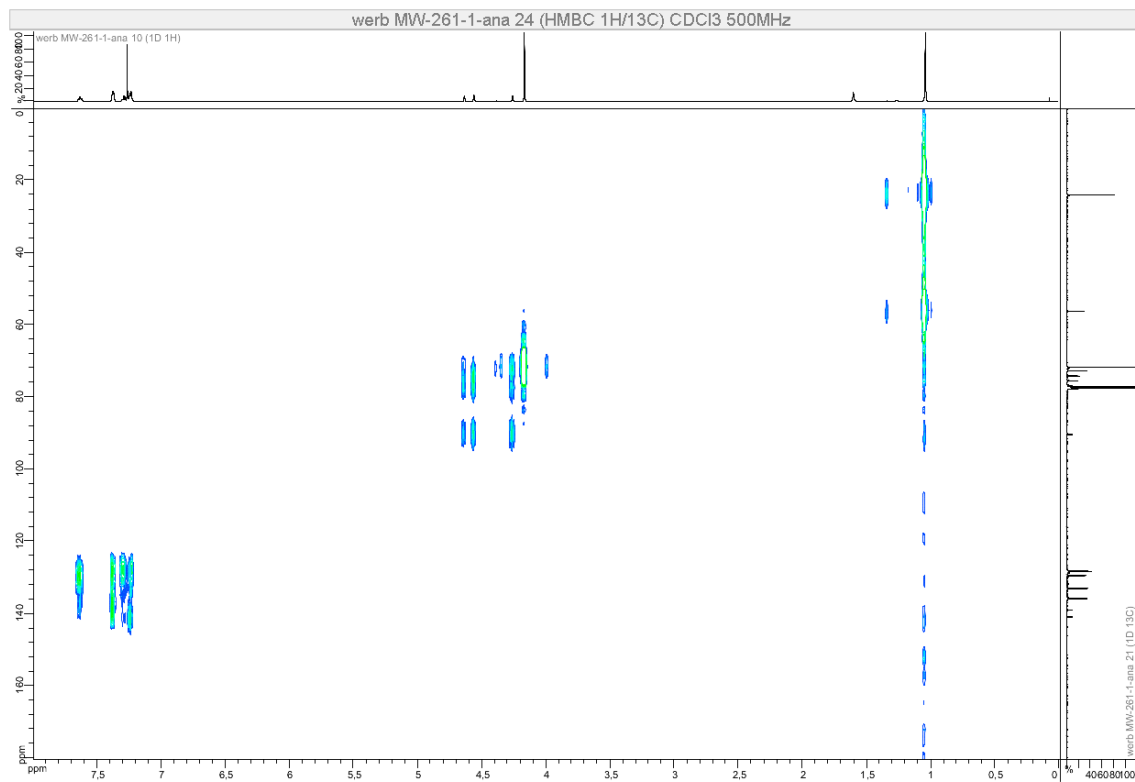
COSY (500 MHz, CDCl₃)



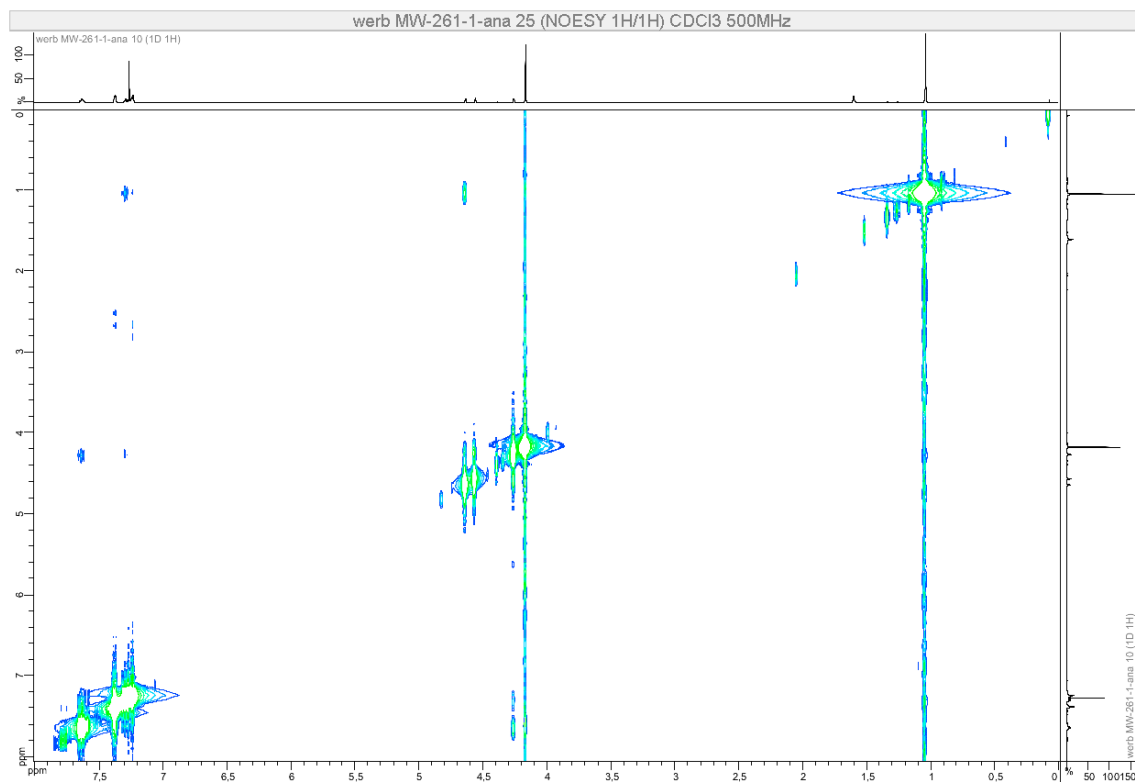
HSQC (500 MHz, CDCl₃)



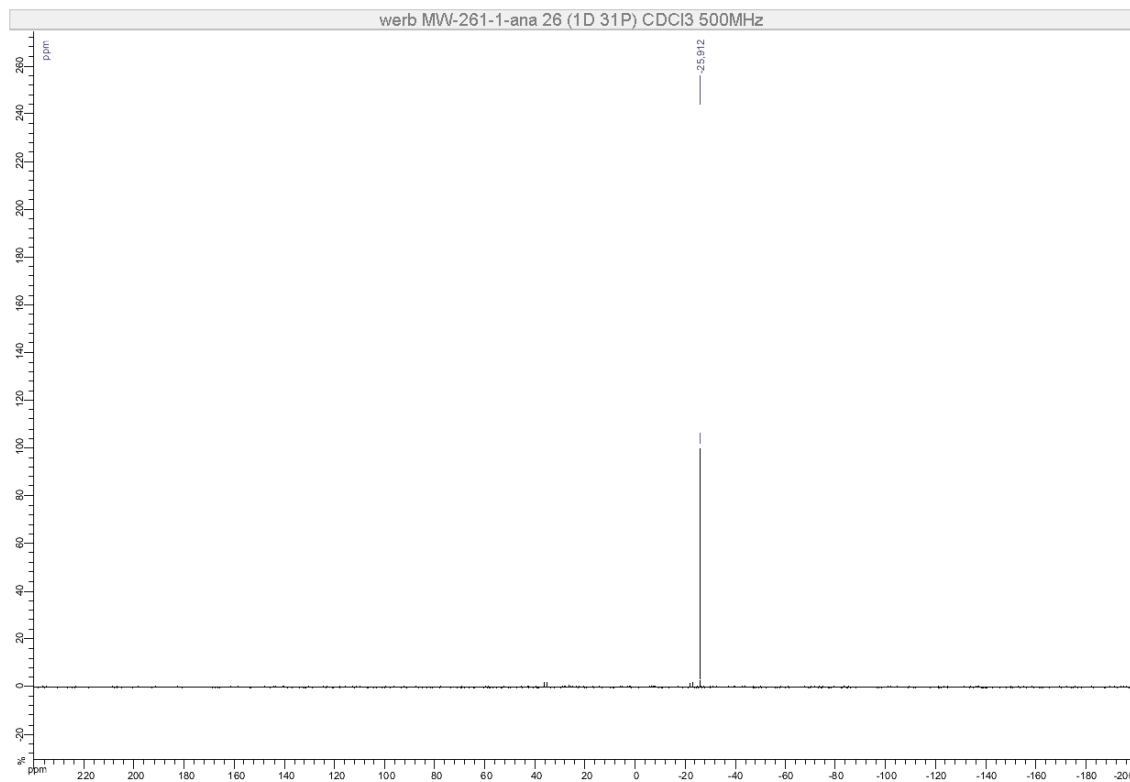
HMBC (500 MHz, CDCl₃)



NOESY (500 MHz, CDCl₃)

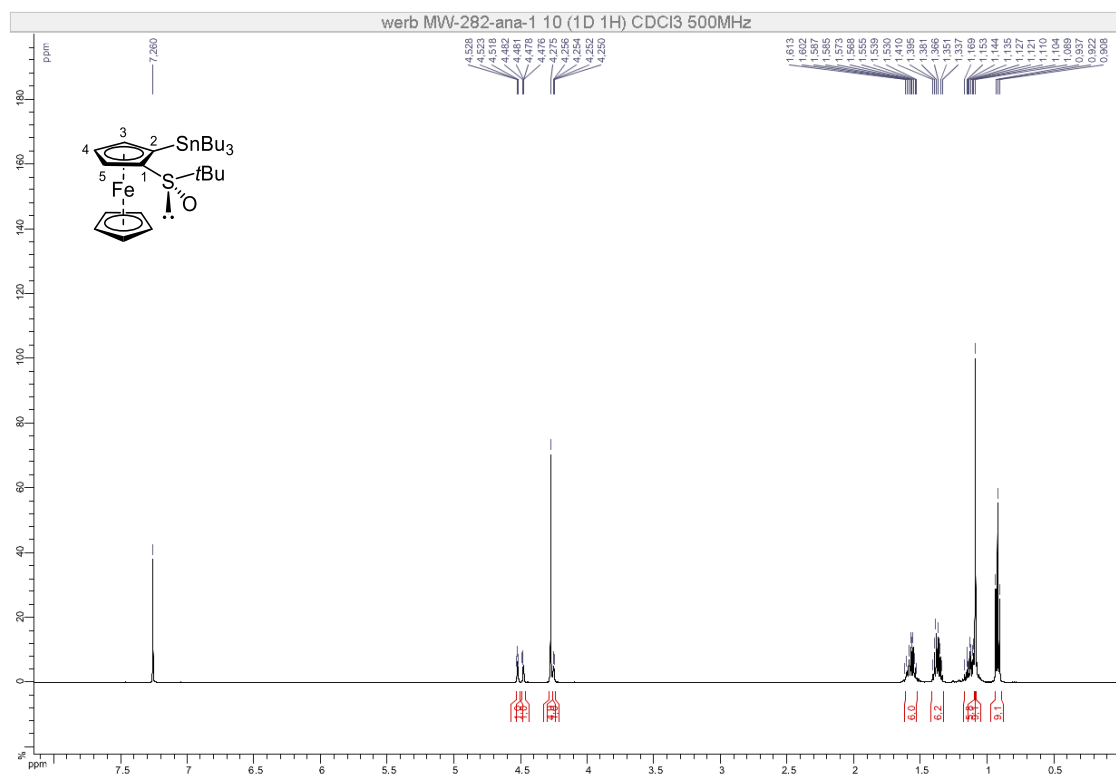


^{31}P NMR (202 MHz, CDCl_3)

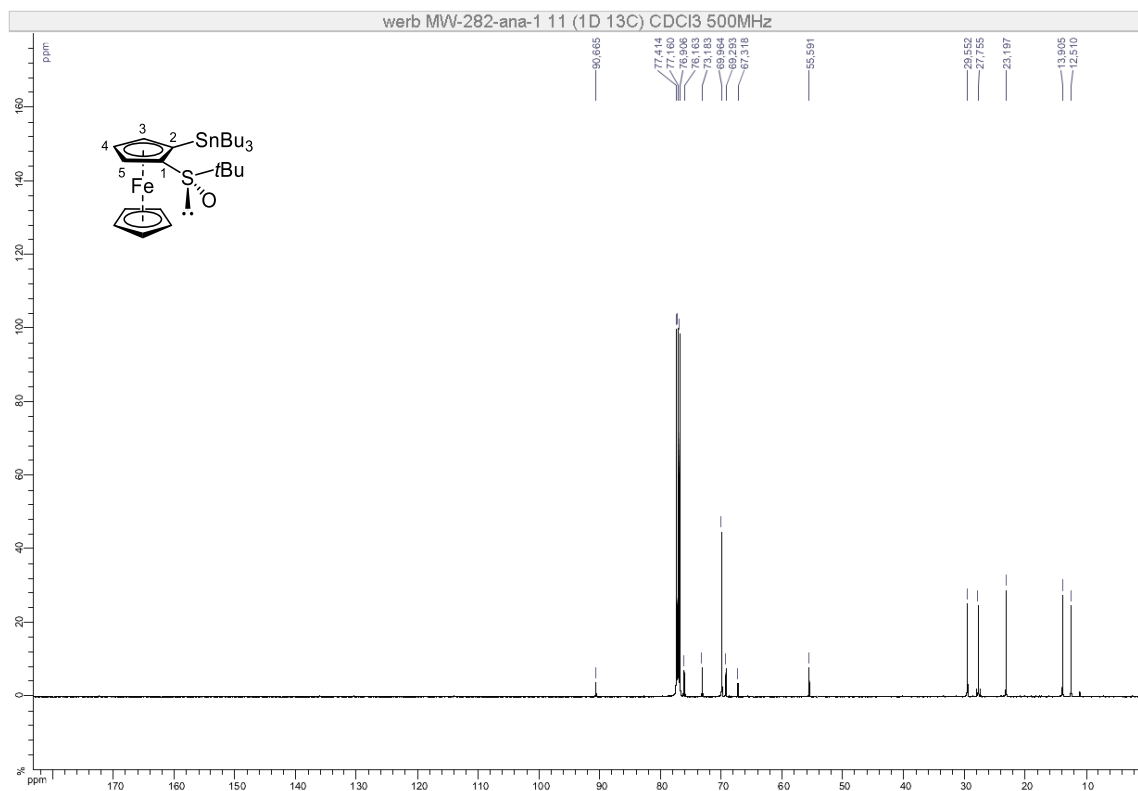


(*S,R_P*)-*S*-tert-Butyl-2-(tributylstannyl)ferrocenesulfoxide (*S,R_P*-1f)

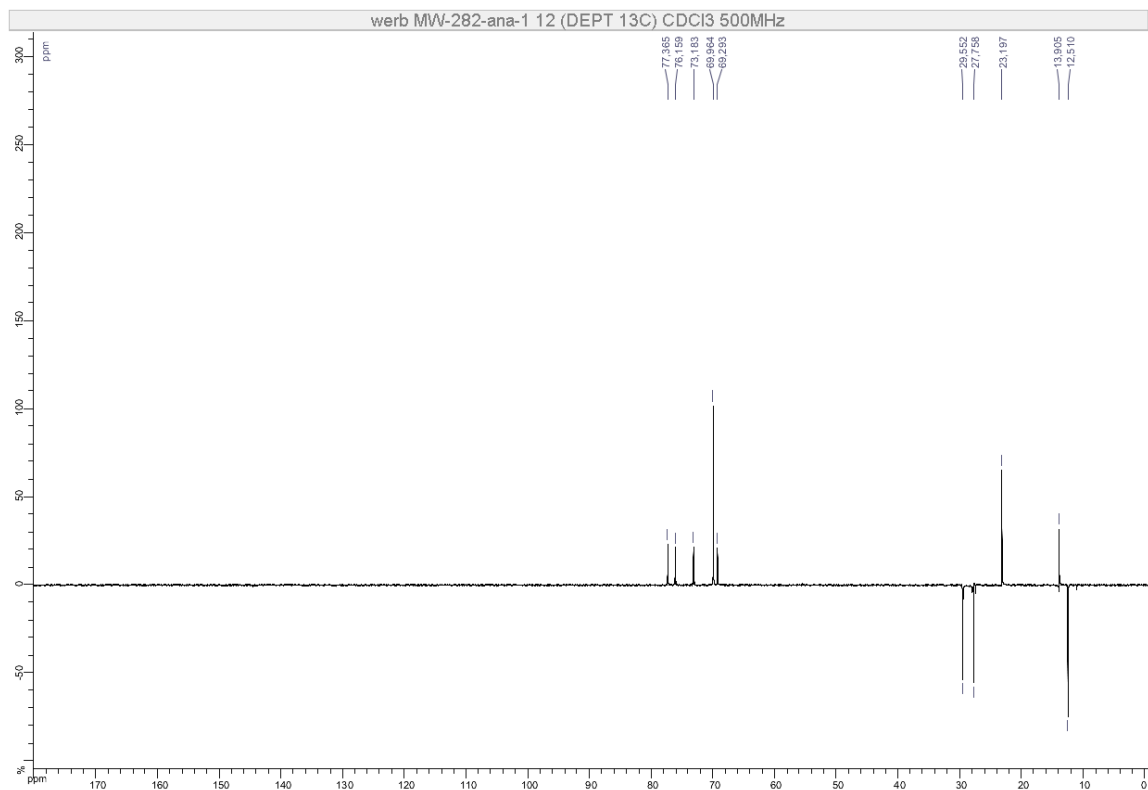
^1H NMR (500 MHz, CDCl_3)



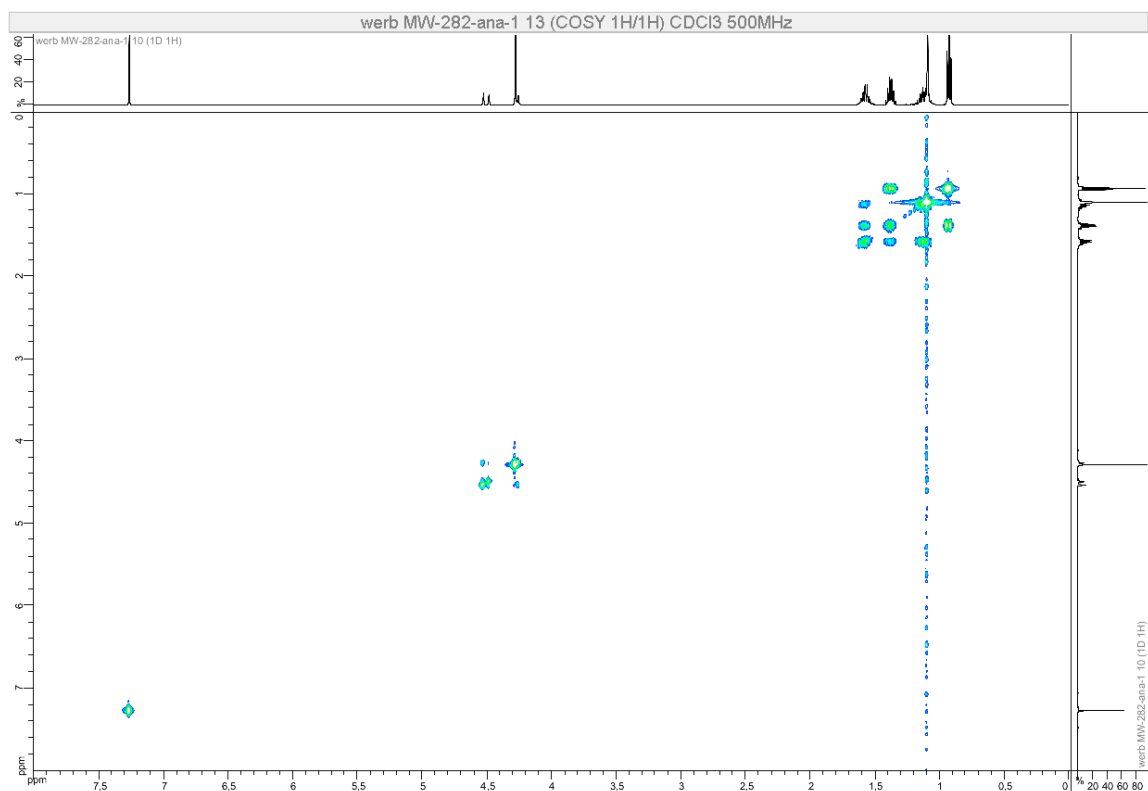
^{13}C NMR (126 MHz, CDCl_3)



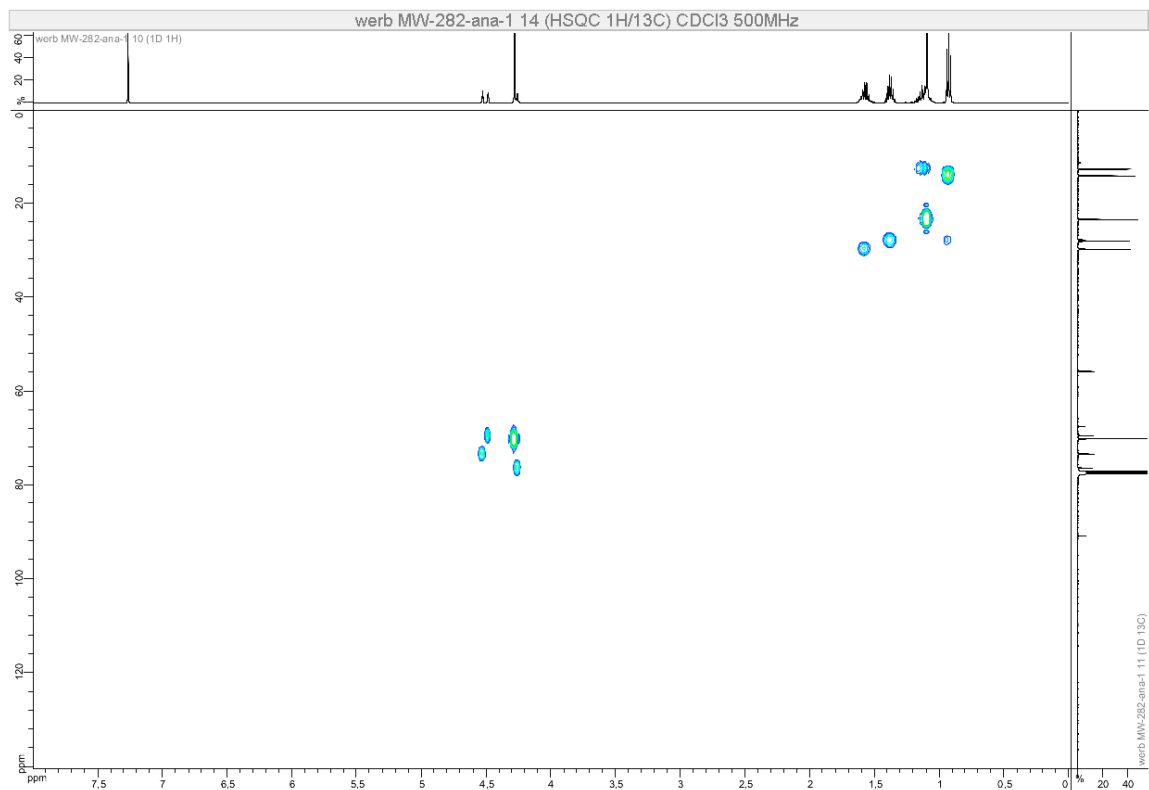
DEPT 135 (126 MHz, CDCl₃)



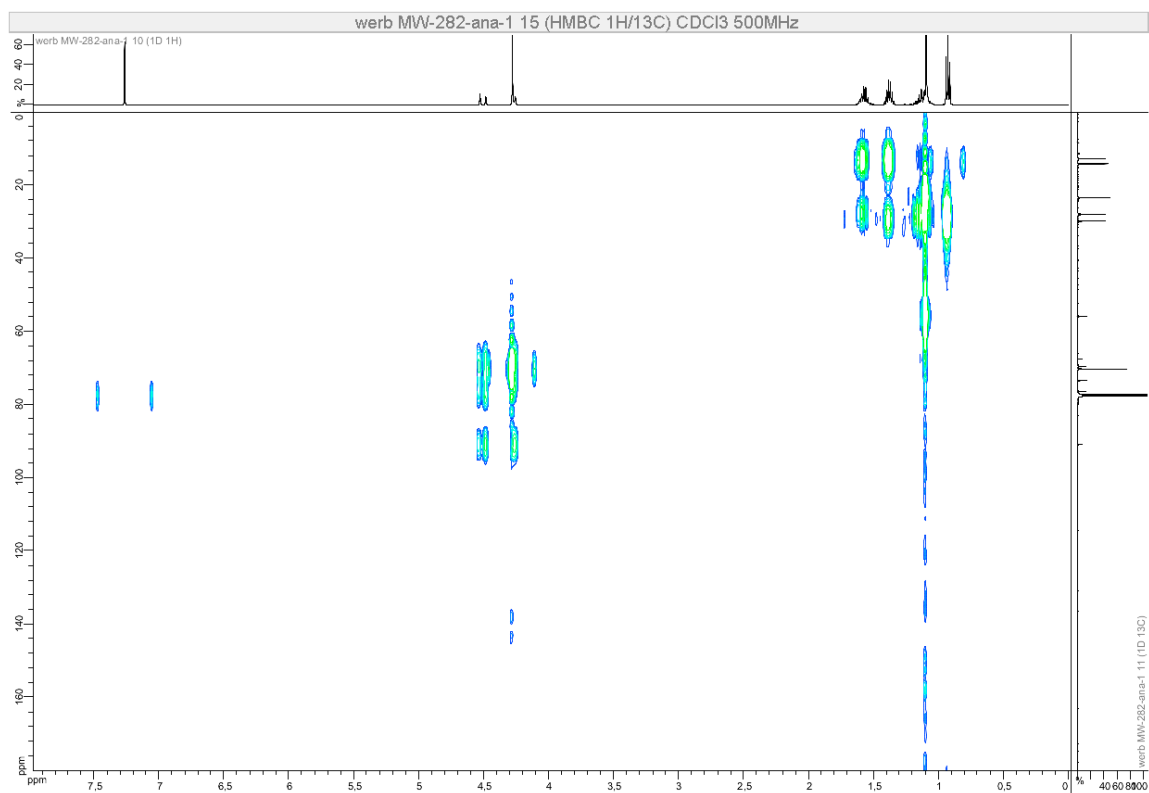
COSY (500 MHz, CDCl₃)



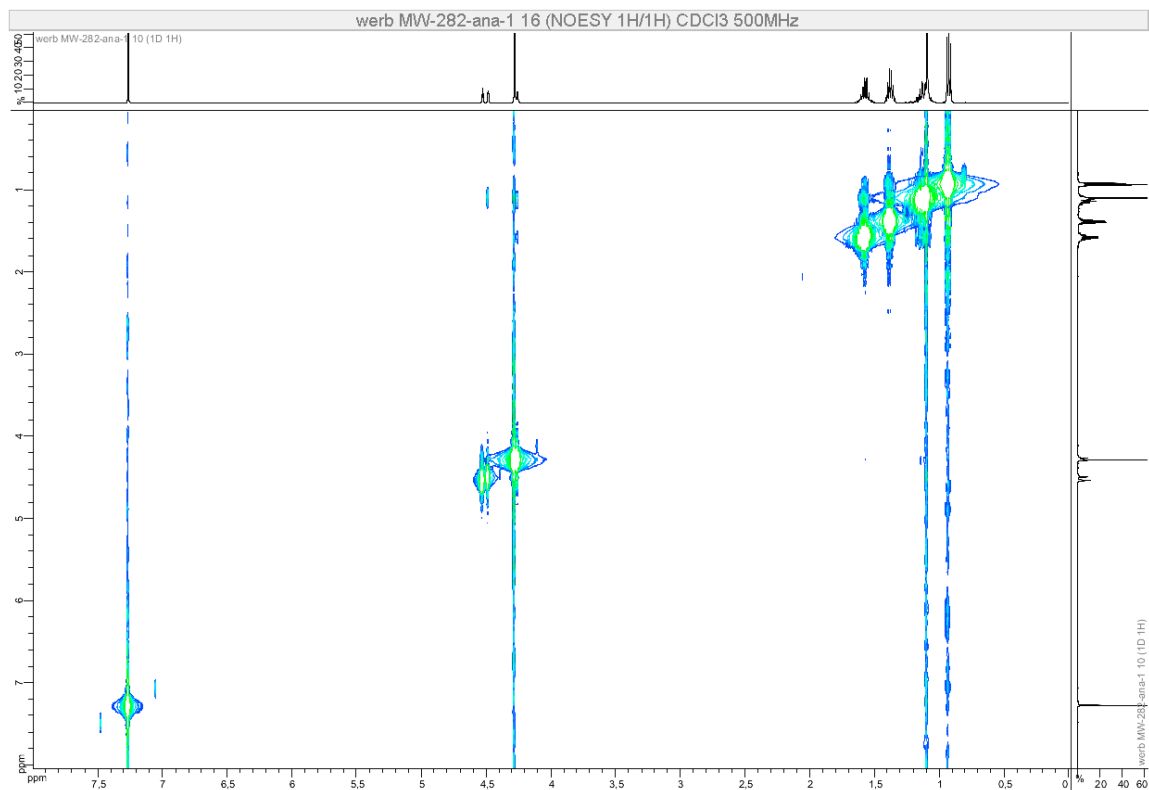
HSQC (500 MHz, CDCl₃)



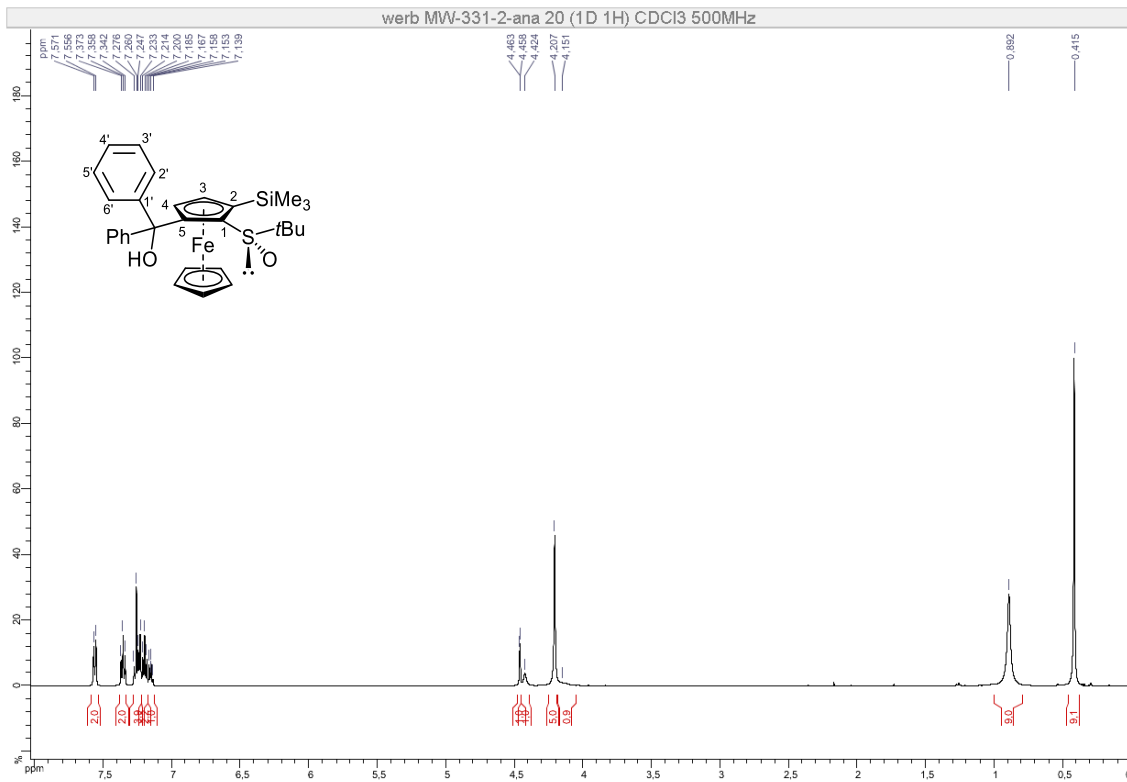
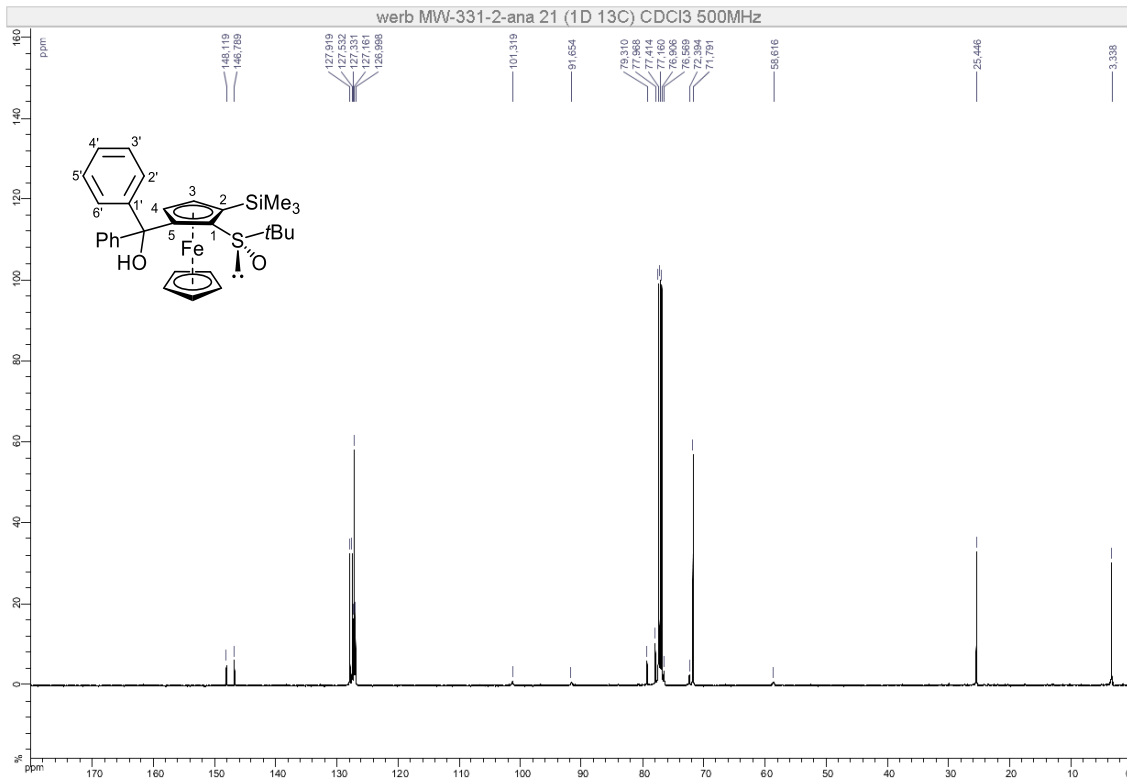
HMBC (500 MHz, CDCl₃)



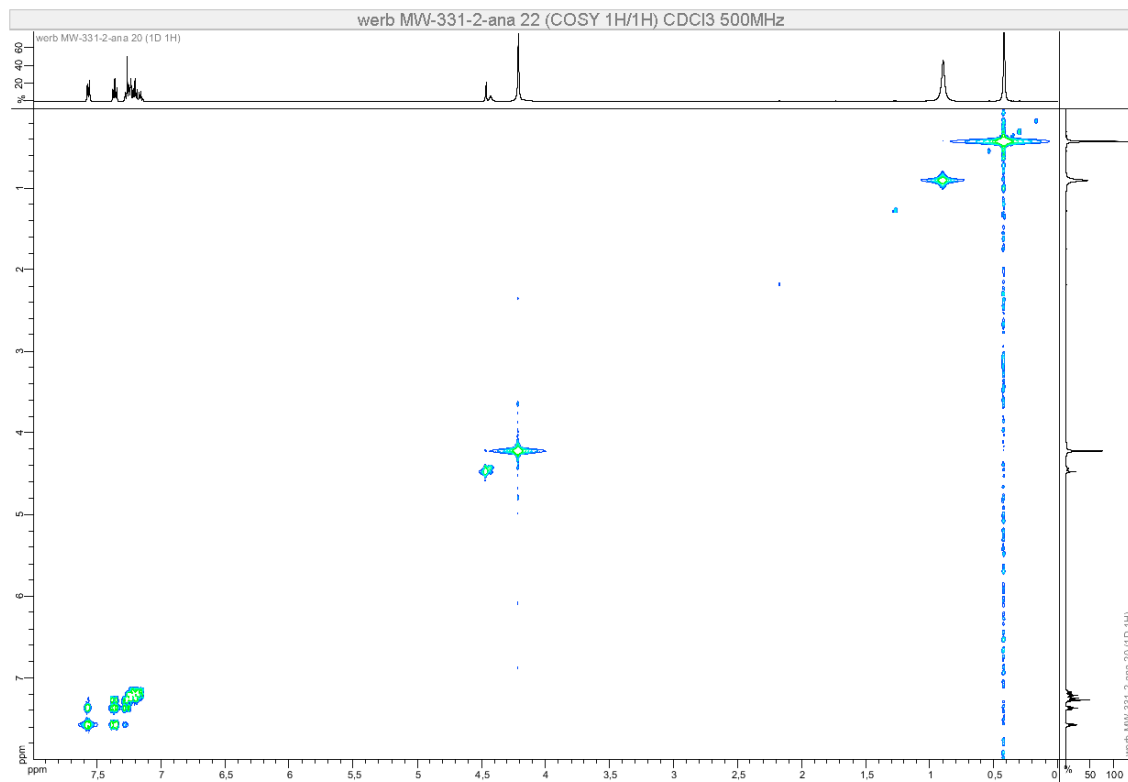
NOESY (500 MHz, CDCl₃)



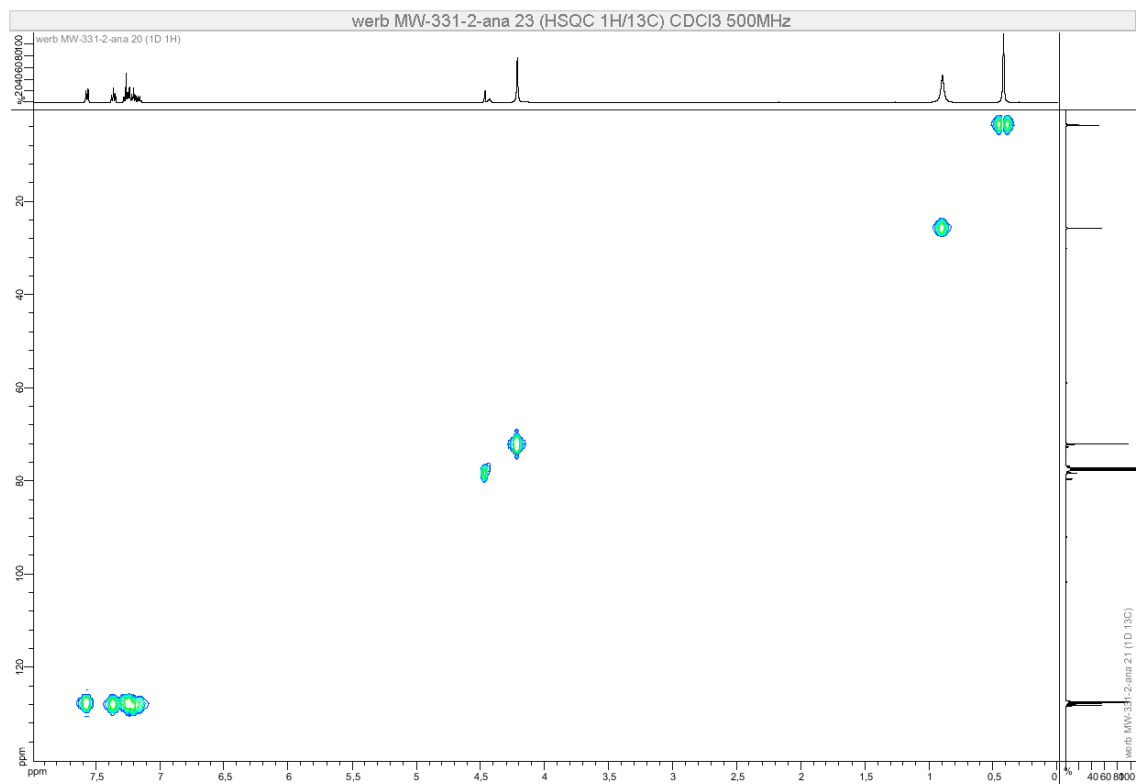
(S,S_P)-S-tert-Butyl-2-[(α,α -diphenyl)hydroxymethyl]-5-(trimethylsilyl)ferrocenesulfoxide (S,S_P-2ag)

¹H NMR (500 MHz, CDCl₃) ^{13}C NMR (126 MHz, CDCl_3)

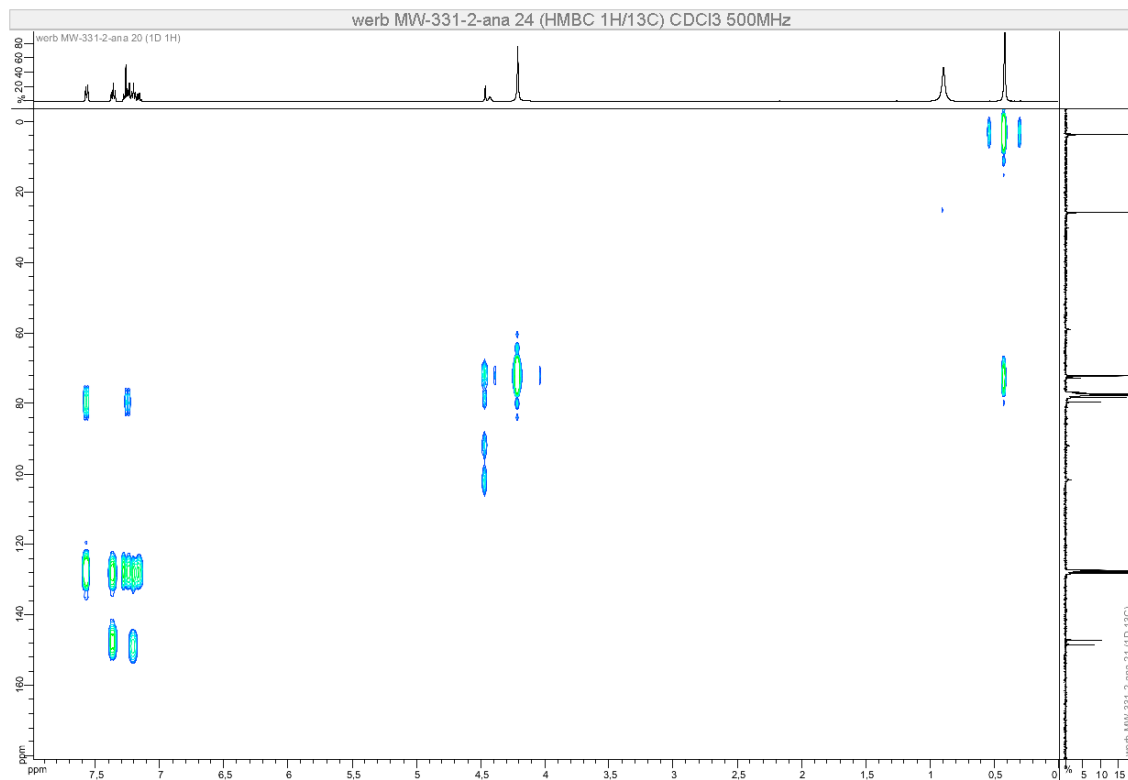
COSY (500 MHz, CDCl₃)



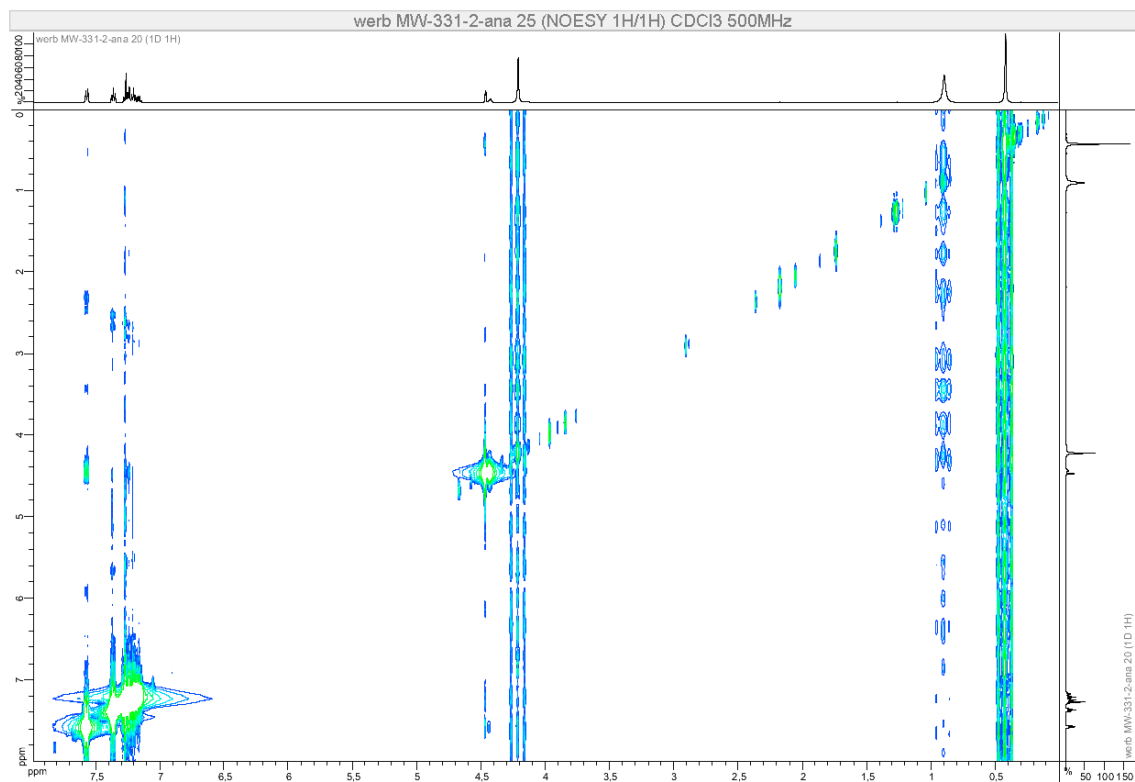
HSQC (500 MHz, CDCl₃)



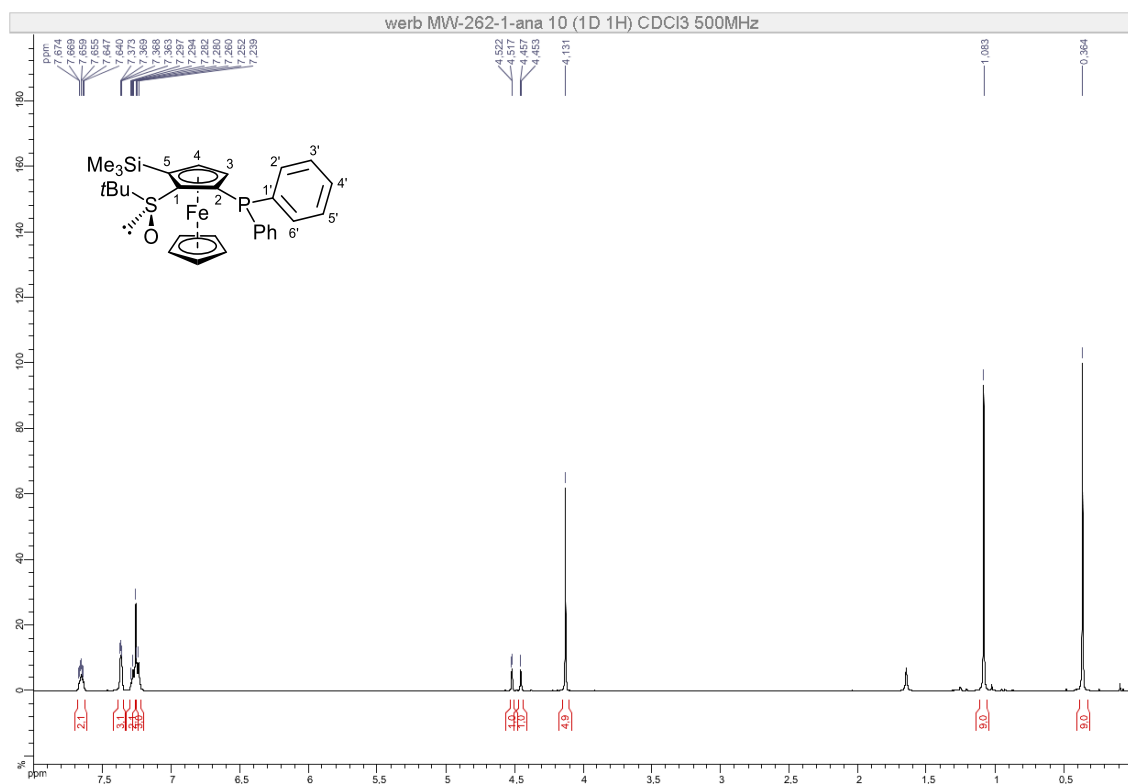
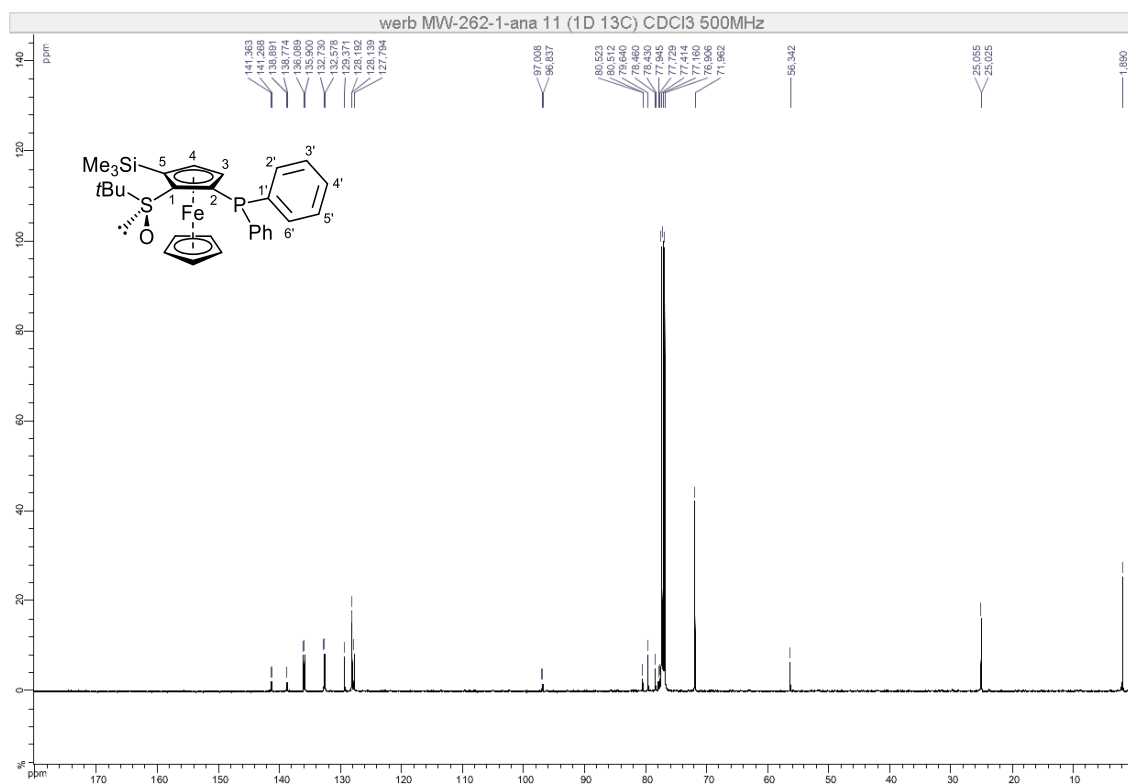
HMBC (500 MHz, CDCl₃)



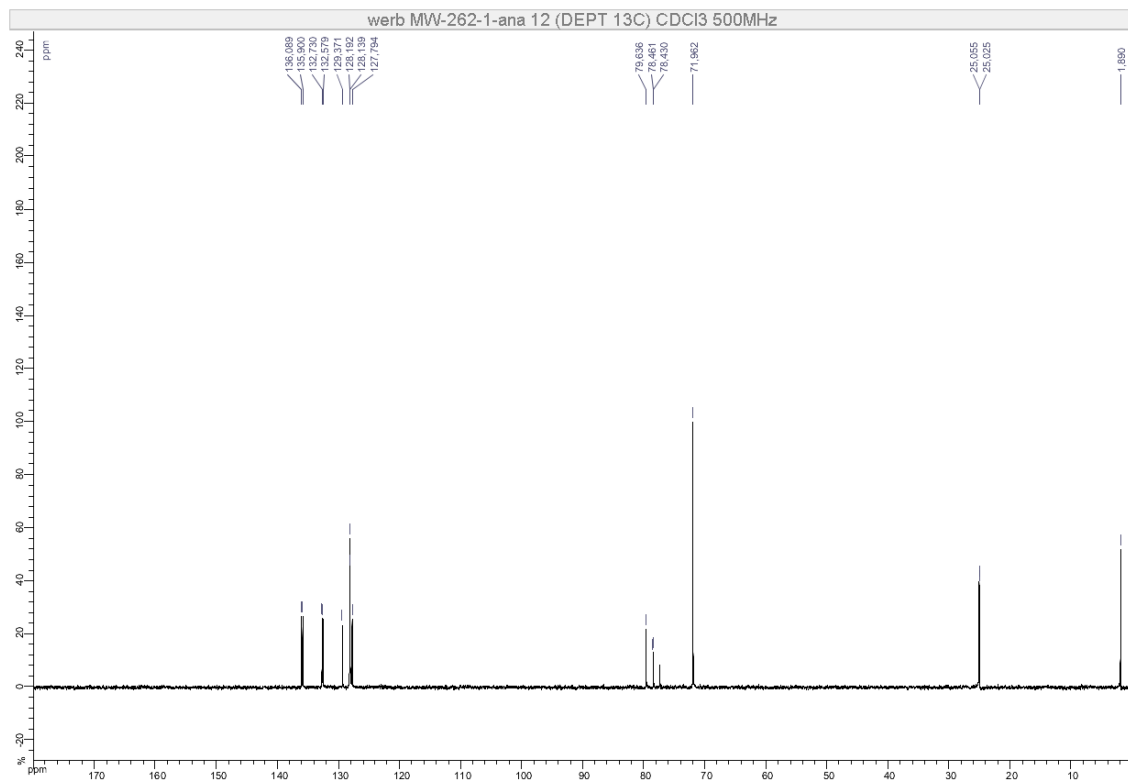
NOESY (500 MHz, CDCl₃)



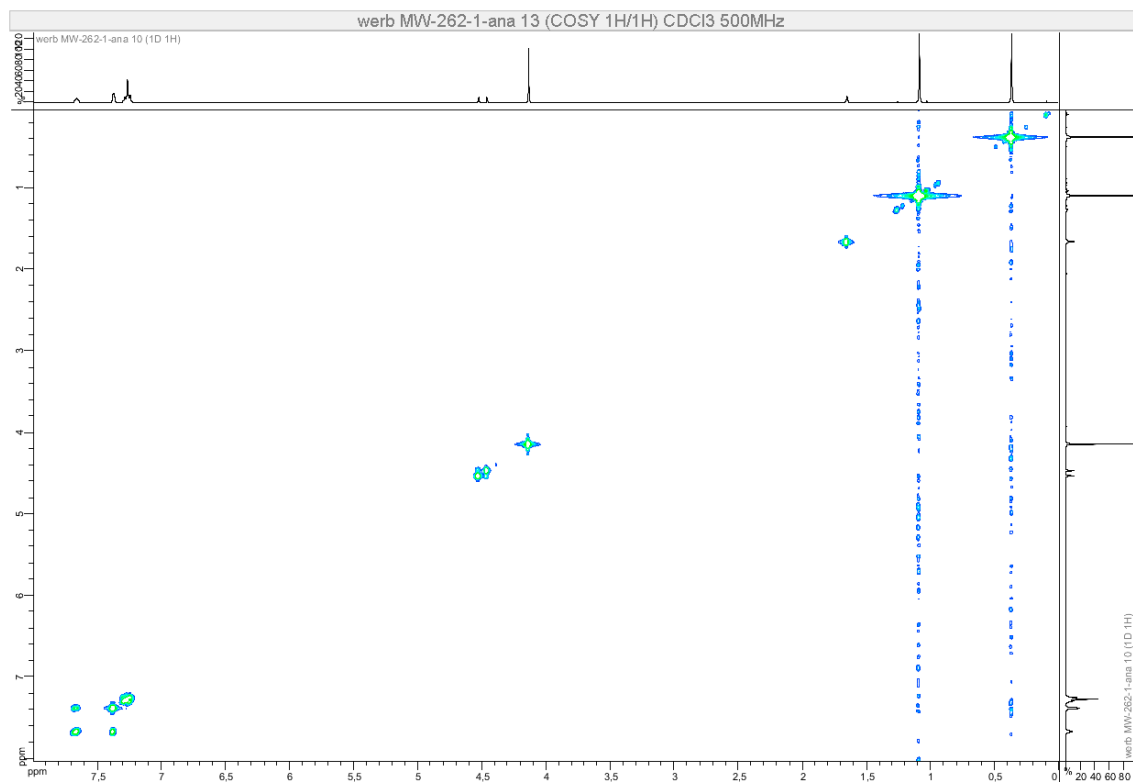
(*S,S*_P)-*S*-*tert*-Butyl-2-(diphenylphosphino)-5-(trimethylsilyl)ferrocenesulfoxide (*S,S*_P-2ea)

¹H NMR (500 MHz, CDCl₃) ^{13}C NMR (126 MHz, CDCl_3)

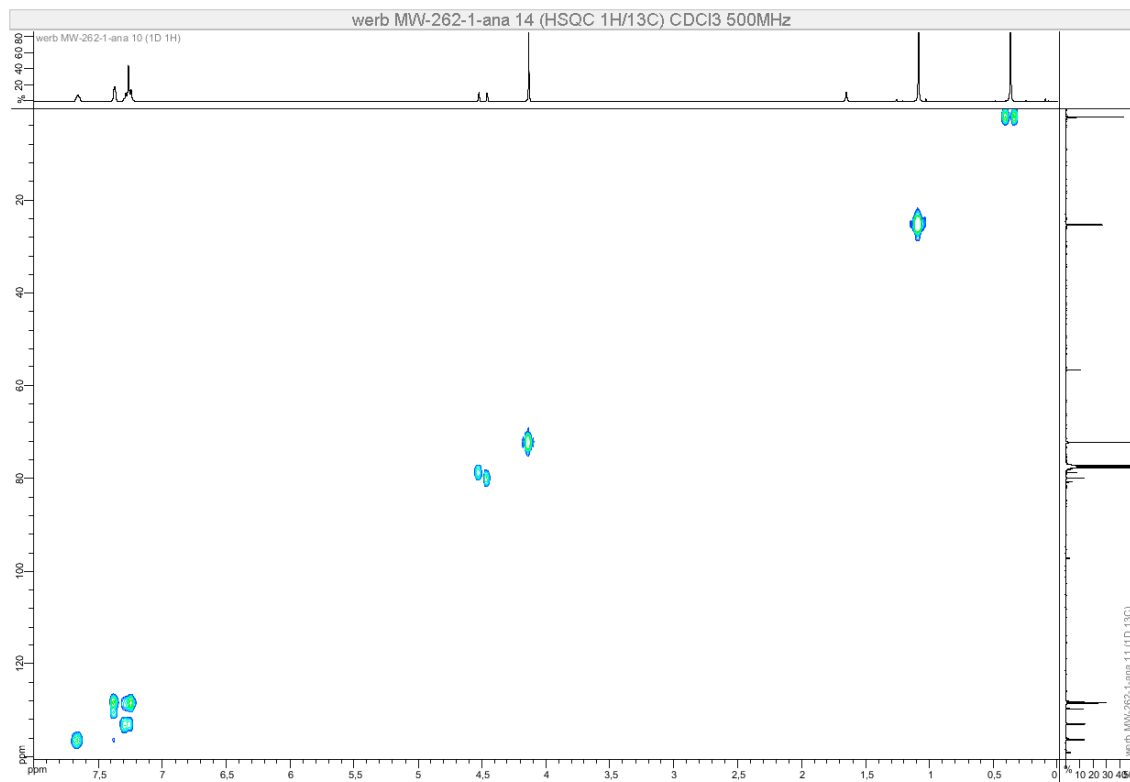
DEPT 135 (126 MHz, CDCl₃)



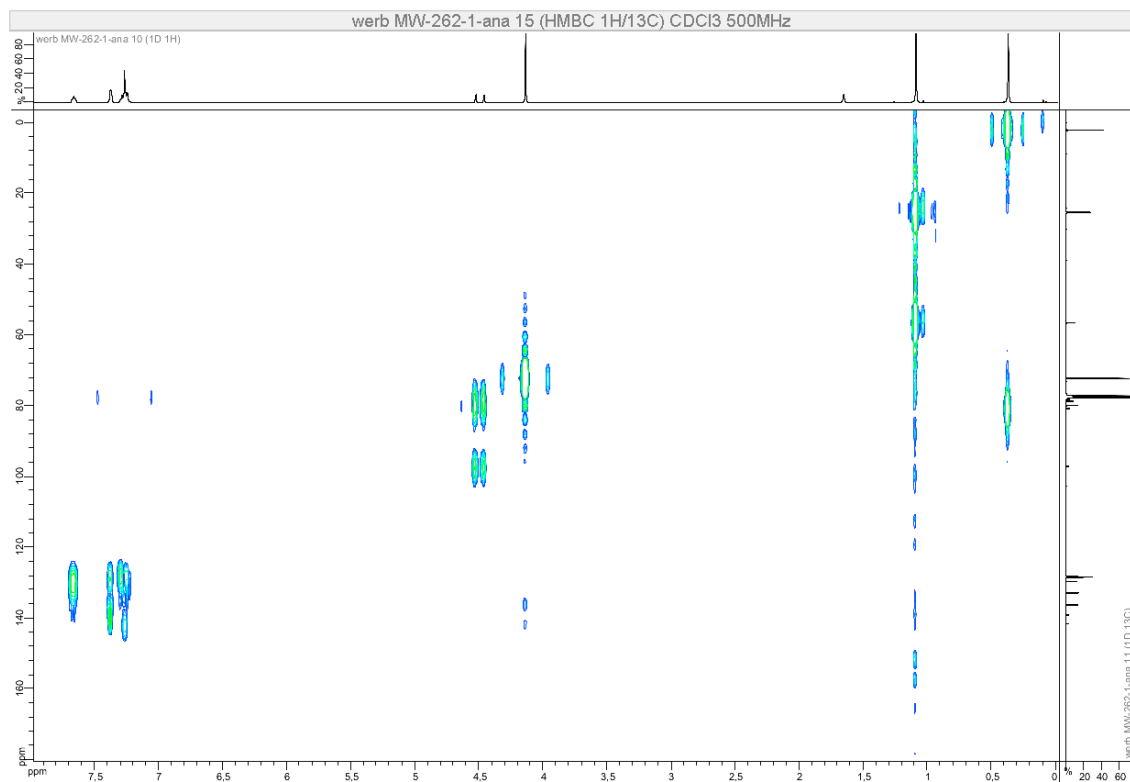
COSY (500 MHz, CDCl₃)



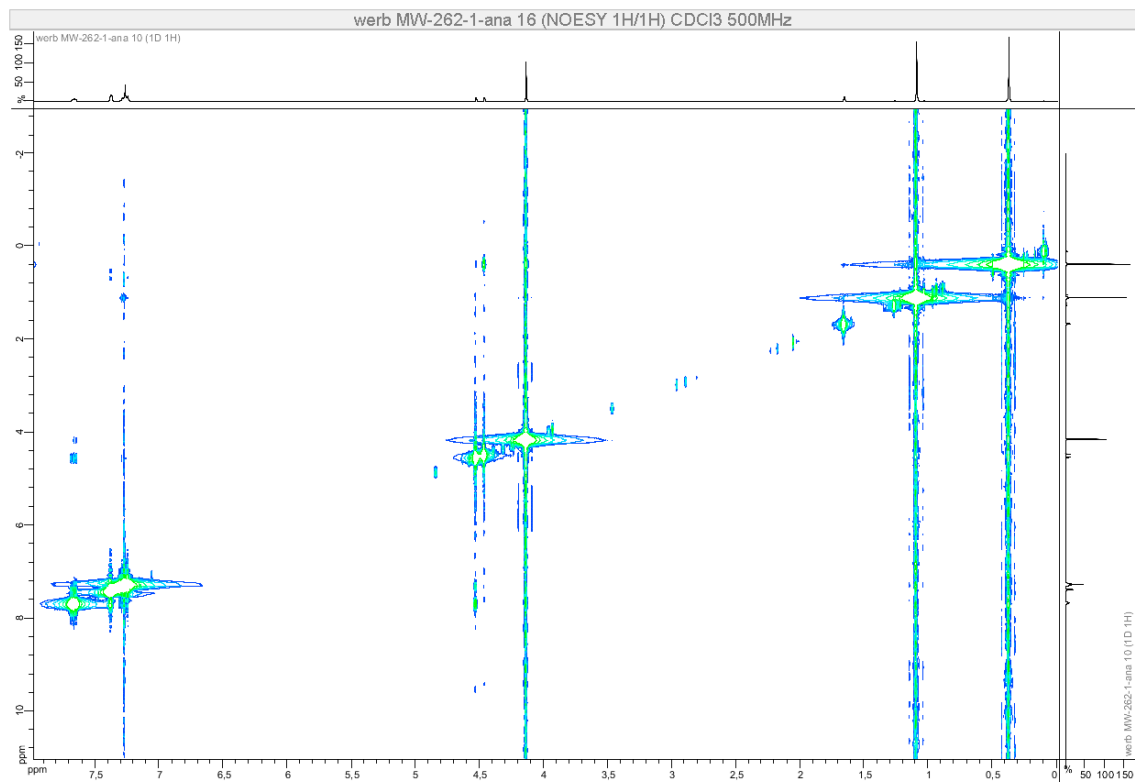
HSQC (500 MHz, CDCl₃)



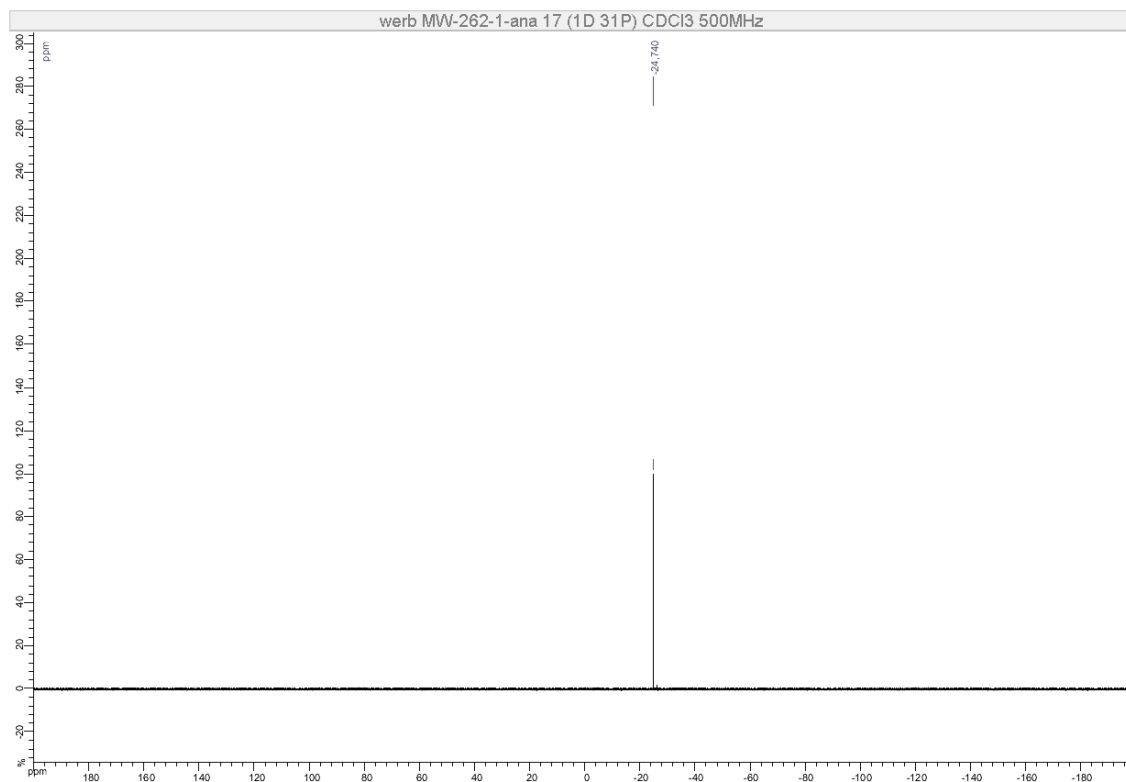
HMBC (500 MHz, CDCl₃)



NOESY (500 MHz, CDCl₃)

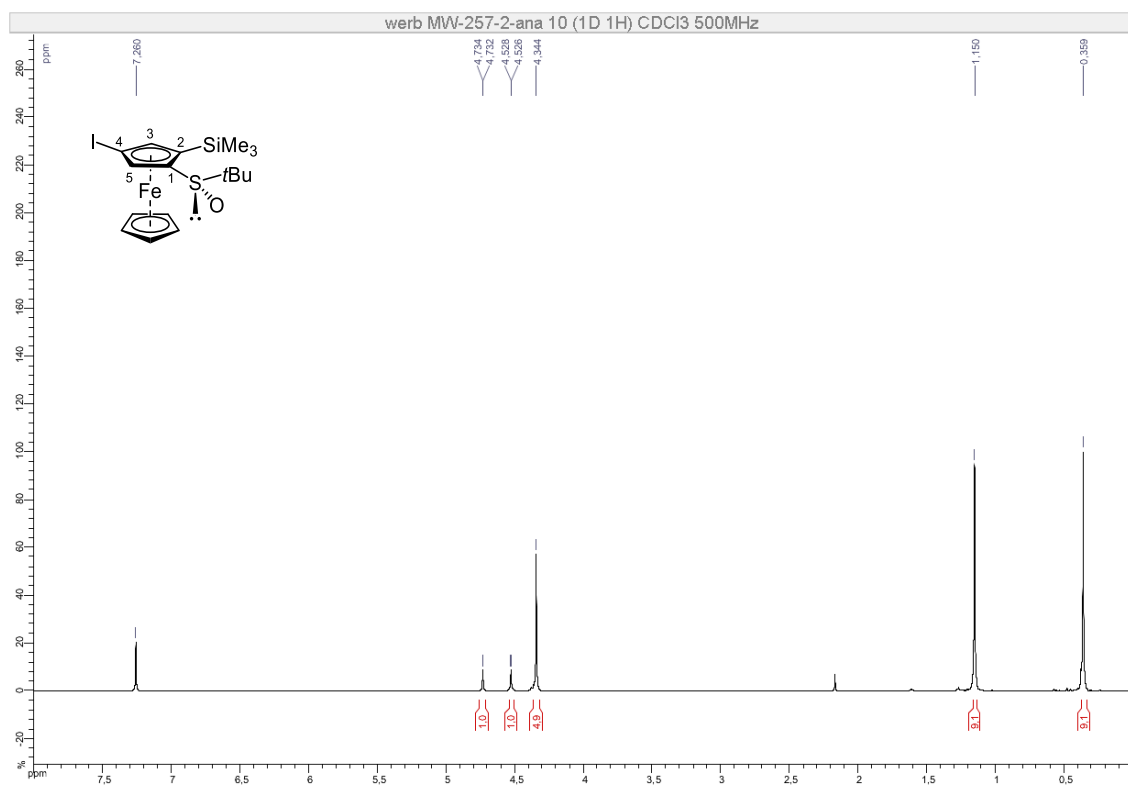


³¹P NMR (202 MHz, CDCl₃)

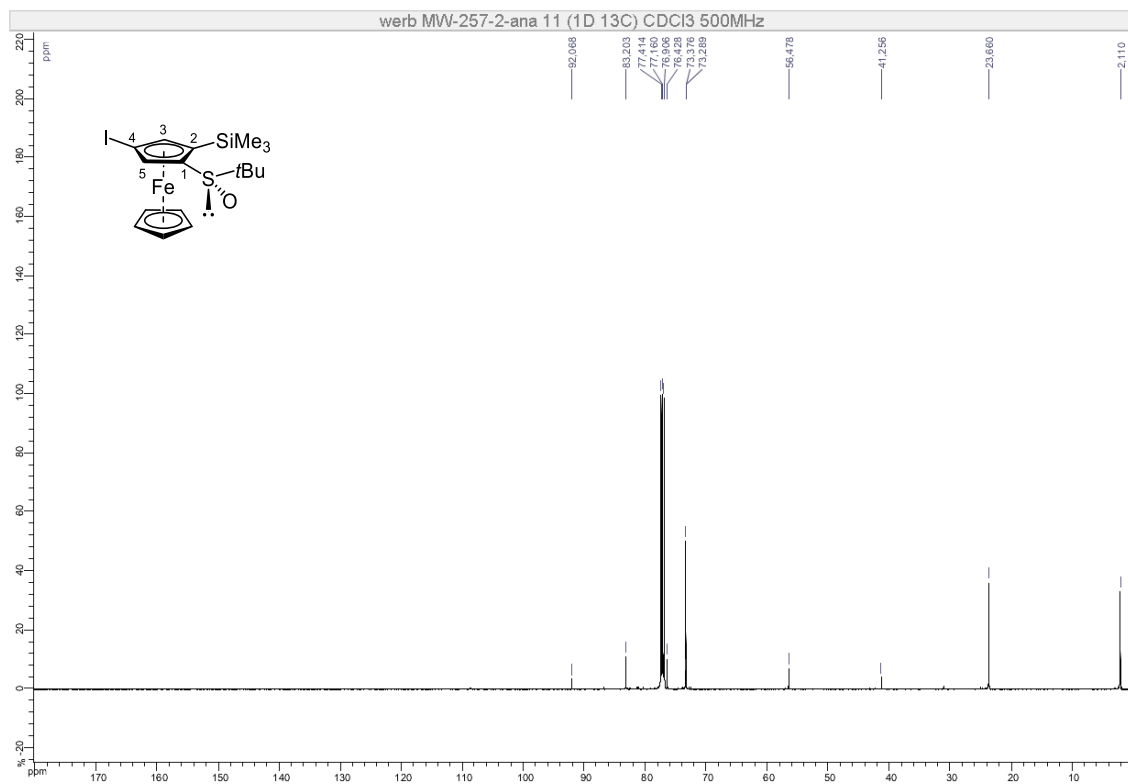


(*S,S*_P)-*S*-tert-Butyl-4-iodo-2-(trimethylsilyl)ferrocenesulfoxide (*S,S*_P-7)

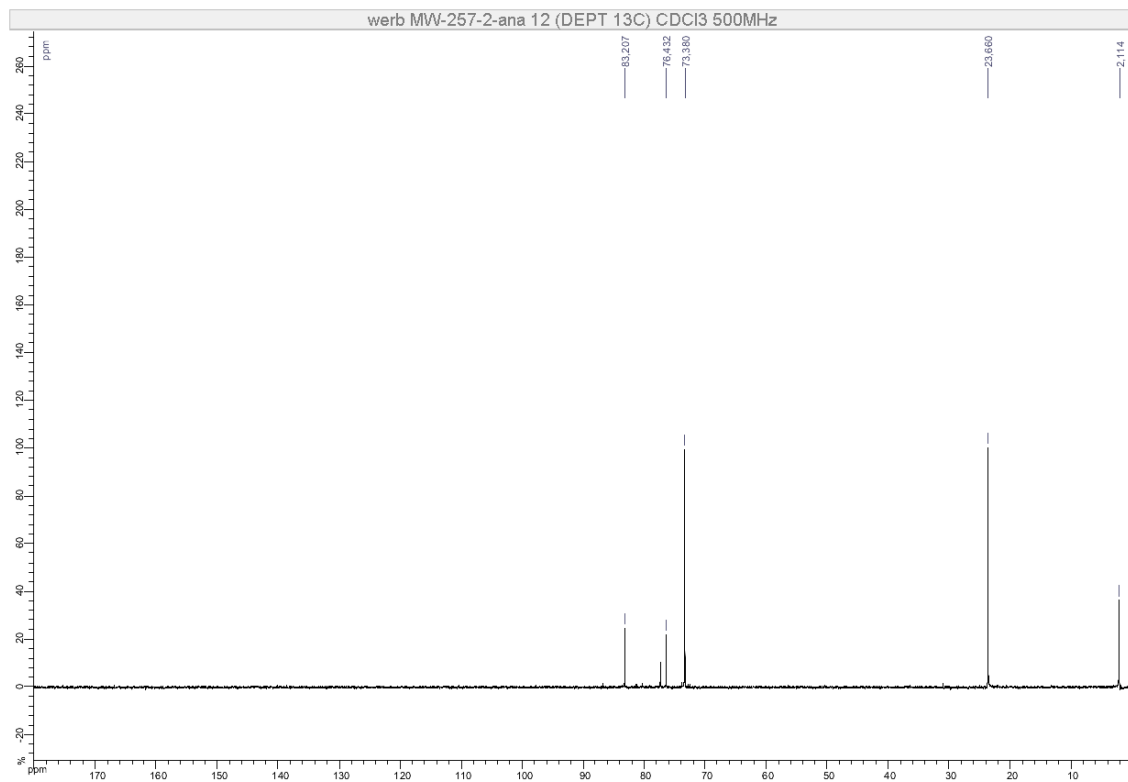
¹H NMR (500 MHz, CDCl₃)



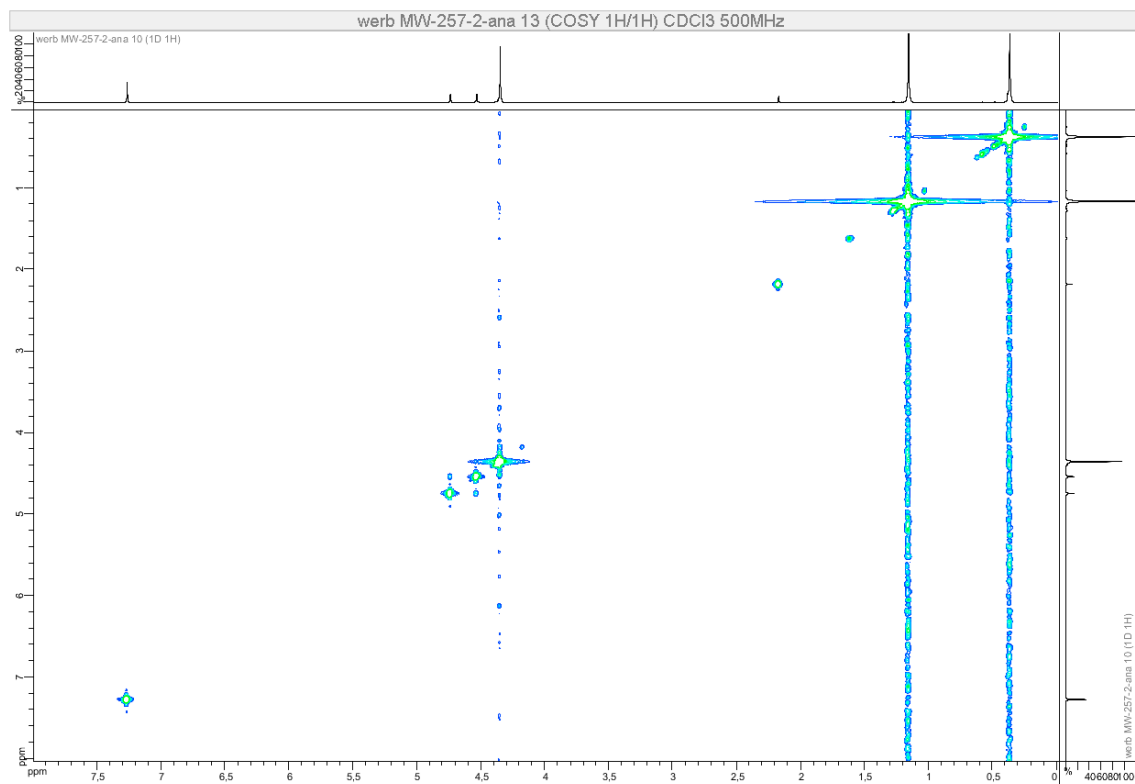
¹³C NMR (126 MHz, CDCl₃)



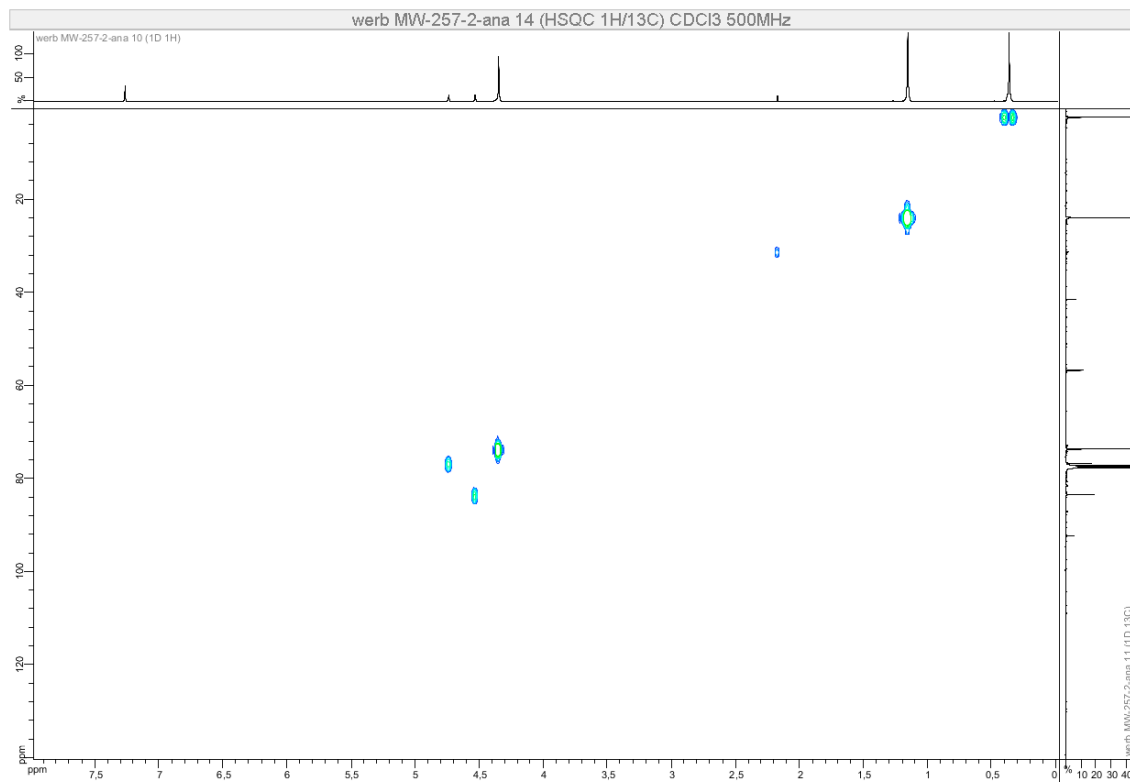
DEPT 135 (126 MHz, CDCl₃)



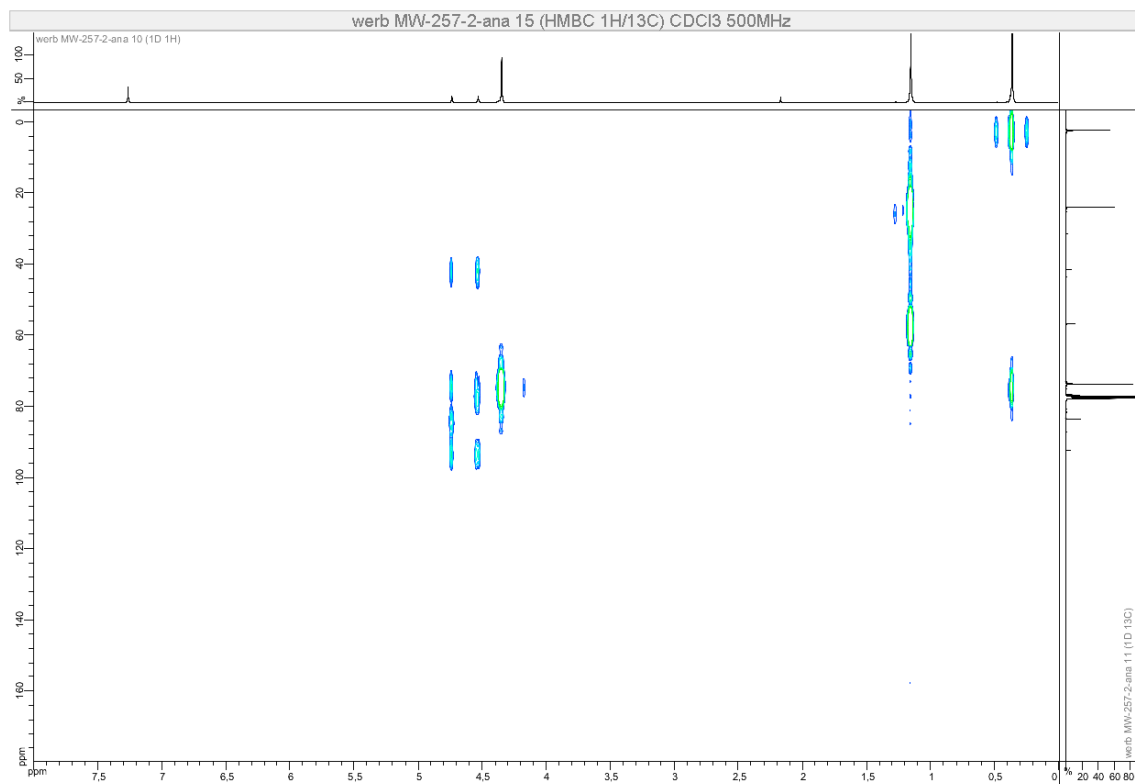
COSY (500 MHz, CDCl₃)



HSQC (500 MHz, CDCl₃)

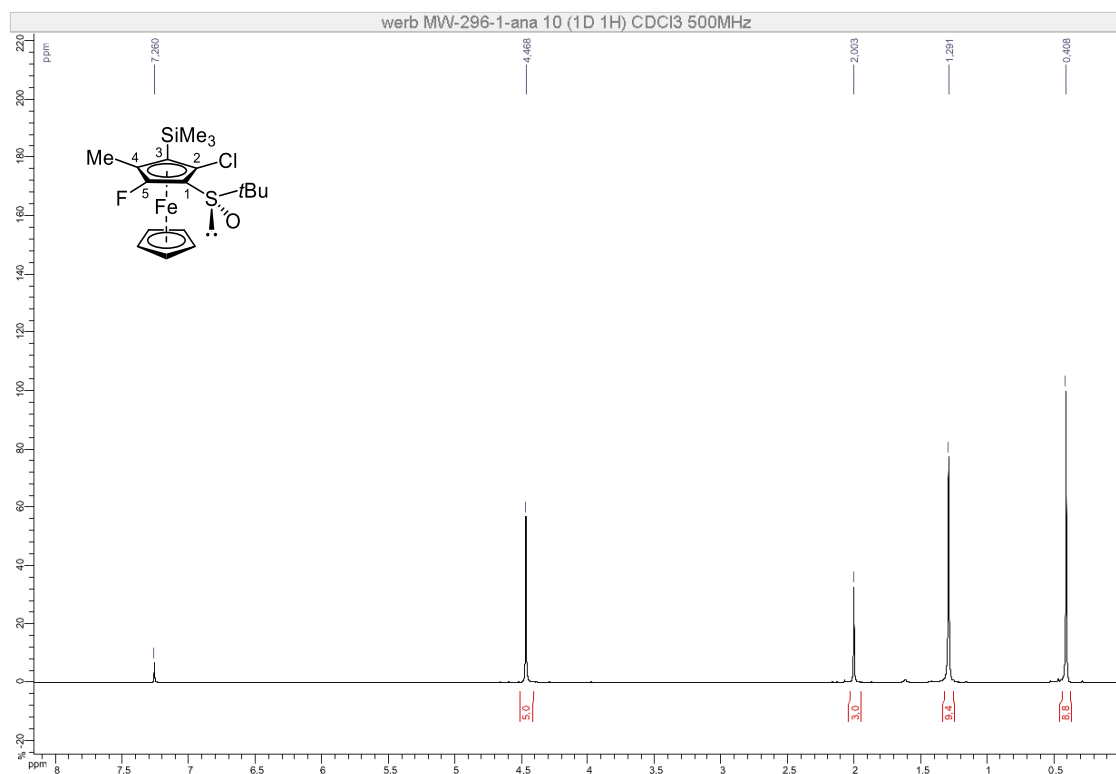


HMBC (500 MHz, CDCl₃)

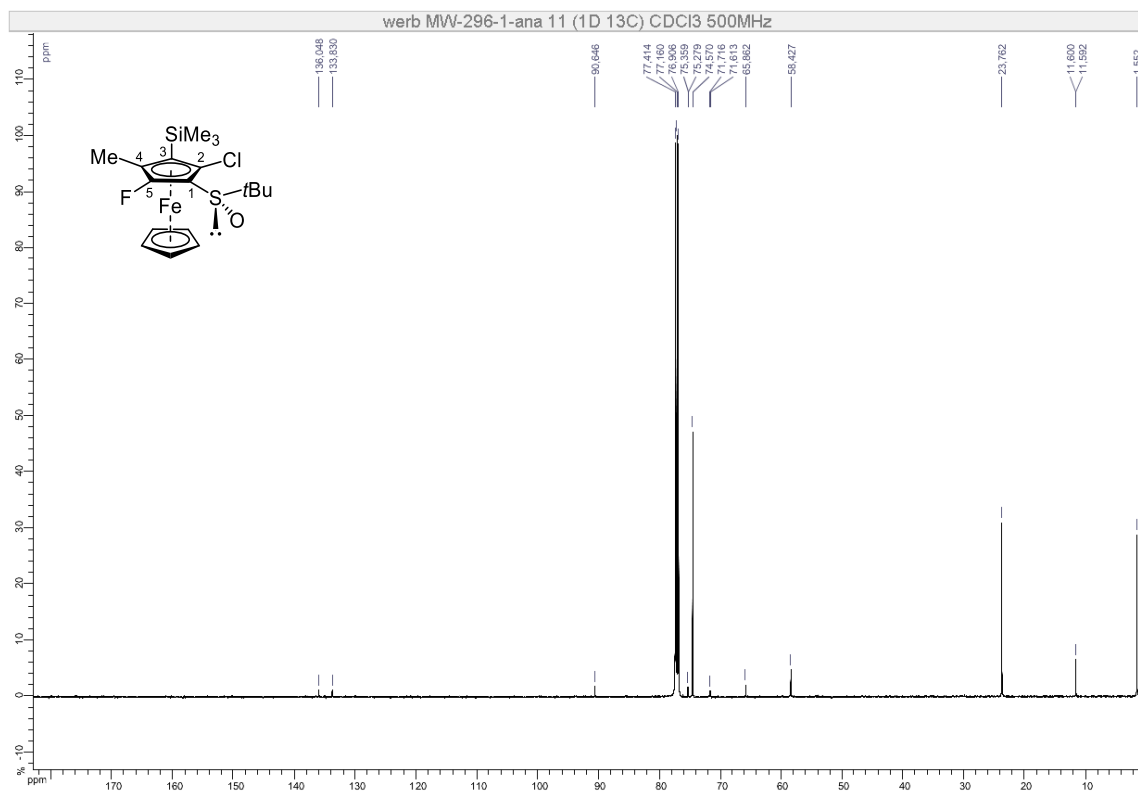


(*S,S*_P)-*S*-tert-Butyl-2-chloro-5-fluoro-4-methyl-3-(trimethylsilyl)ferrocenesulfoxide (*S,S*_P-12)

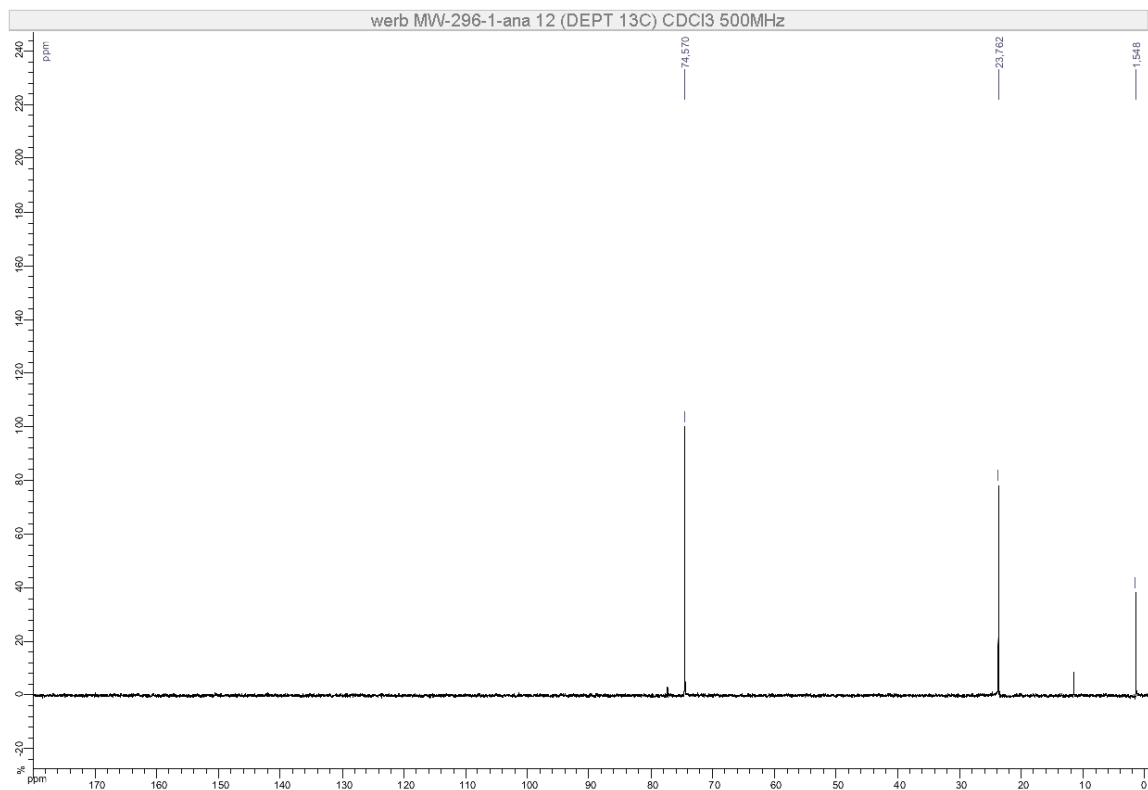
¹H NMR (500 MHz, CDCl₃)



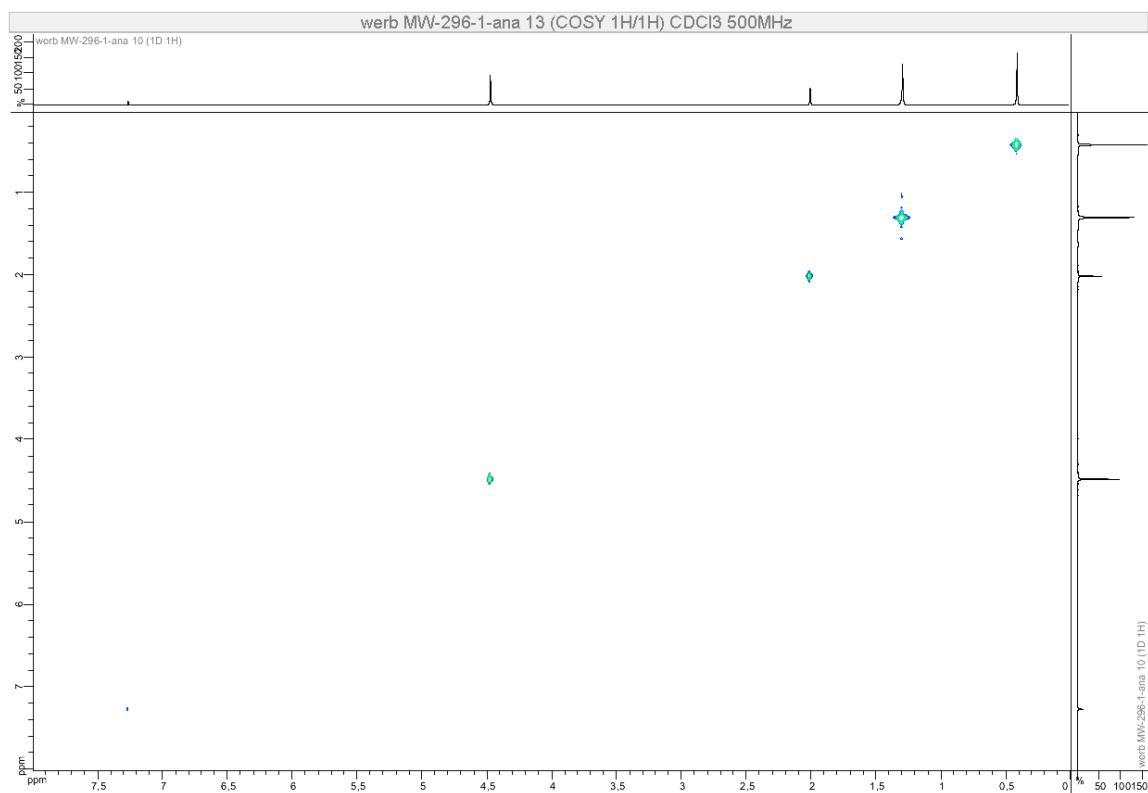
¹³C NMR (126 MHz, CDCl₃)



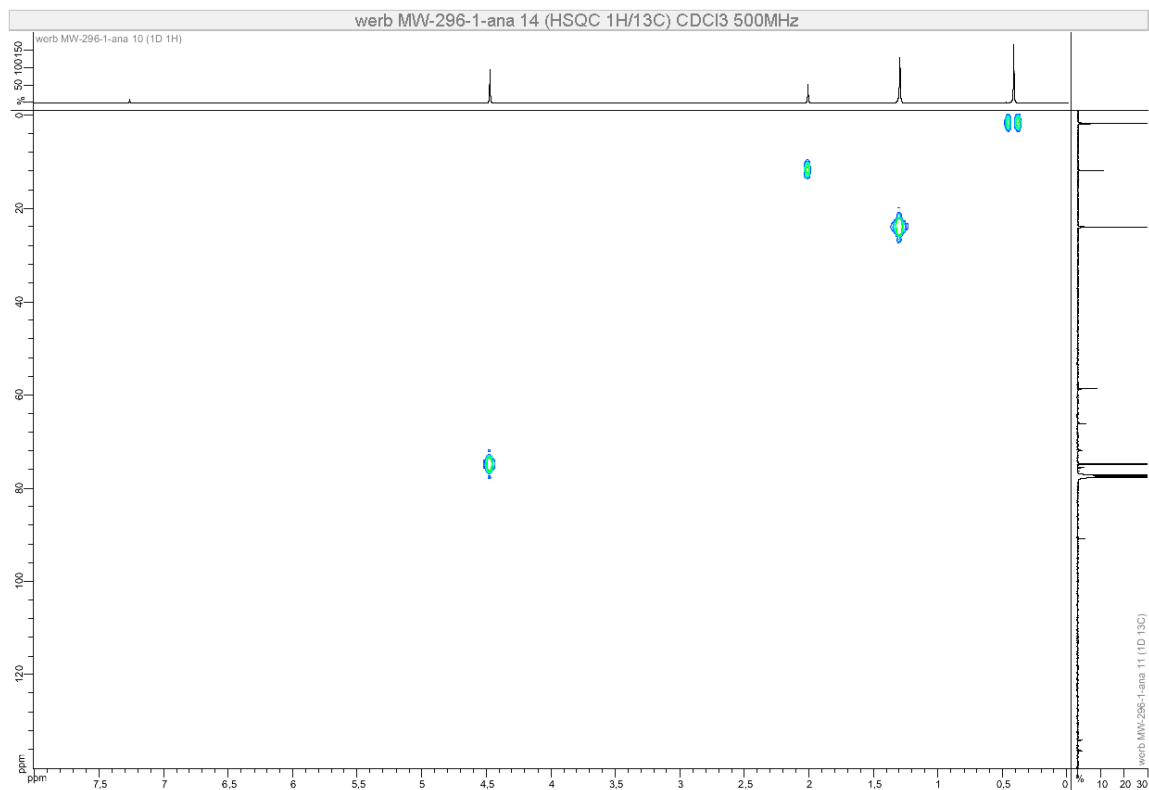
DEPT 135 (126 MHz, CDCl₃)



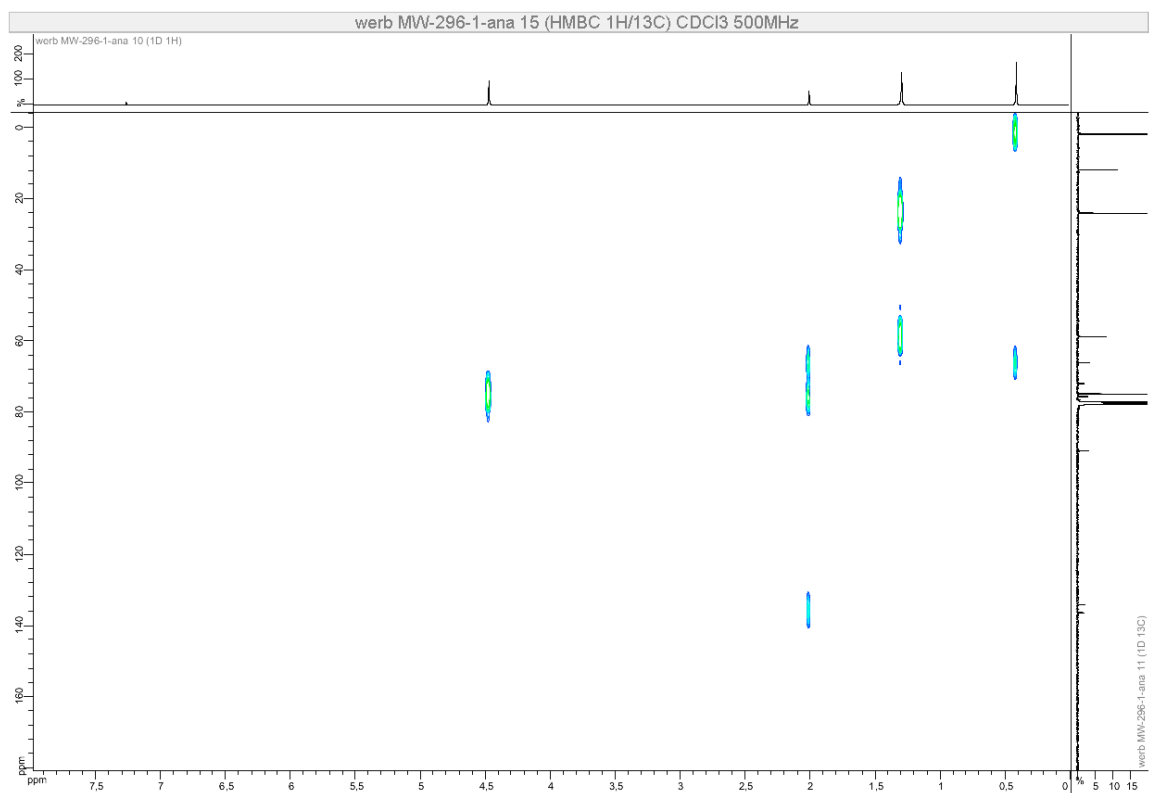
COSY (500 MHz, CDCl₃)



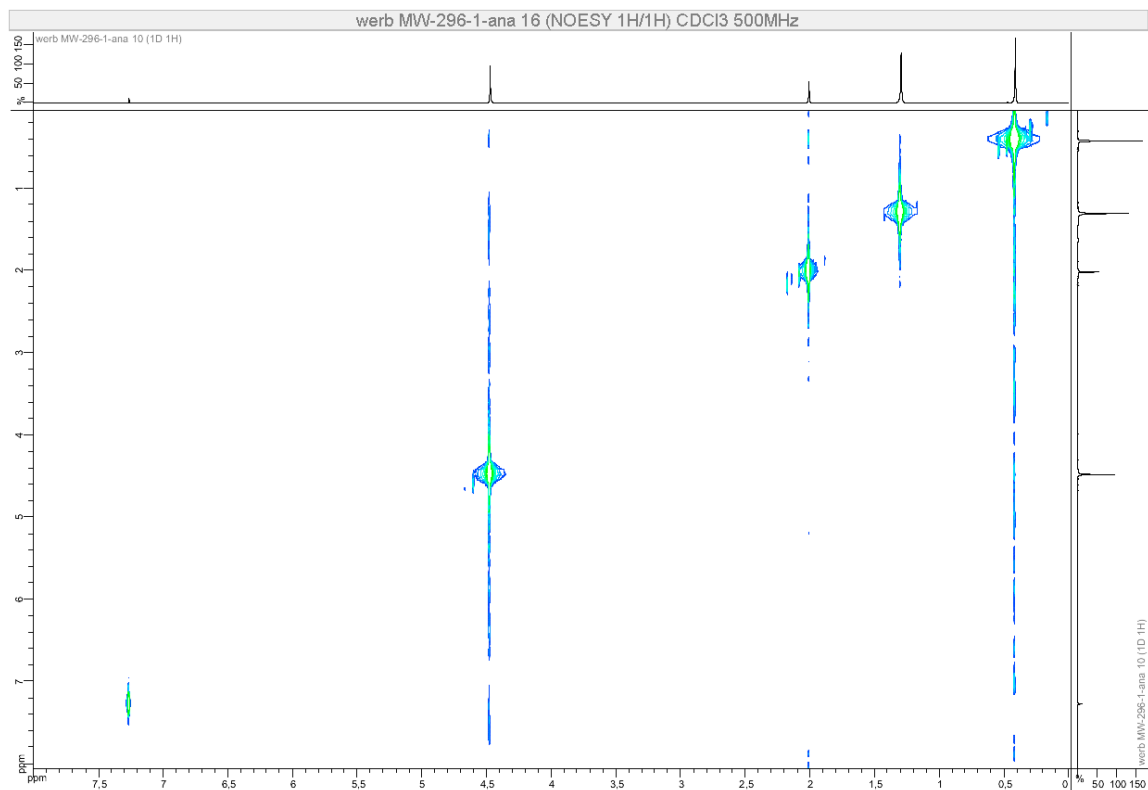
HSQC (500 MHz, CDCl₃)



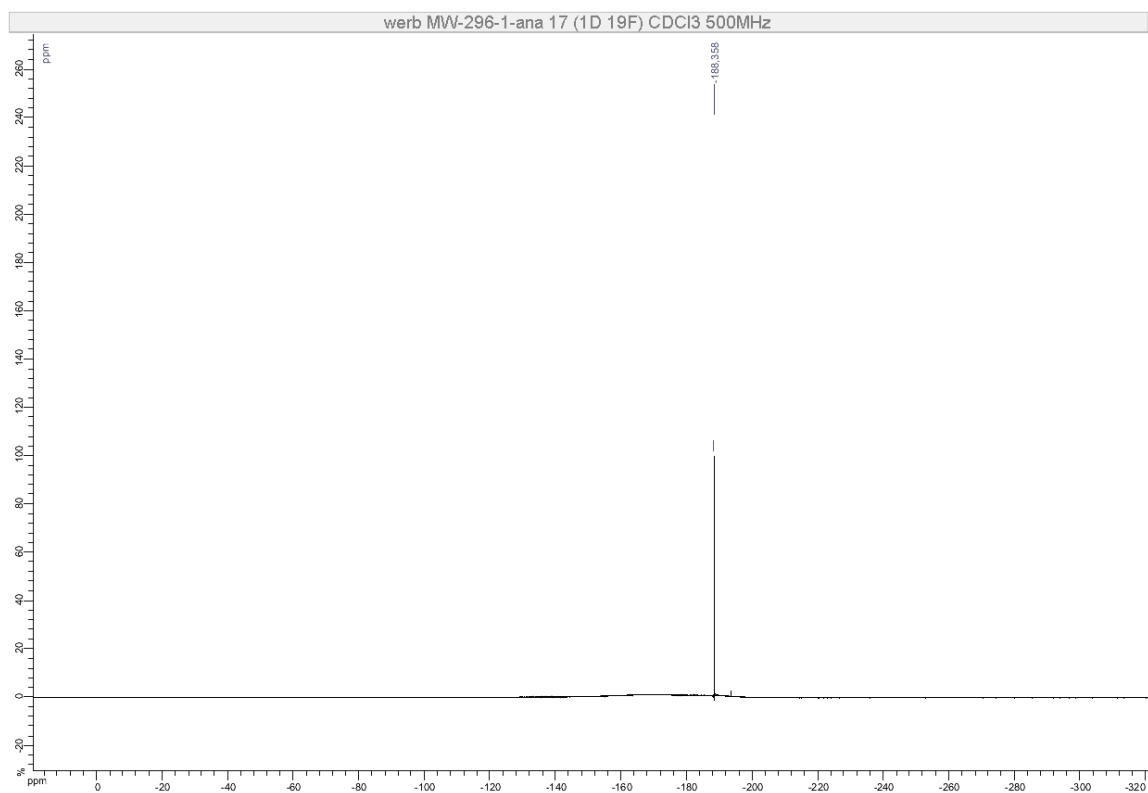
HMBC (500 MHz, CDCl₃)



NOESY (500 MHz, CDCl₃)

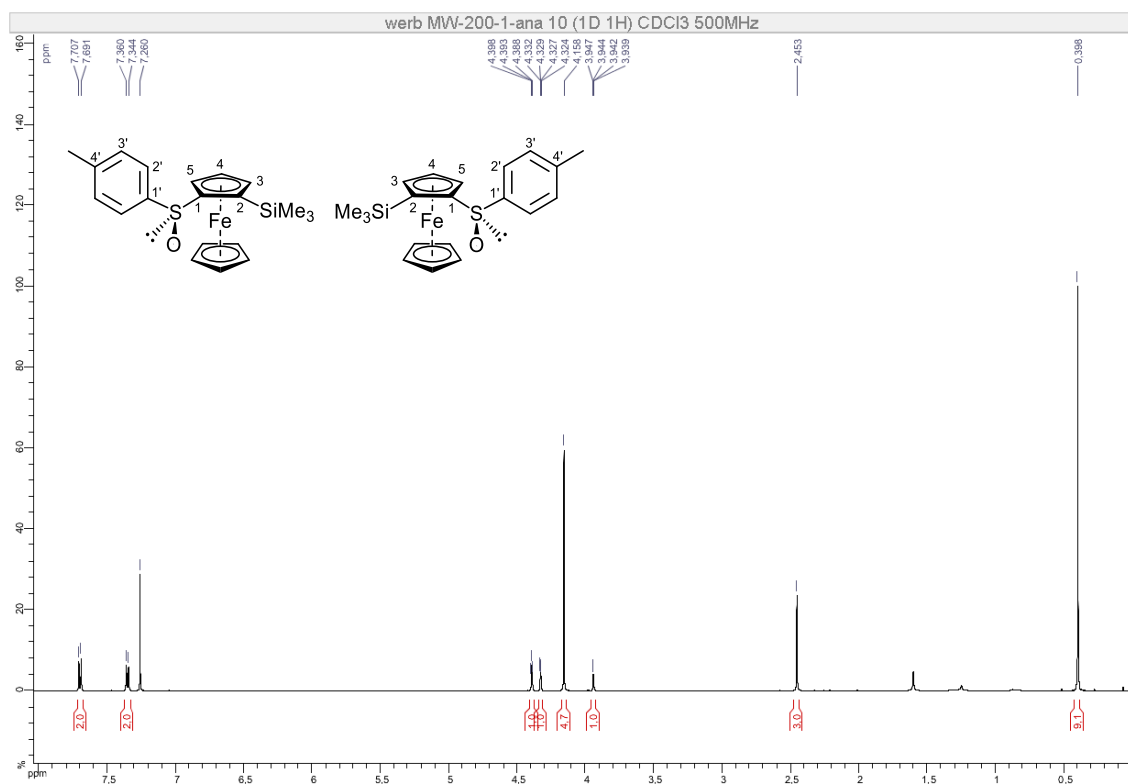


¹⁹F NMR (471 MHz, CDCl₃)

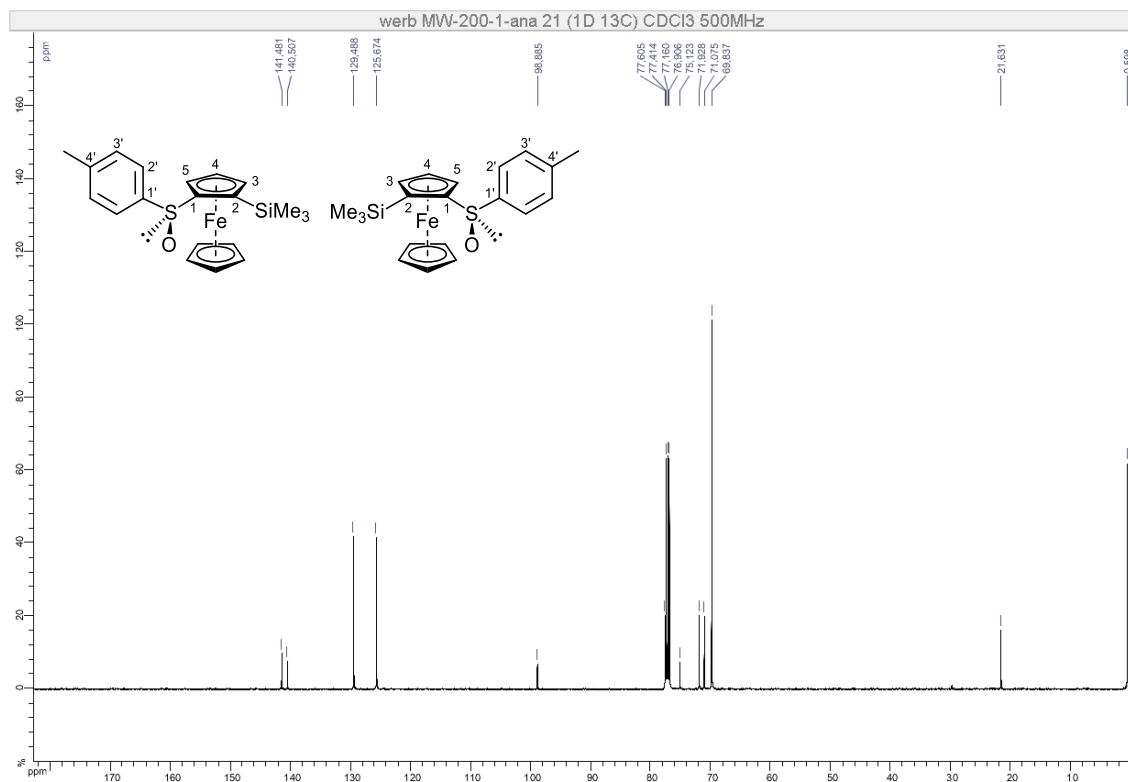


(*R,R*_P)- and (*S,S*_P)-*S*-(4-Tolyl)-2-(trimethylsilyl)ferrocenesulfoxide (*R,R*_P/*S,S*_P-3a)

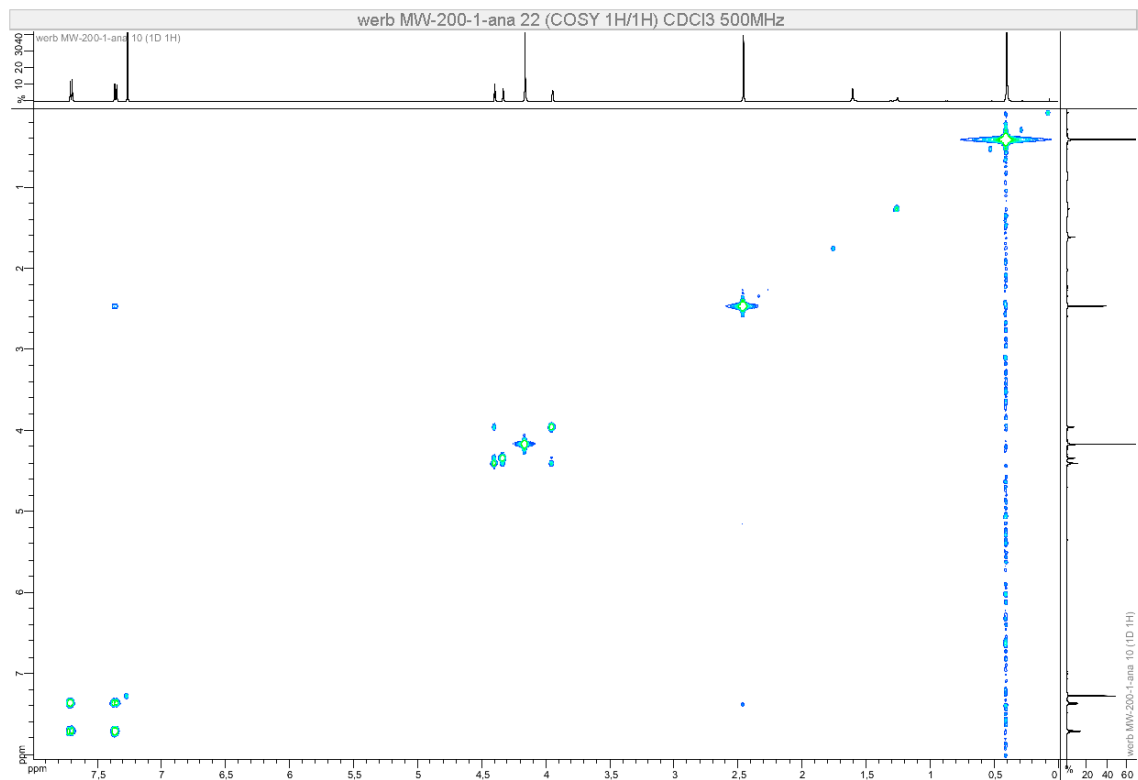
¹H NMR (500 MHz, CDCl₃)



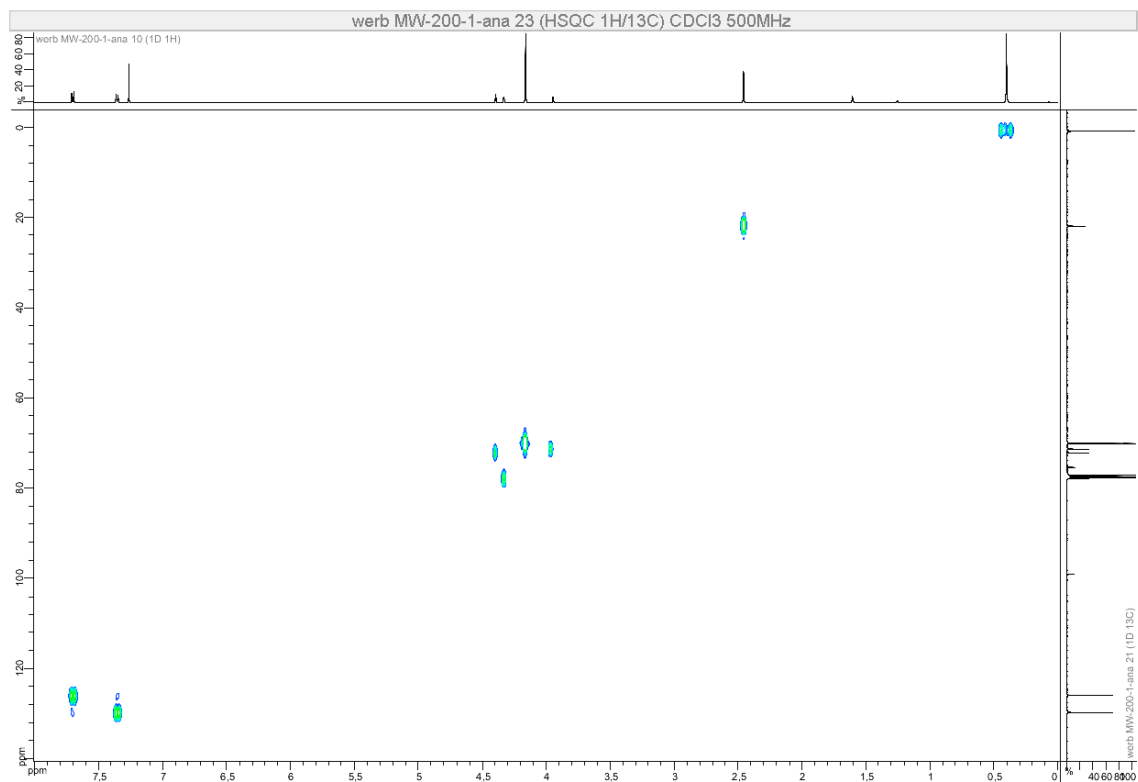
¹³C NMR (126 MHz, CDCl₃)



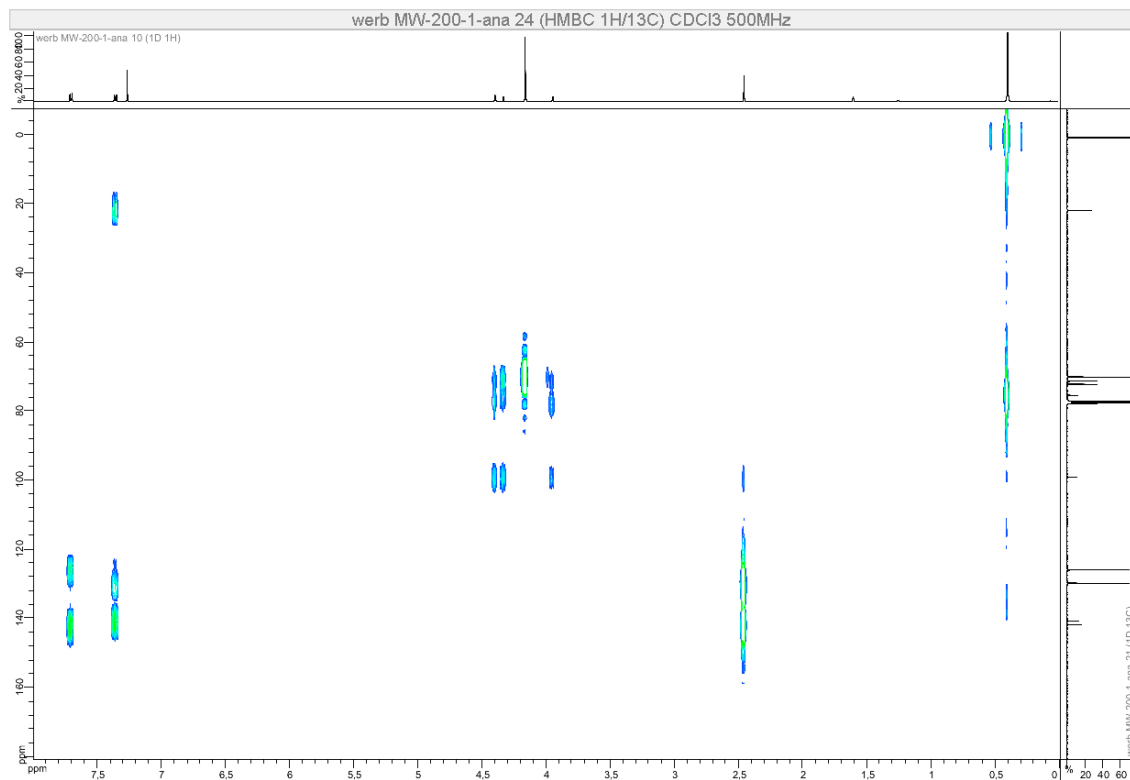
COSY (500 MHz, CDCl₃)



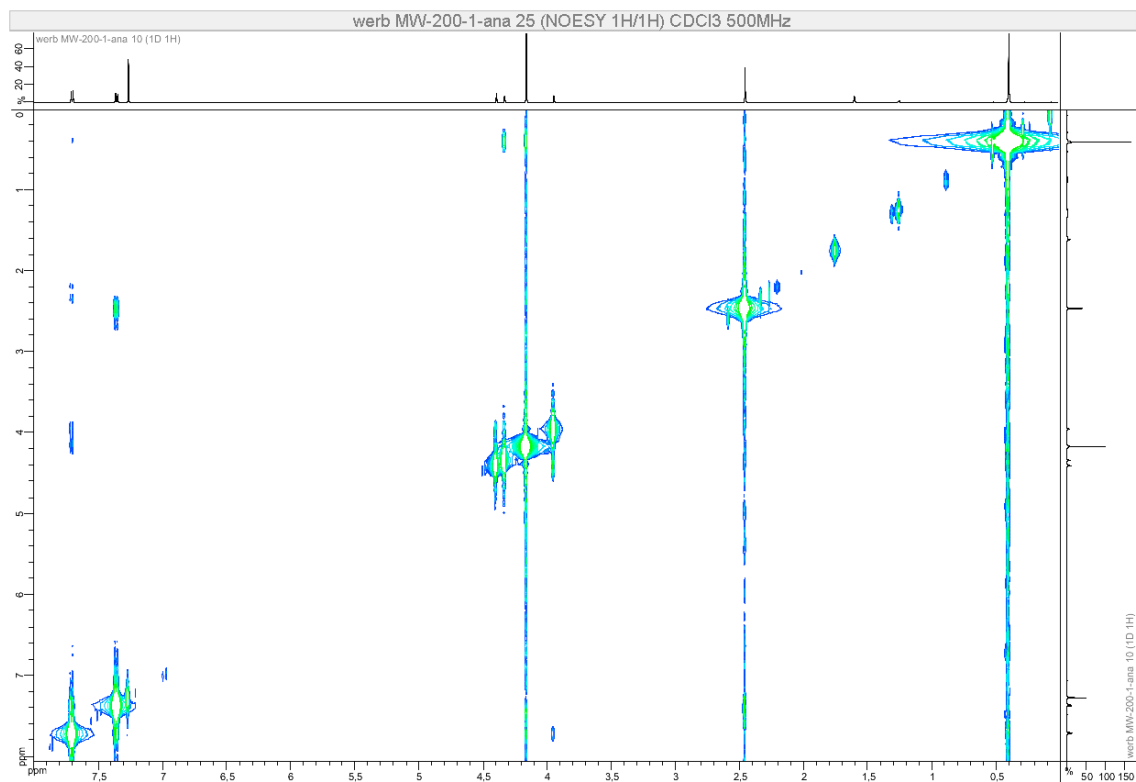
HSQC (500 MHz, CDCl₃)



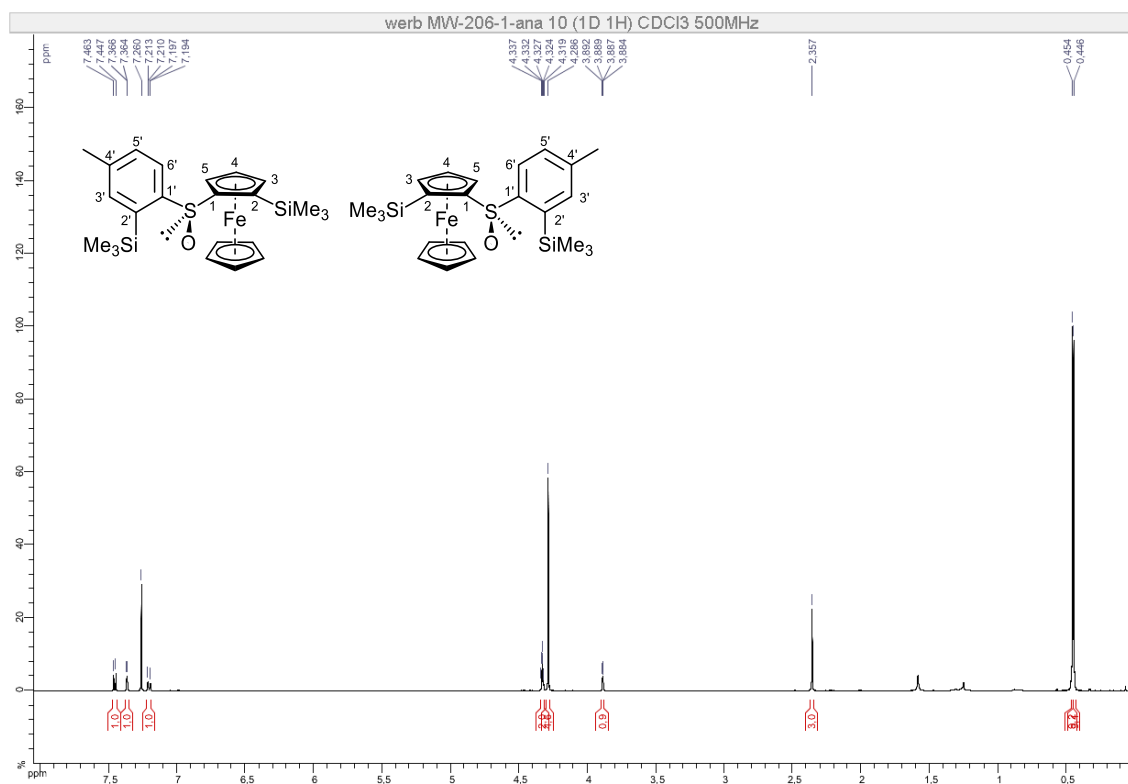
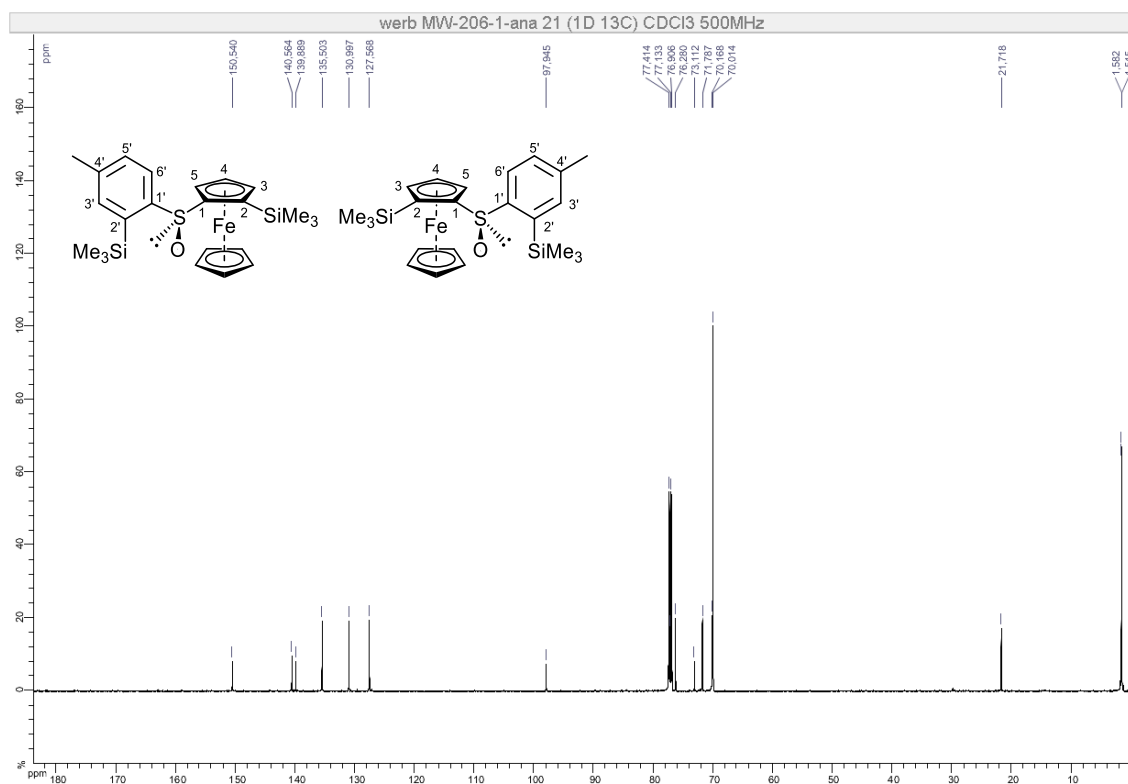
HMBC (500 MHz, CDCl₃)



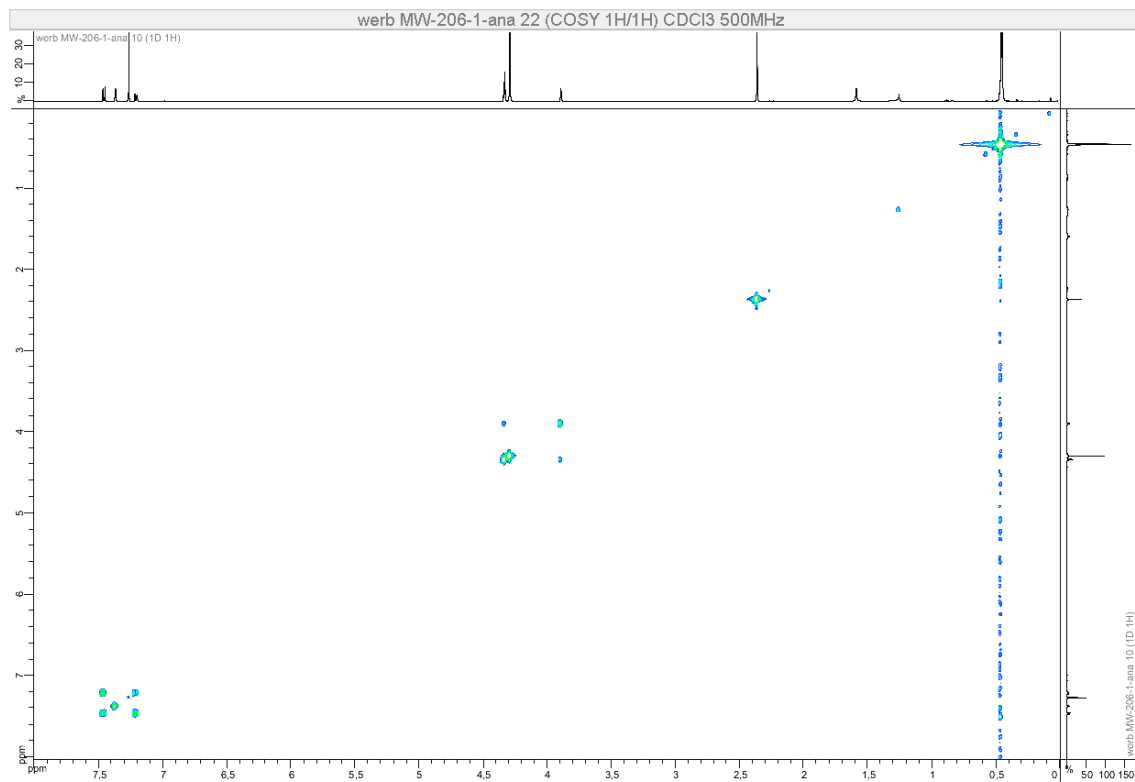
NOESY (500 MHz, CDCl₃)



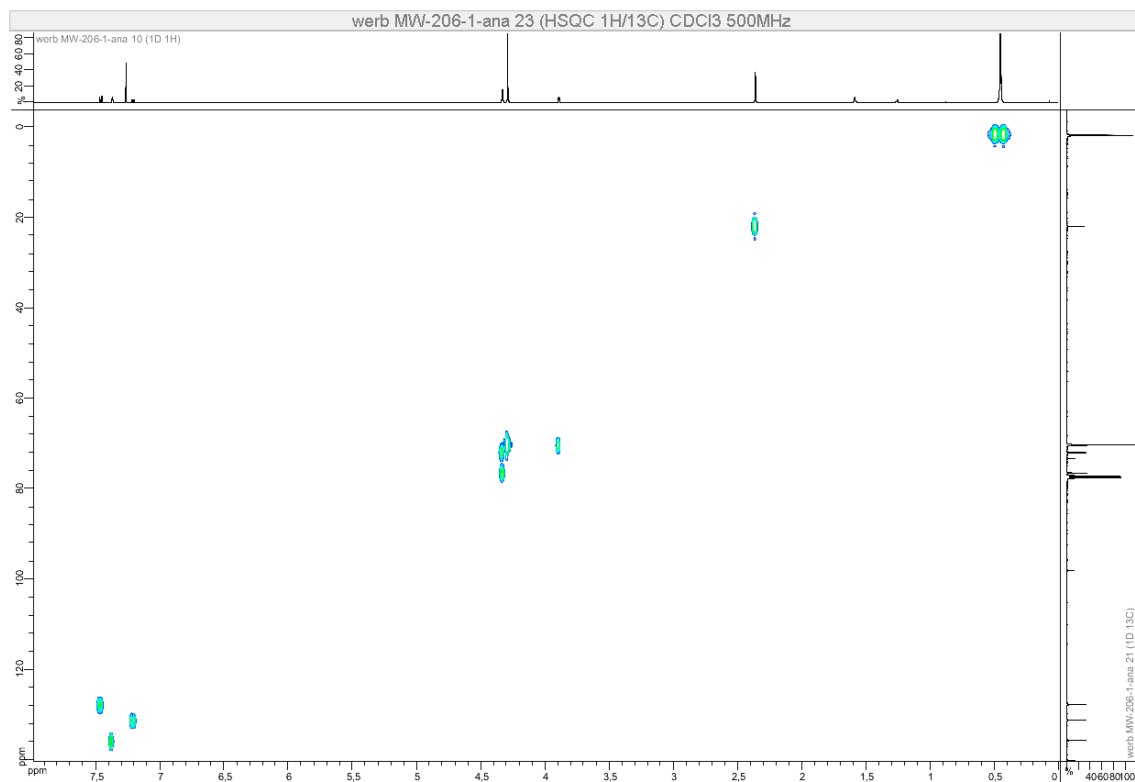
(*R,R*)- and (*S,S*)-*S*-[4-Methyl-2-(trimethylsilyl)phenyl]-2-(trimethylsilyl)ferrocenesulfoxide (*R,R*/*S,S*-3a')

¹H NMR (500 MHz, CDCl₃) ^{13}C NMR (126 MHz, CDCl_3)

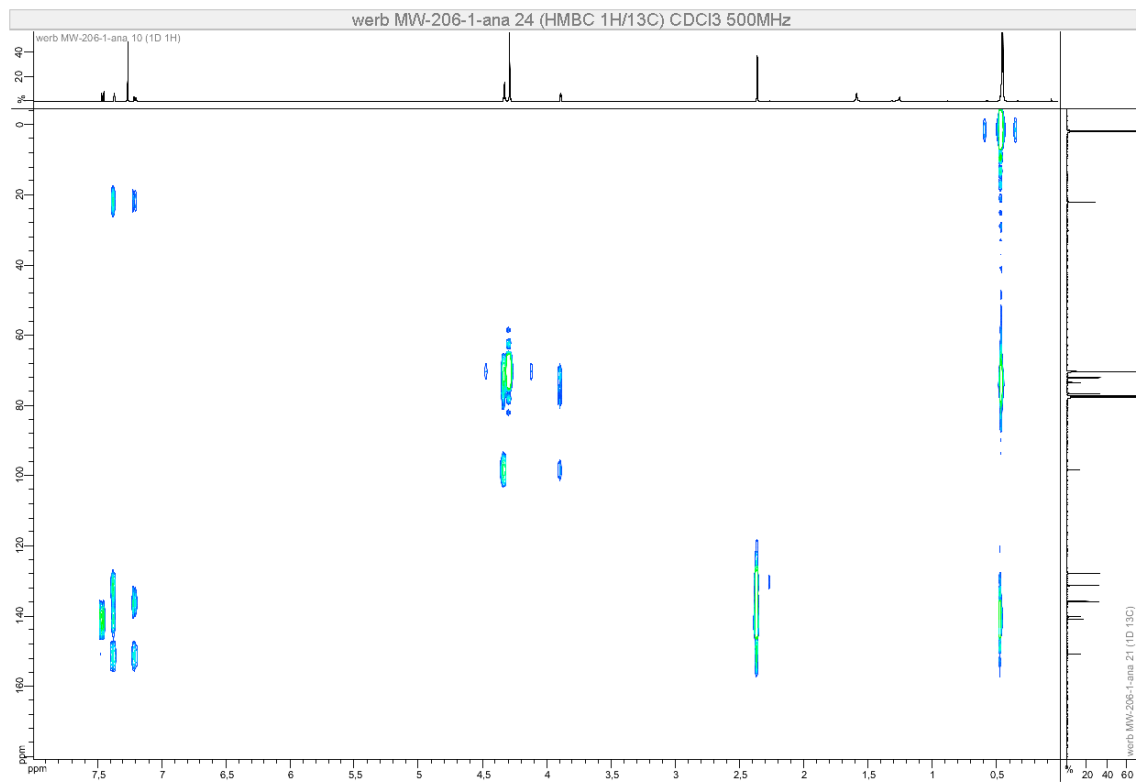
COSY (500 MHz, CDCl₃)



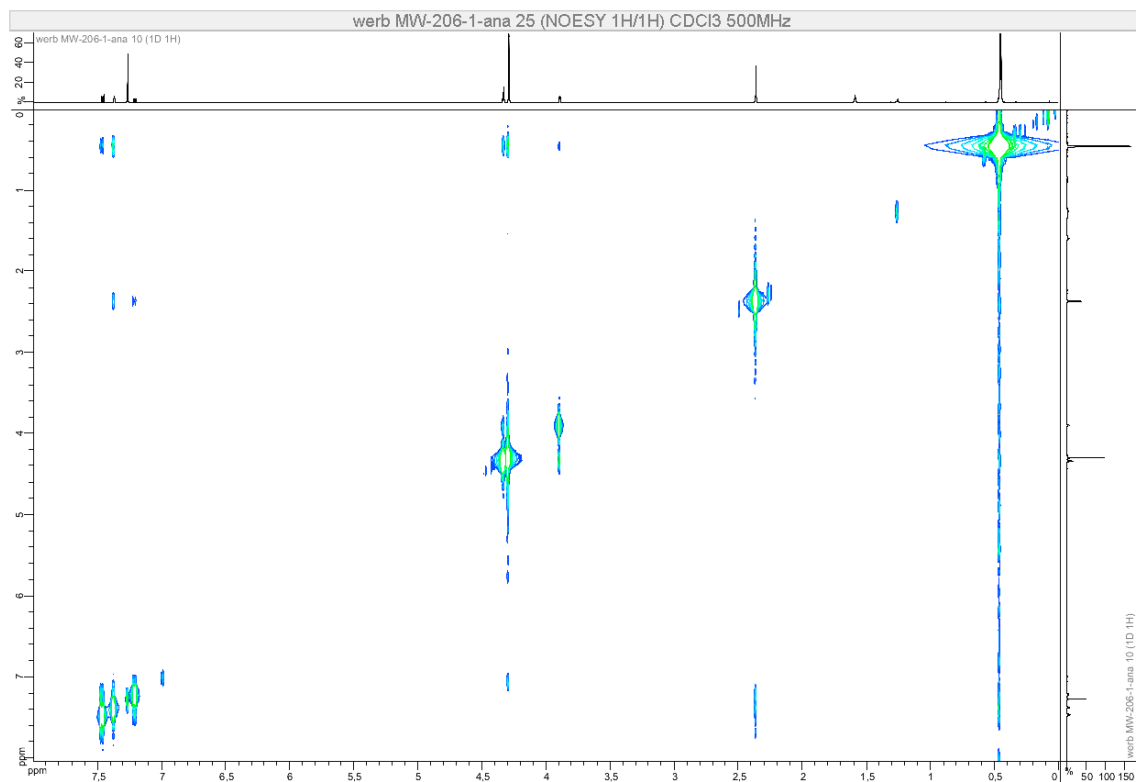
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

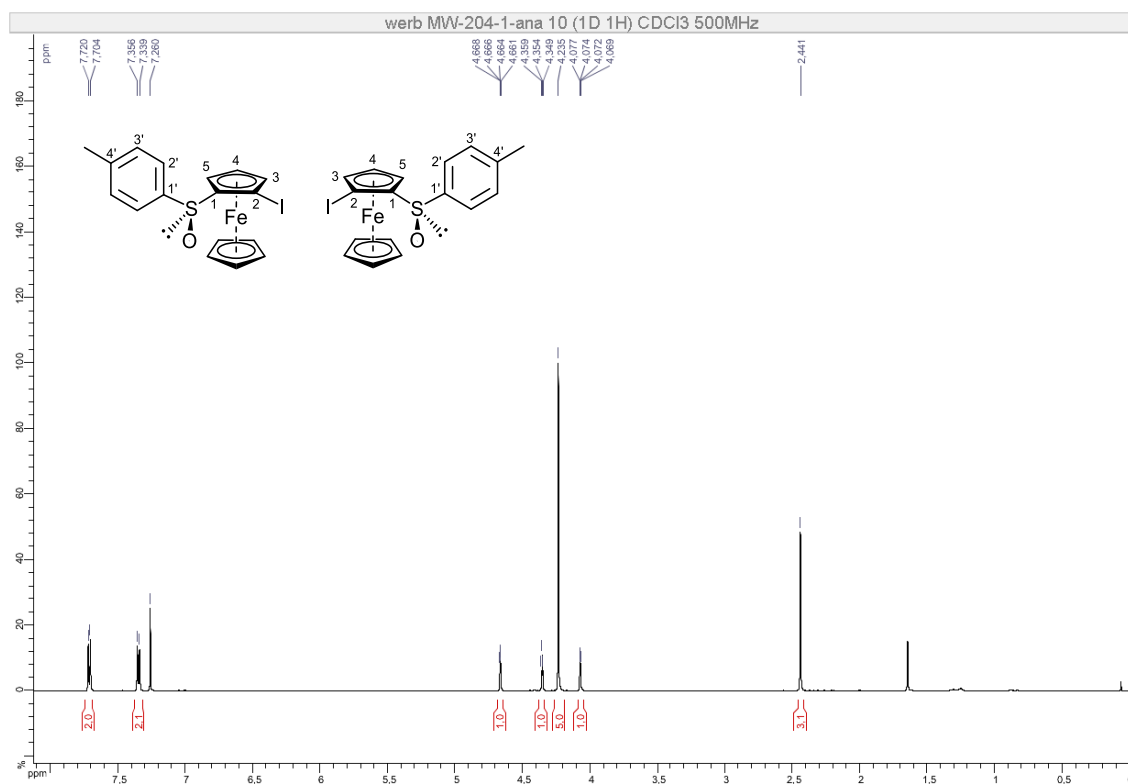


NOESY (500 MHz, CDCl₃)

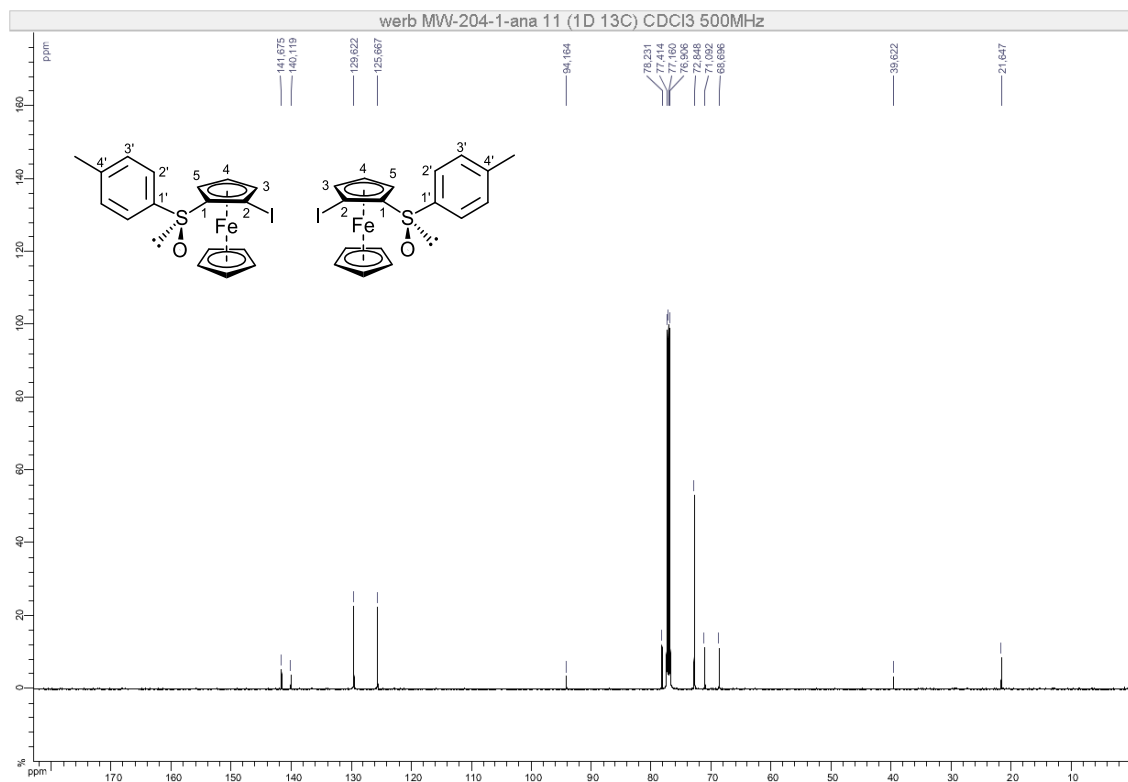


(*R,S_P*)- and (*S,R_P*)-2-Iodo-*S*-(4-tolyl)ferrocenesulfoxide (*R,S_P*/*S,R_P*-3b)

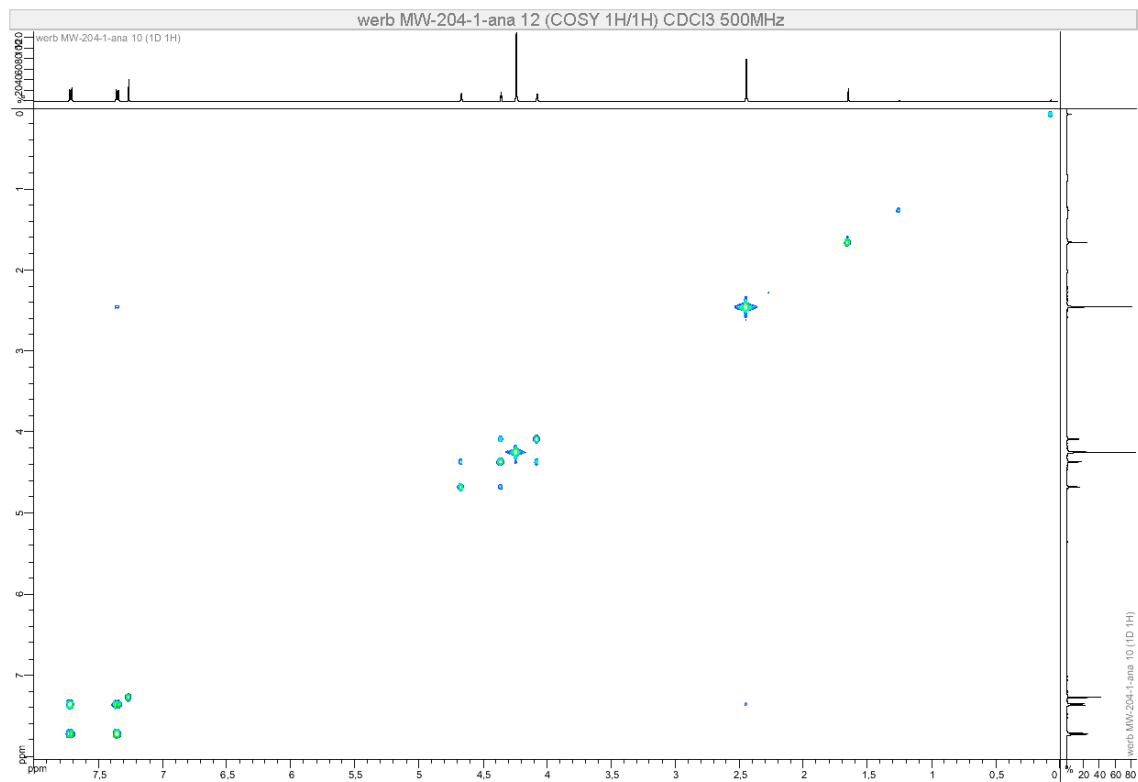
¹H NMR (500 MHz, CDCl₃)



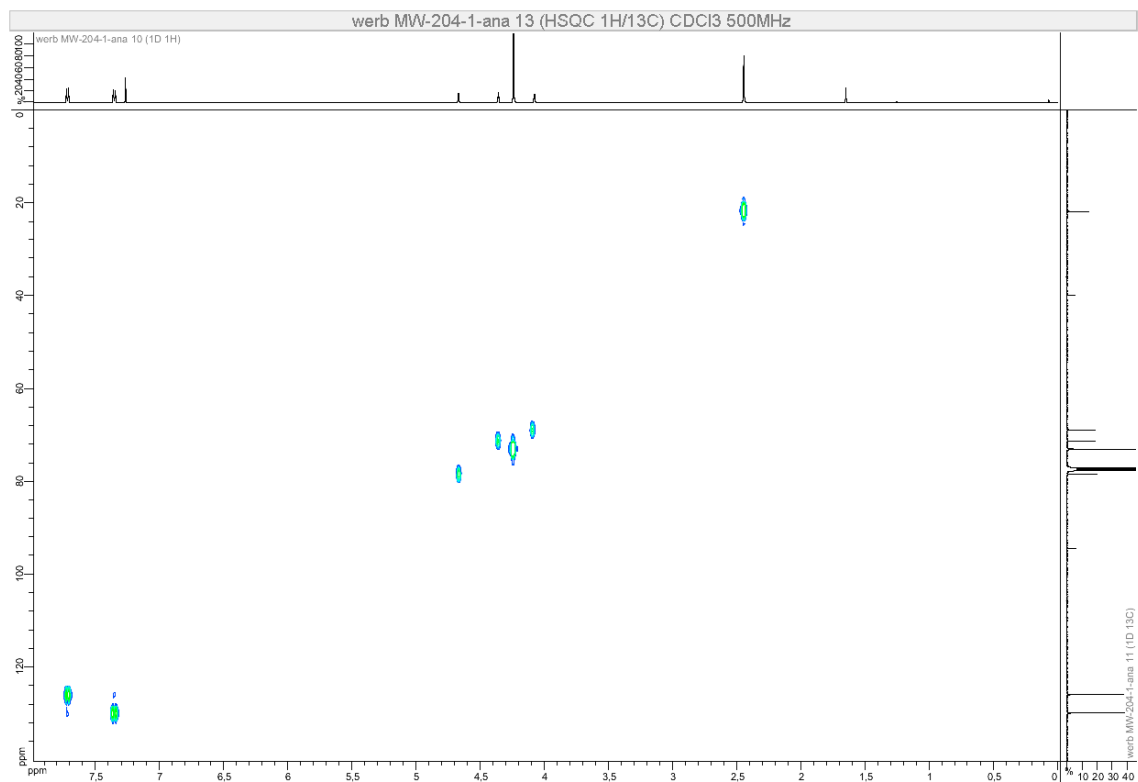
¹³C NMR (126 MHz, CDCl₃)



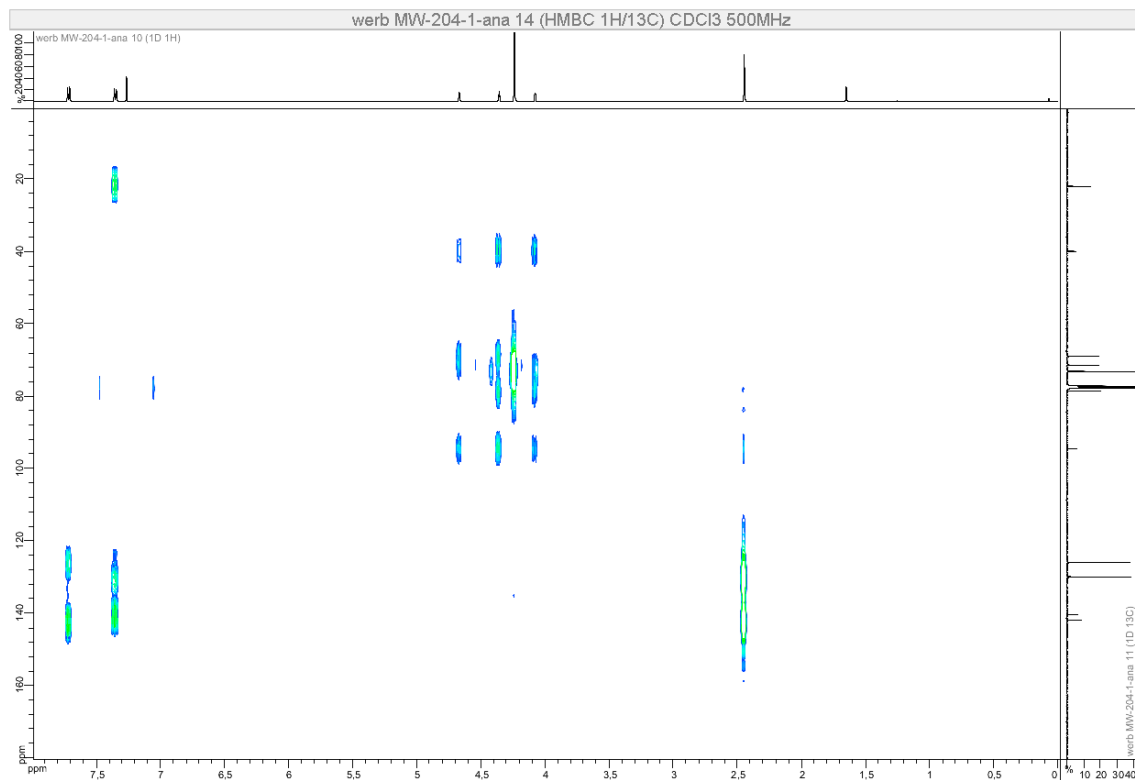
COSY (500 MHz, CDCl₃)



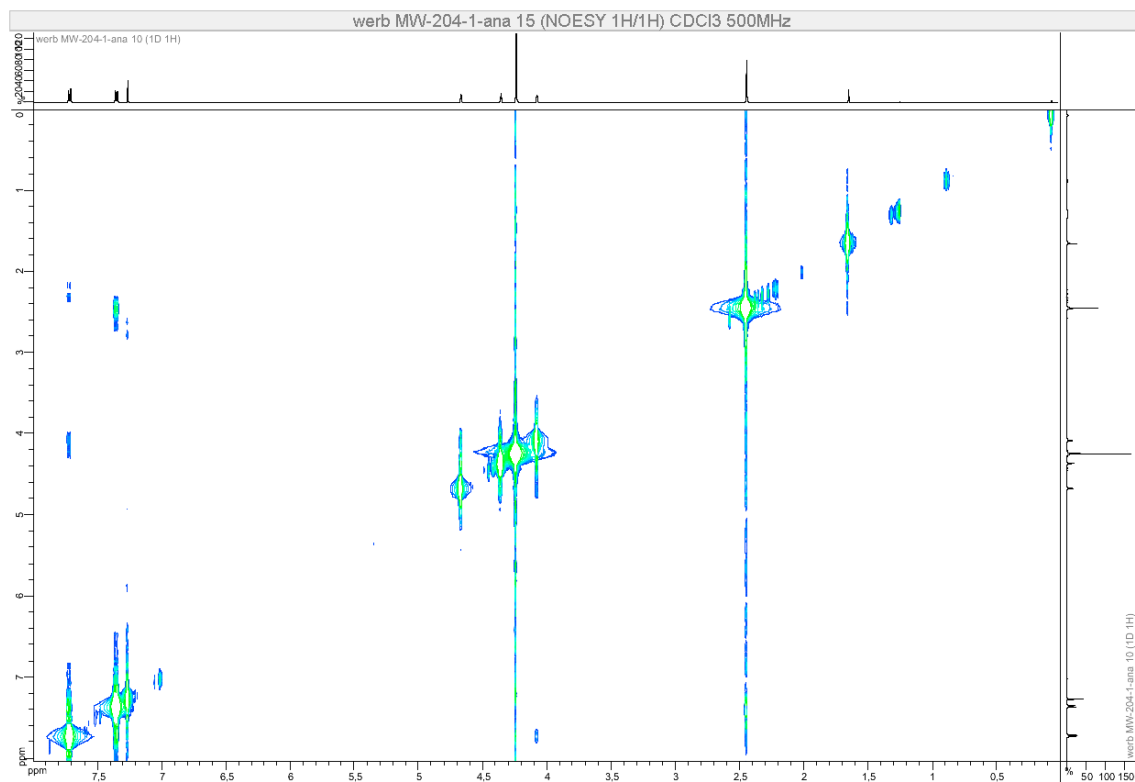
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

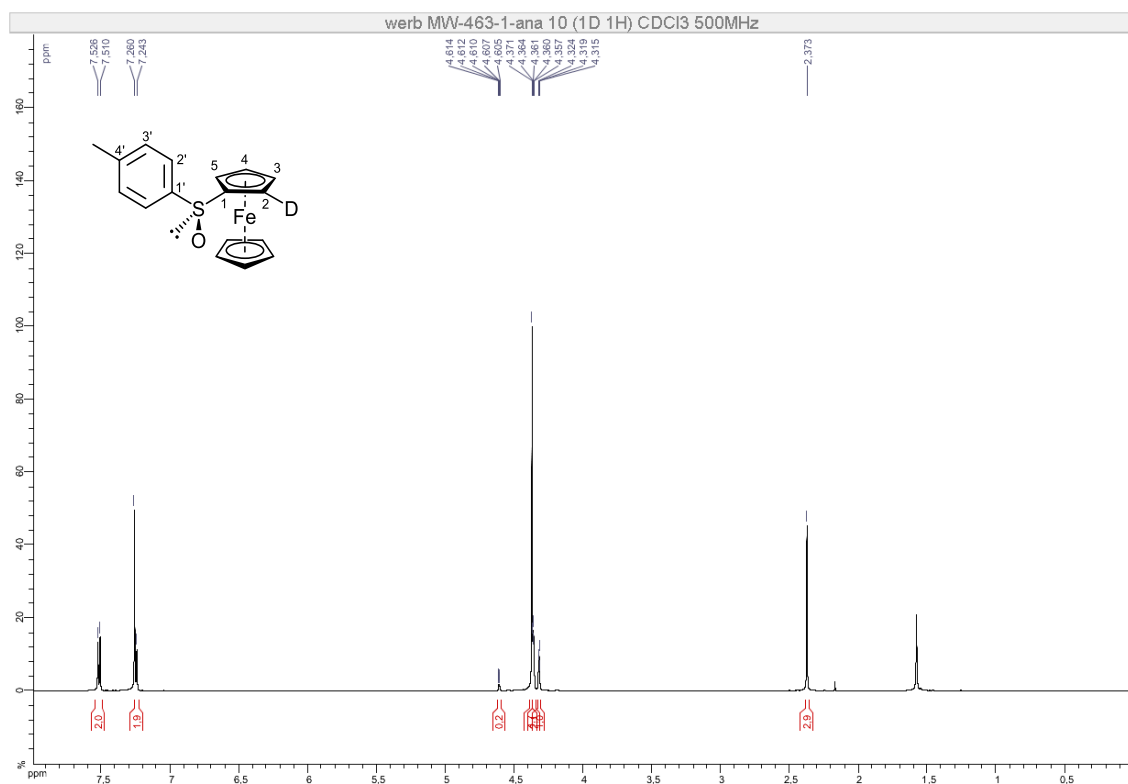


NOESY (500 MHz, CDCl₃)

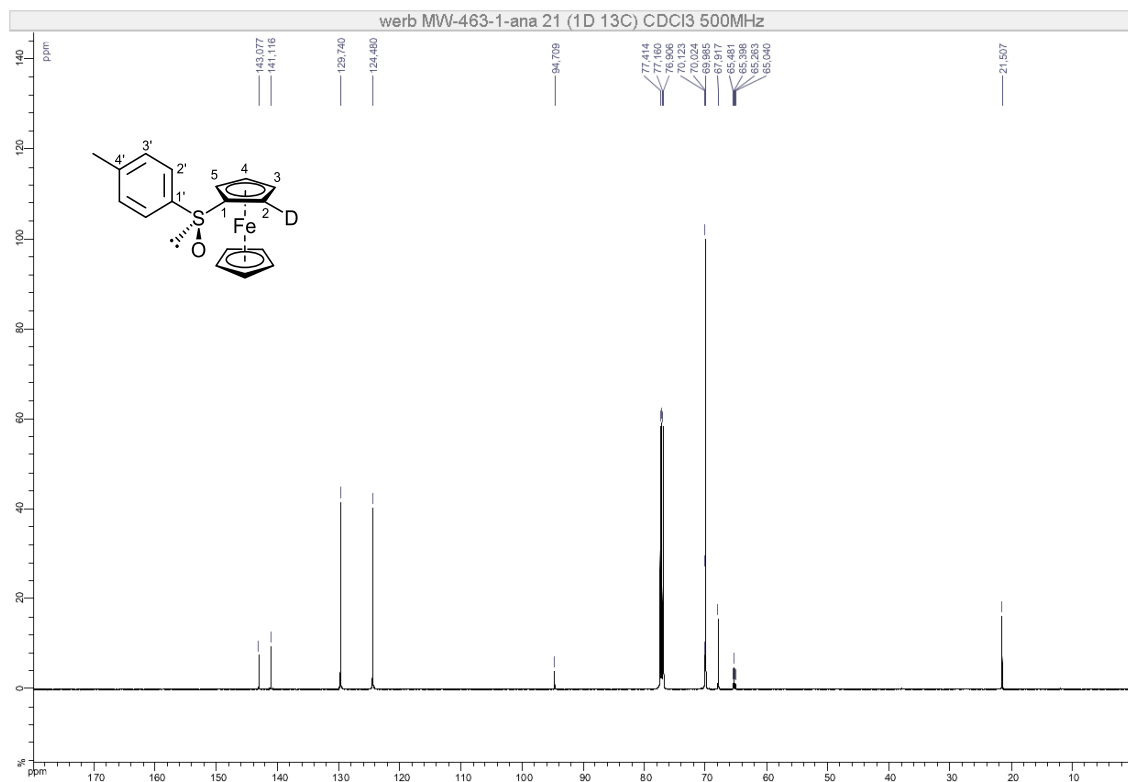


(*S,S*)-2-Deuterio-*S*-(4-tolyl)ferrocenesulfoxide (*S,S*-3c)

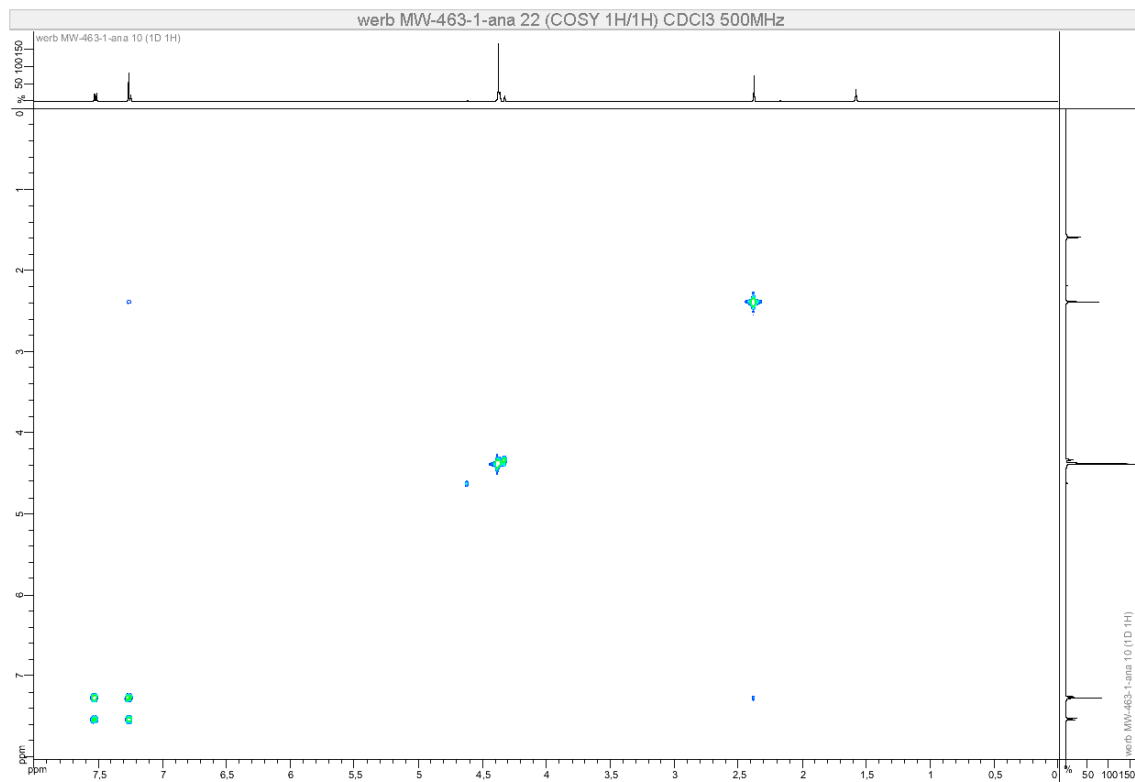
^1H NMR (500 MHz, CDCl_3)



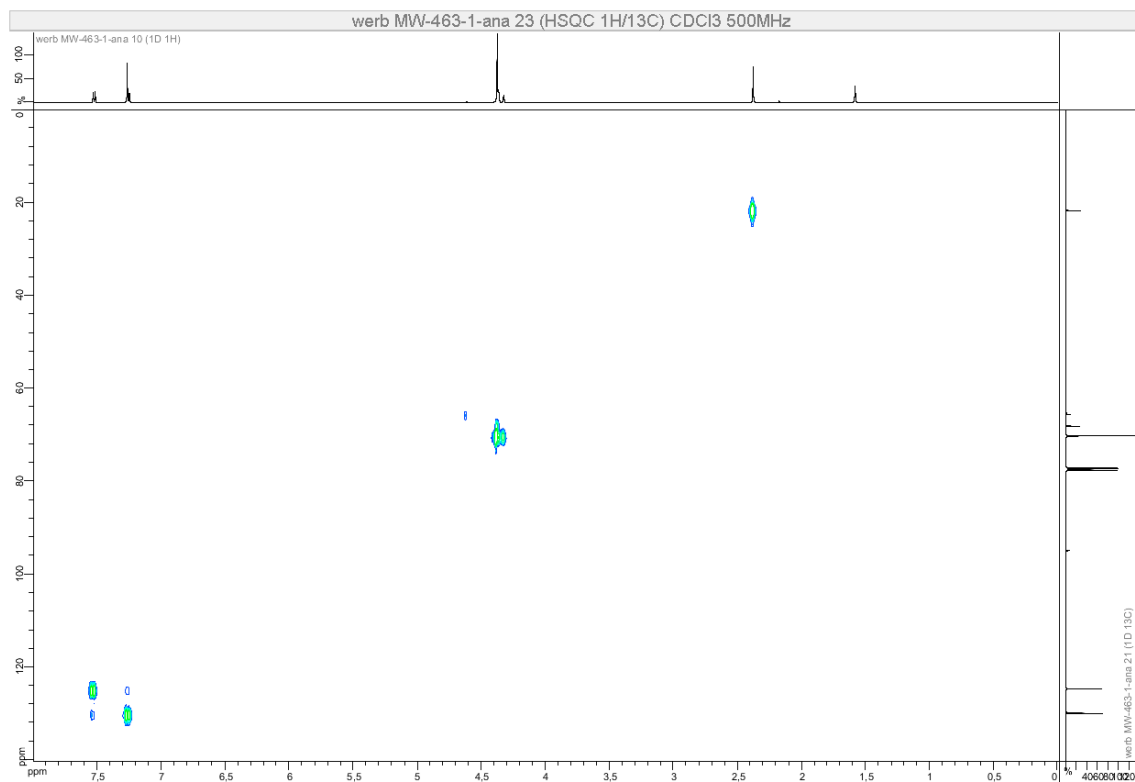
^{13}C NMR (126 MHz, CDCl_3)



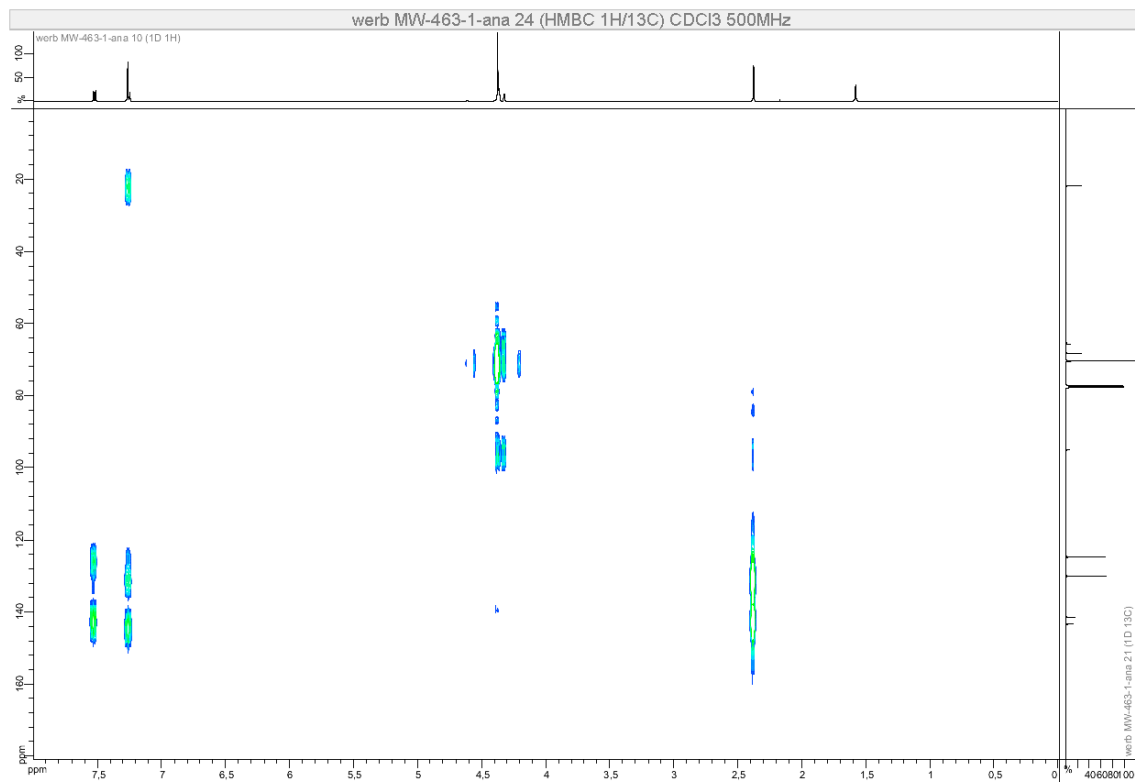
COSY (500 MHz, CDCl₃)



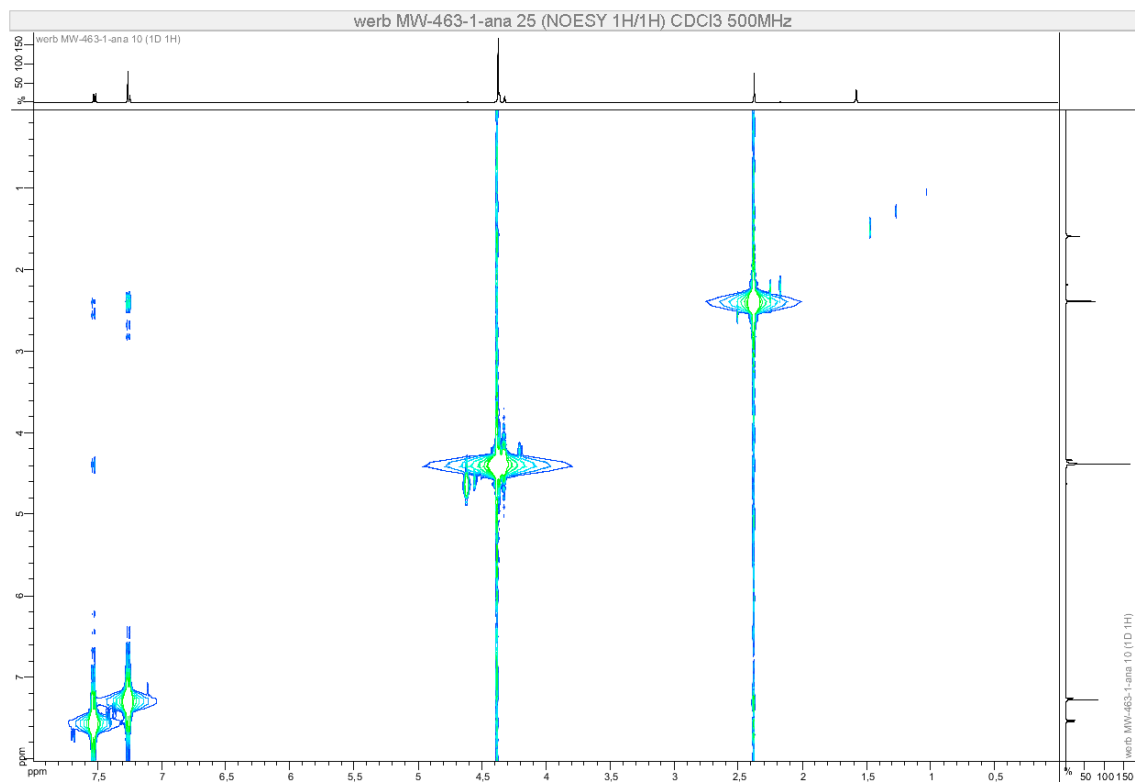
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

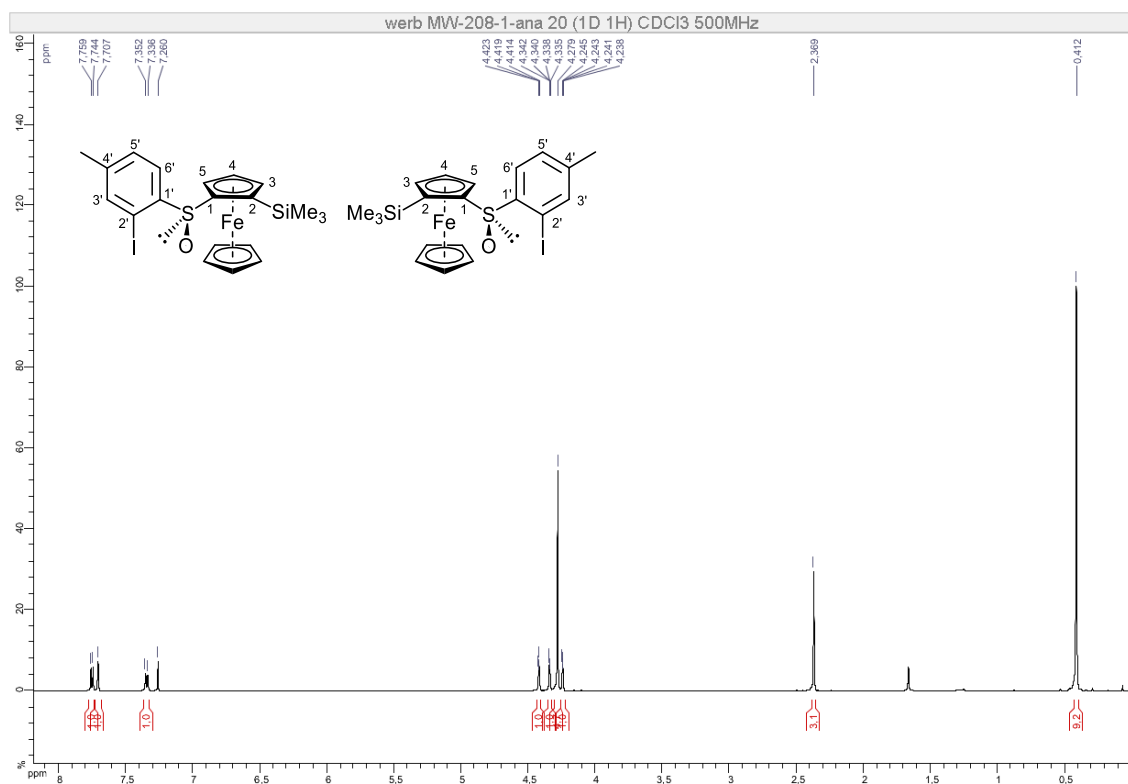


NOESY (500 MHz, CDCl₃)

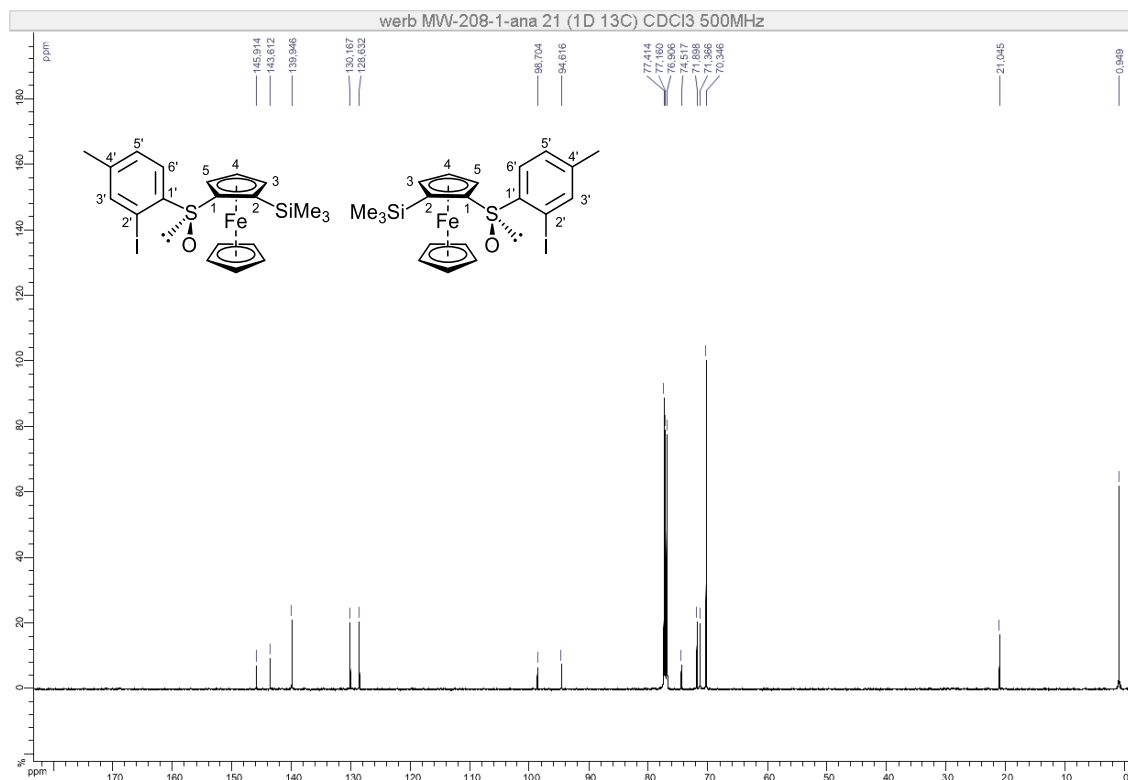


(*R,R*_P)- and (*S,S*_P)-*S*-(2-Iodo-4-tolyl)-2-(trimethylsilyl)ferrocenesulfoxide (*R,R*_P/*S,S*_P-4)

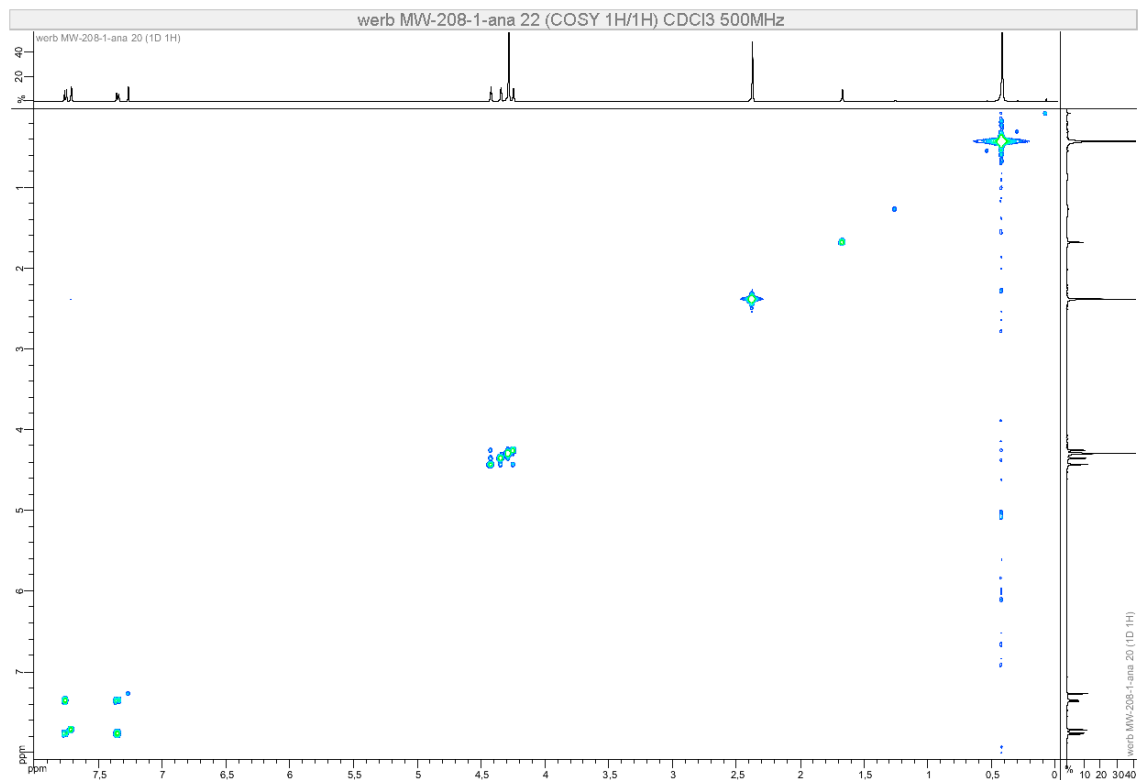
¹H NMR (500 MHz, CDCl₃)



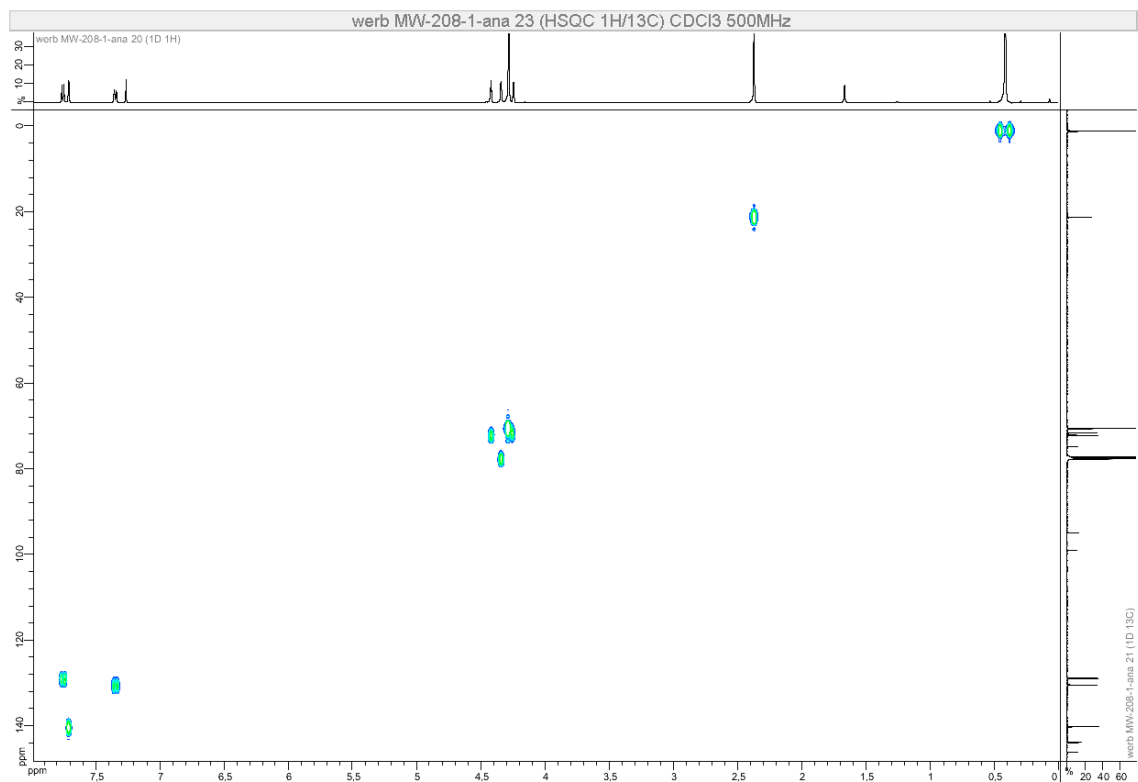
¹³C NMR (126 MHz, CDCl₃)



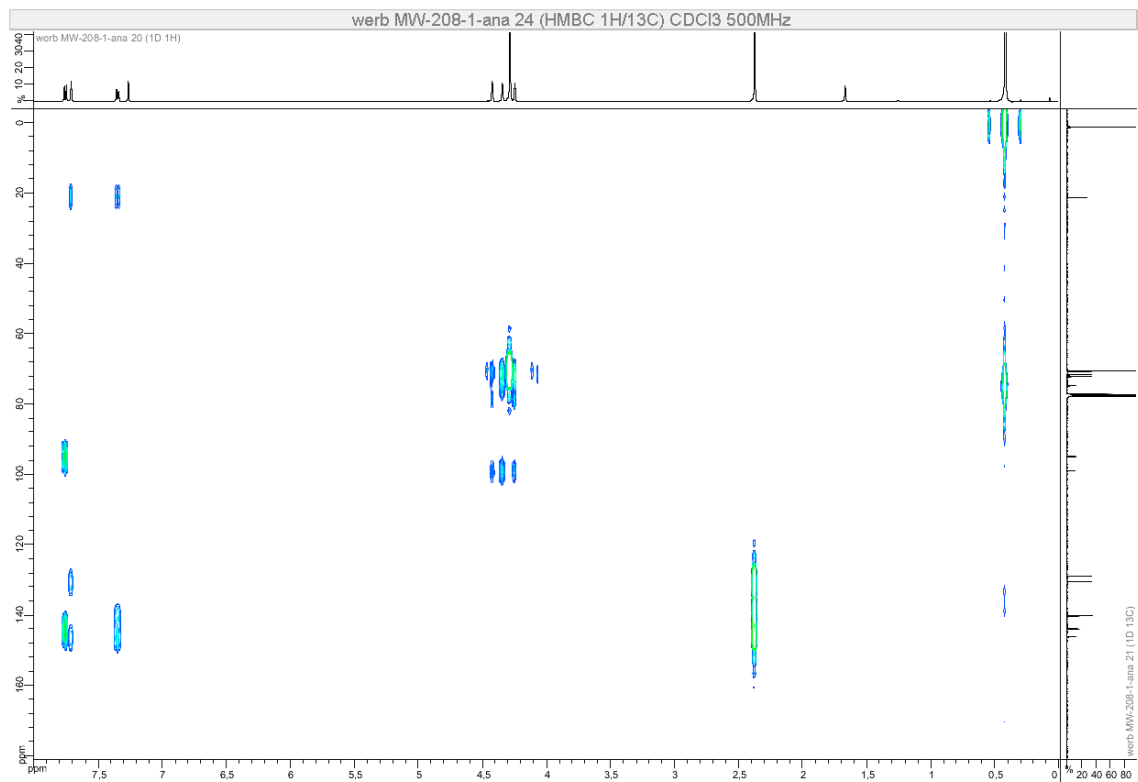
COSY (500 MHz, CDCl₃)



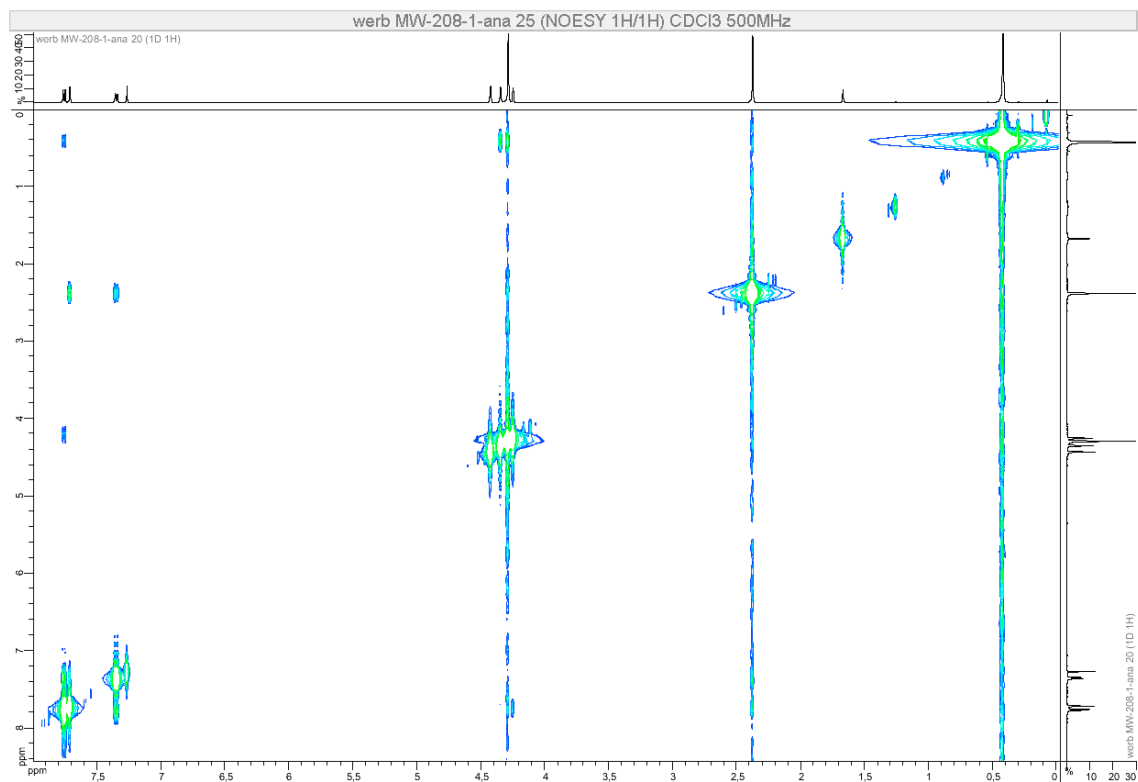
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

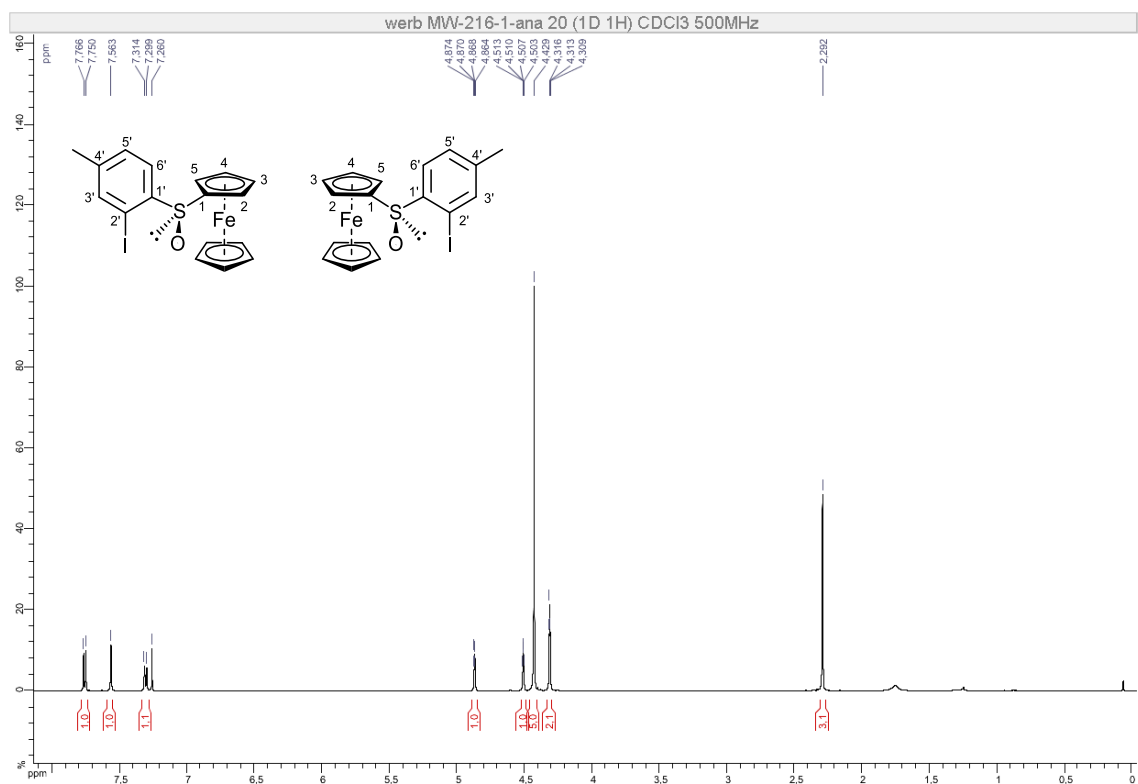


NOESY (500 MHz, CDCl₃)

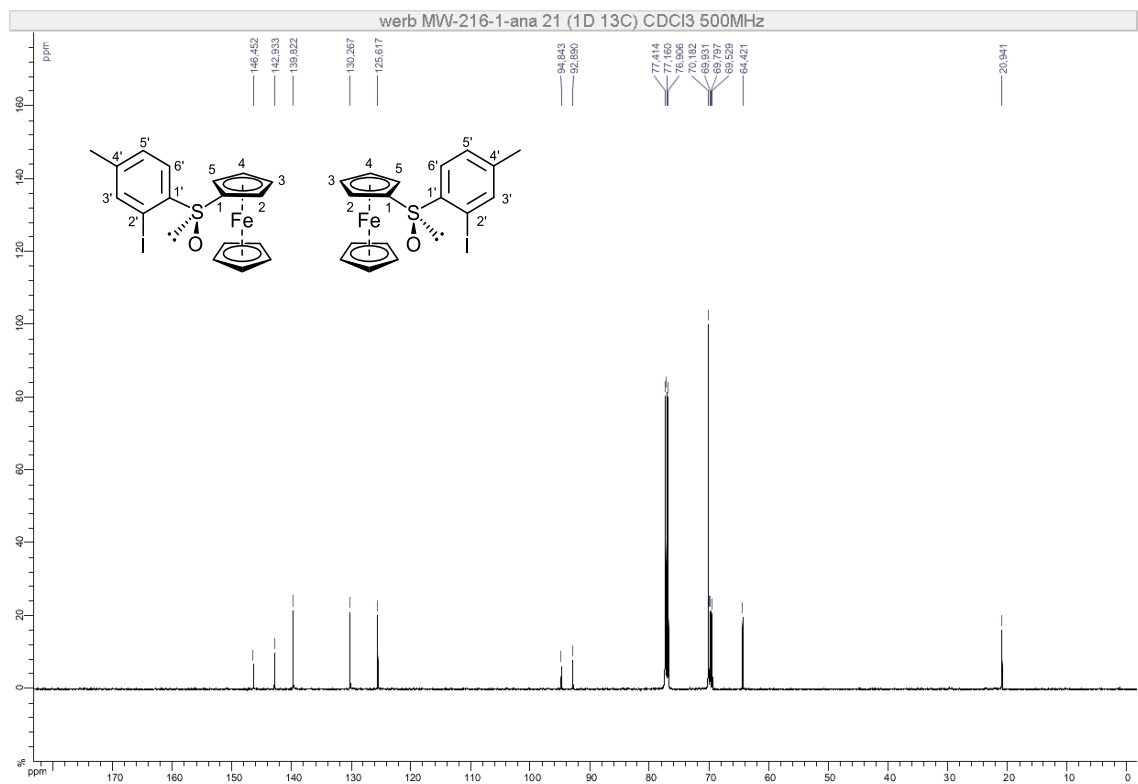


Racemic *S*-(2-Iodo-4-tolyl)ferrocenesulfoxide (*rac*-5)

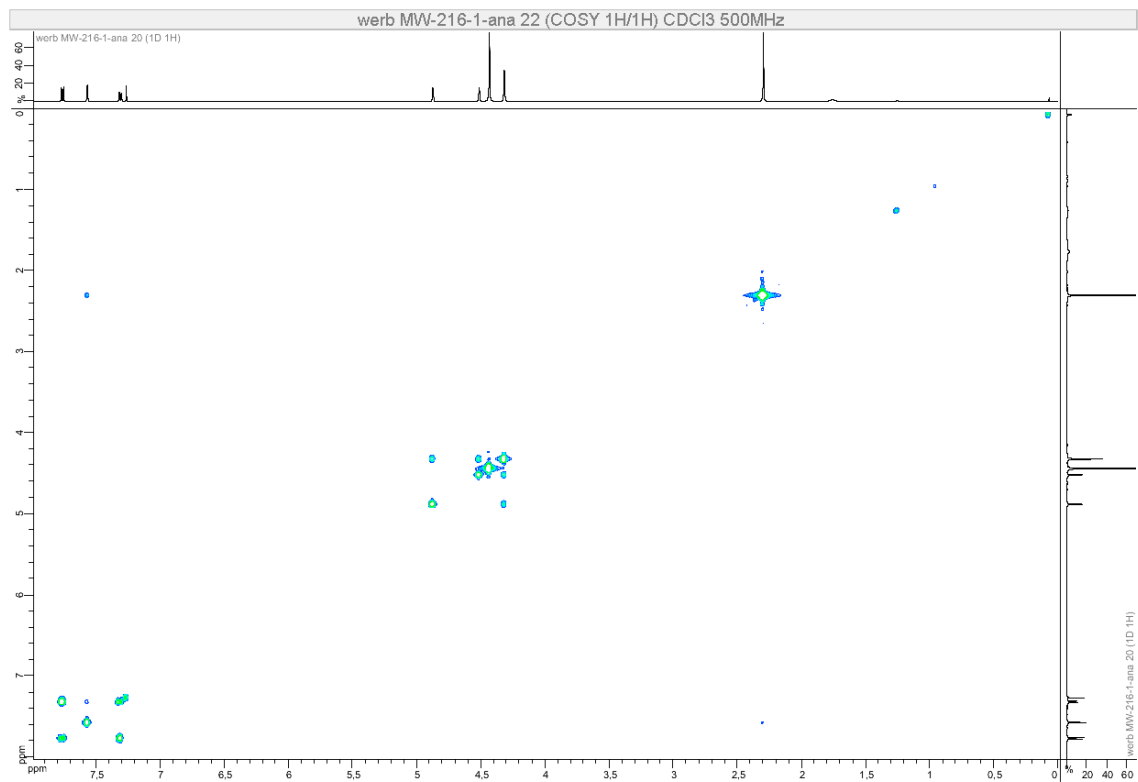
^1H NMR (500 MHz, CDCl_3)



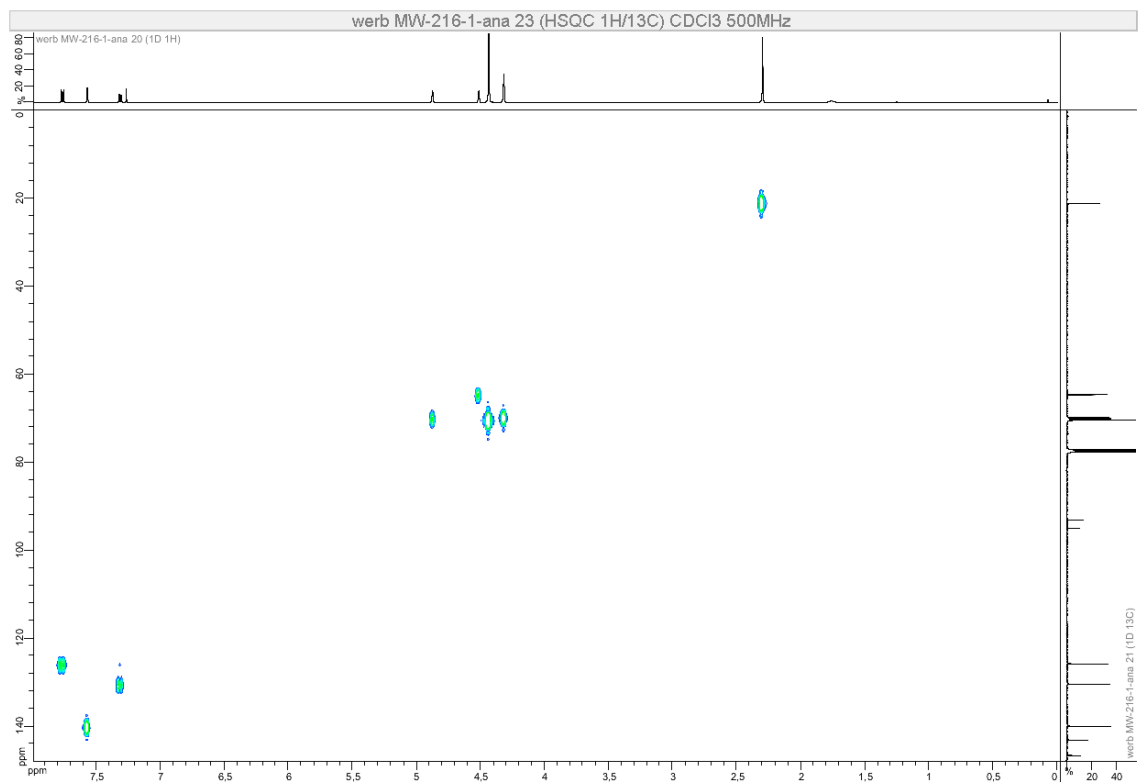
^{13}C NMR (126 MHz, CDCl_3)



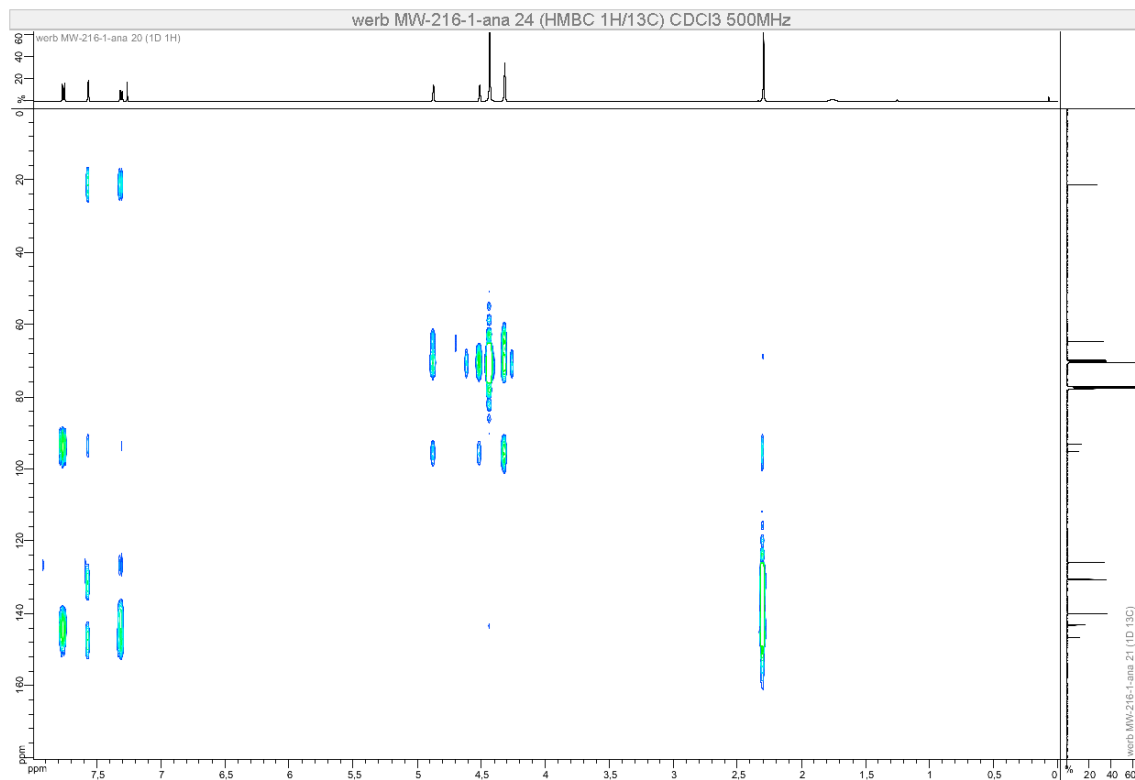
COSY (500 MHz, CDCl₃)



HSQC (500 MHz, CDCl₃)

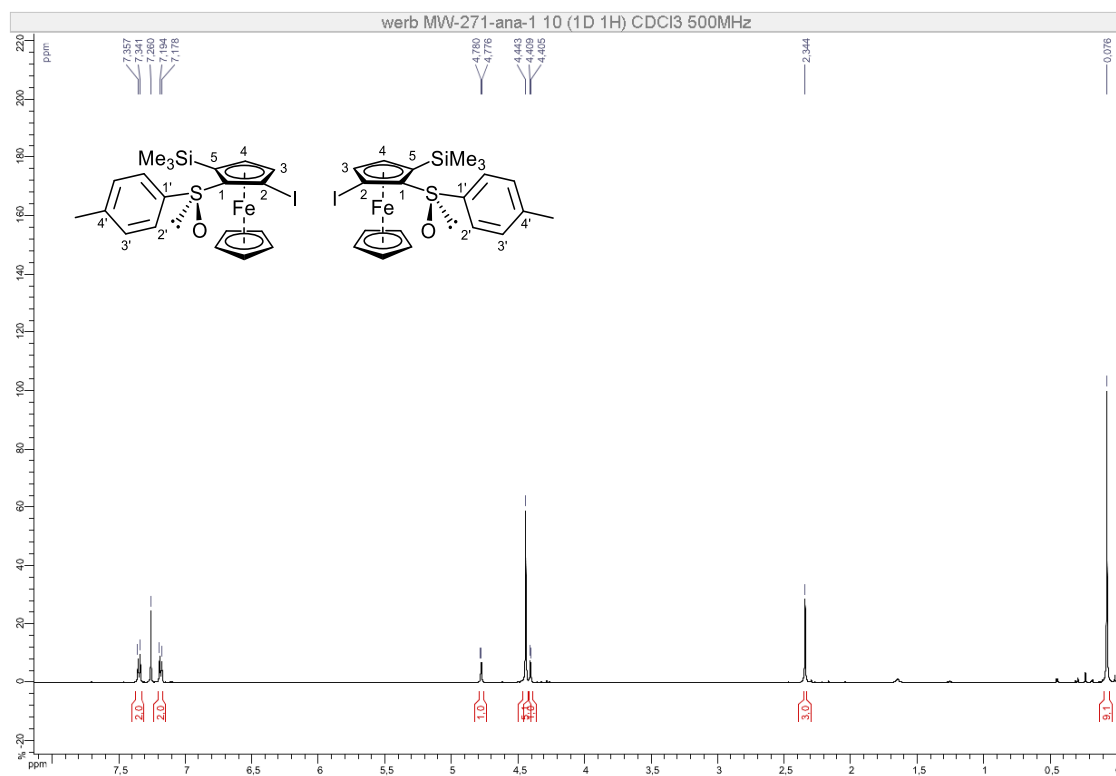


HMBC (500 MHz, CDCl₃)

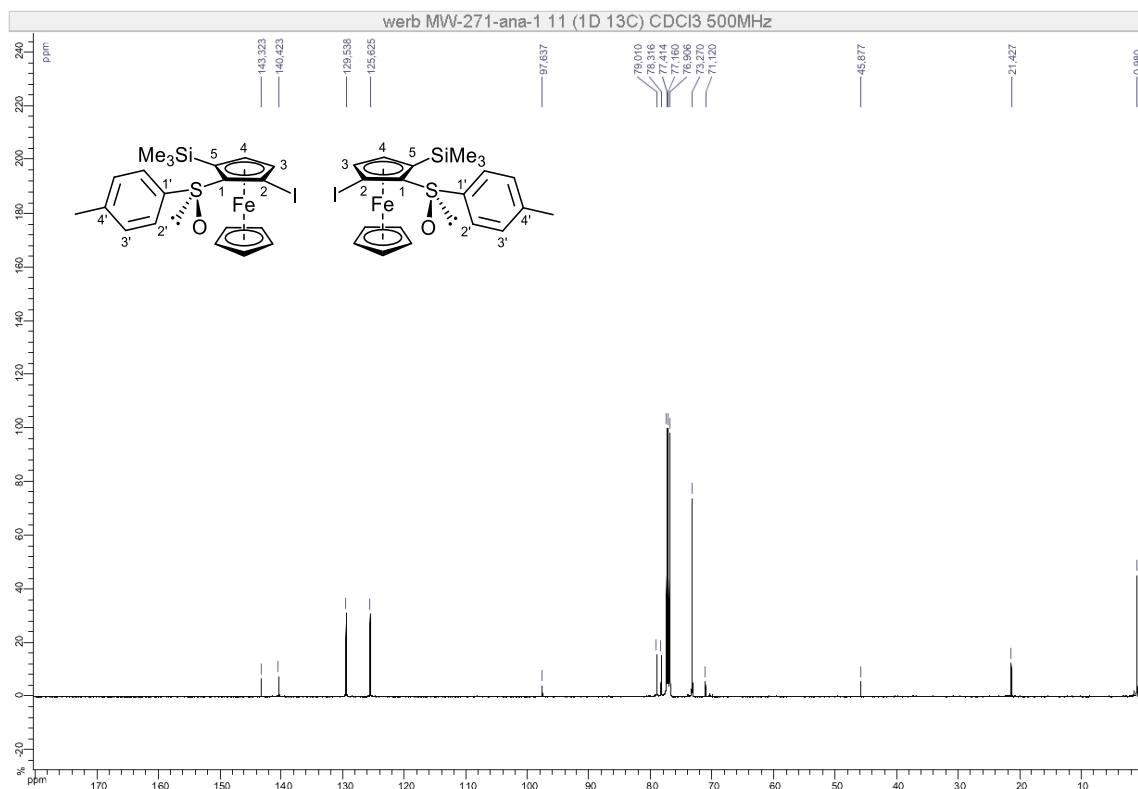


(*R,S*_P)- and (*S,R*_P)-2-Iodo-*S*-(4-tolyl)-5-(trimethylsilyl)ferrocenesulfoxide (*R,S*_P/*S,R*_P-6)

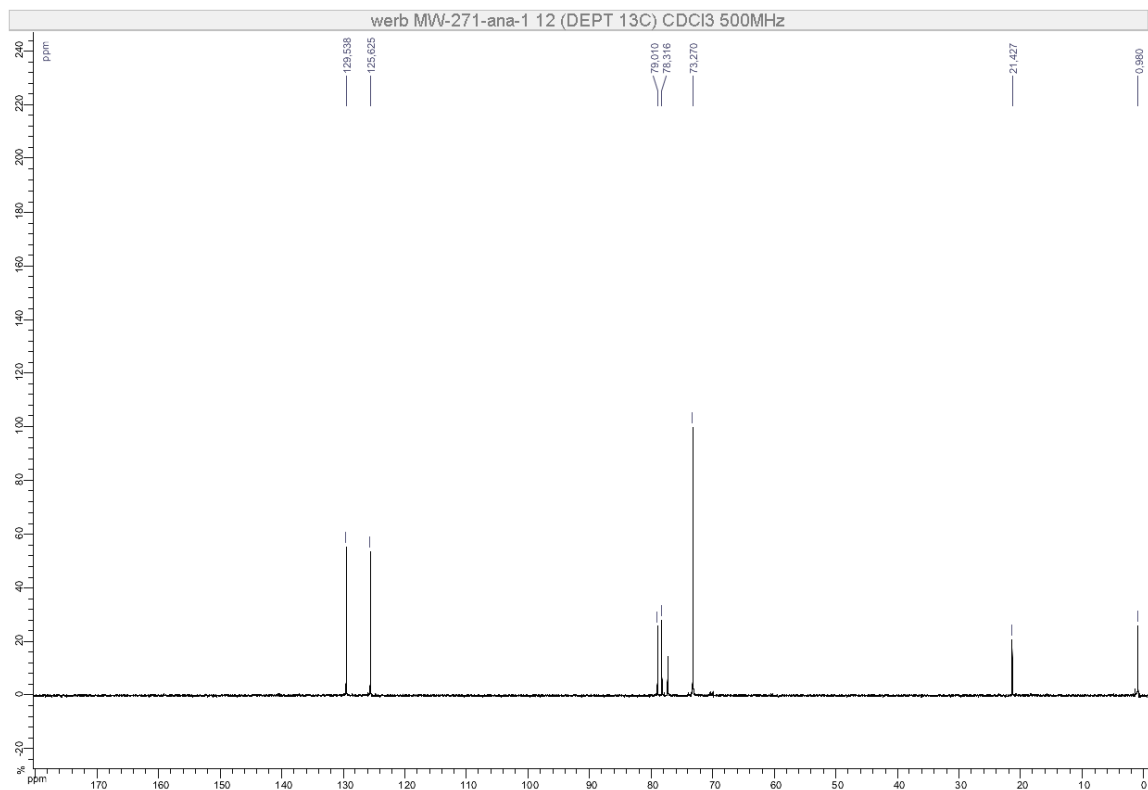
¹H NMR (500 MHz, CDCl₃)



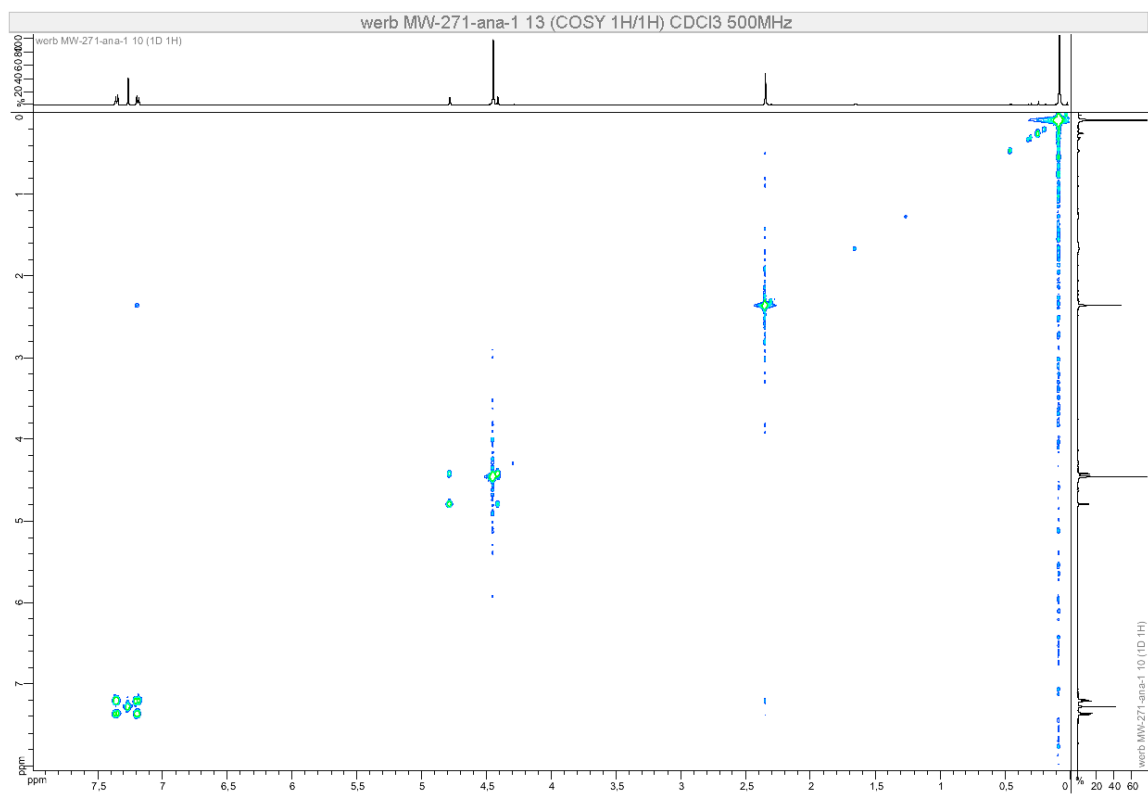
¹³C NMR (126 MHz, CDCl₃)



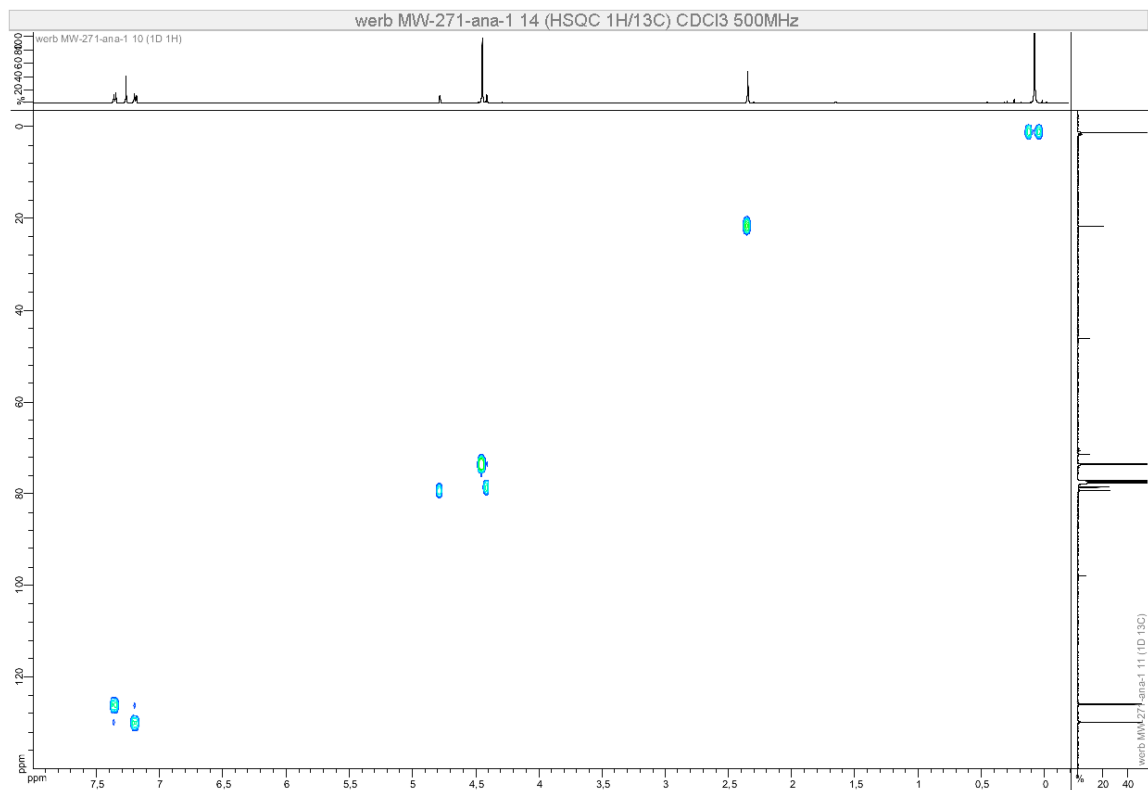
DEPT 135 (126 MHz, CDCl₃)



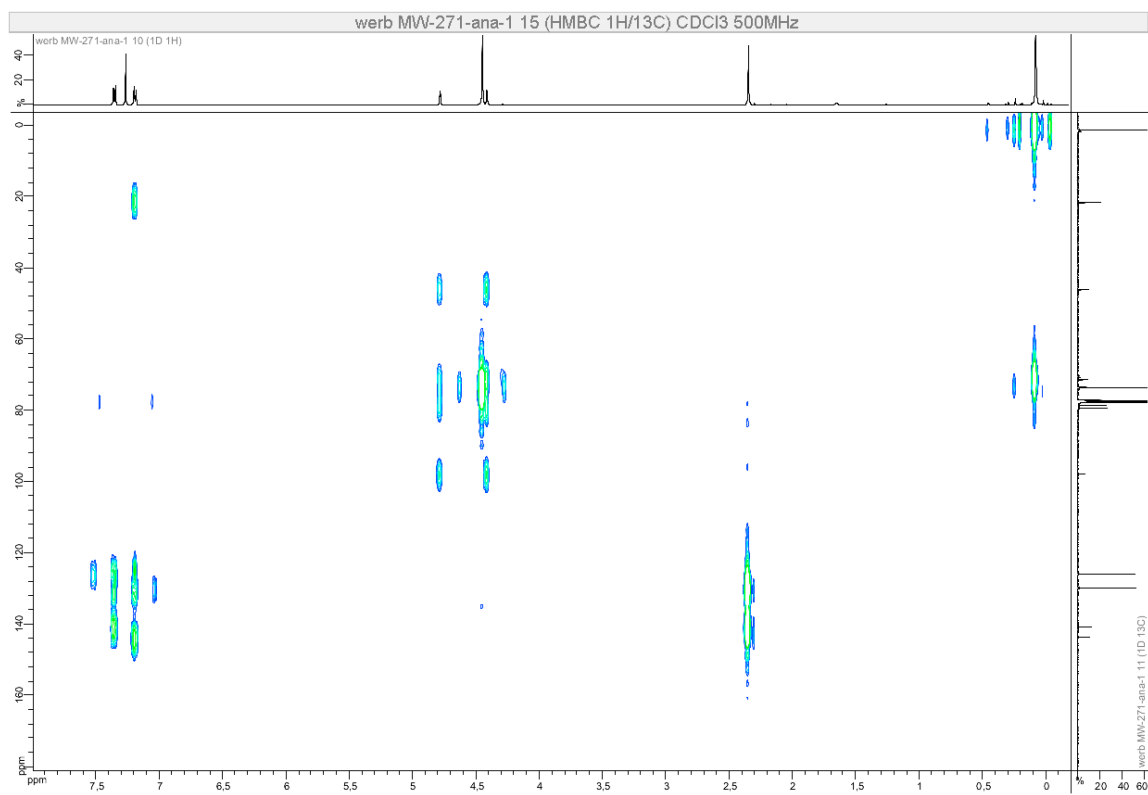
COSY (500 MHz, CDCl₃)



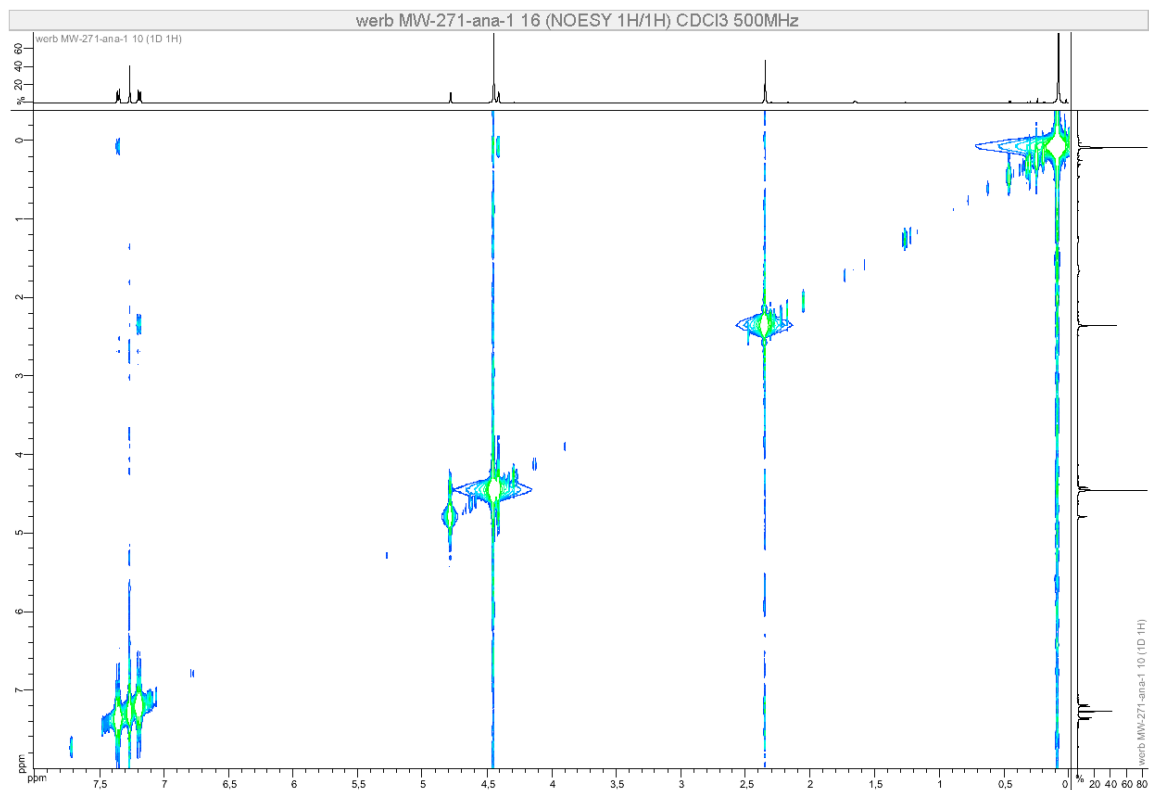
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

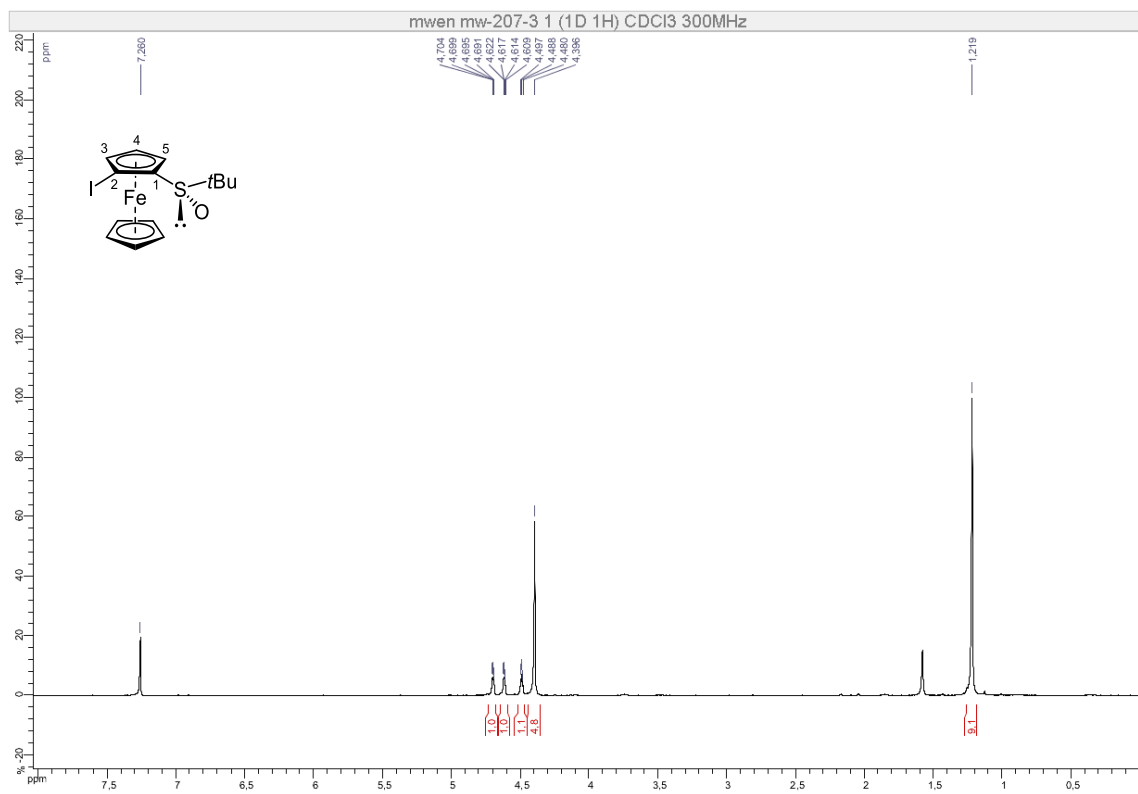


NOESY (500 MHz, CDCl₃)



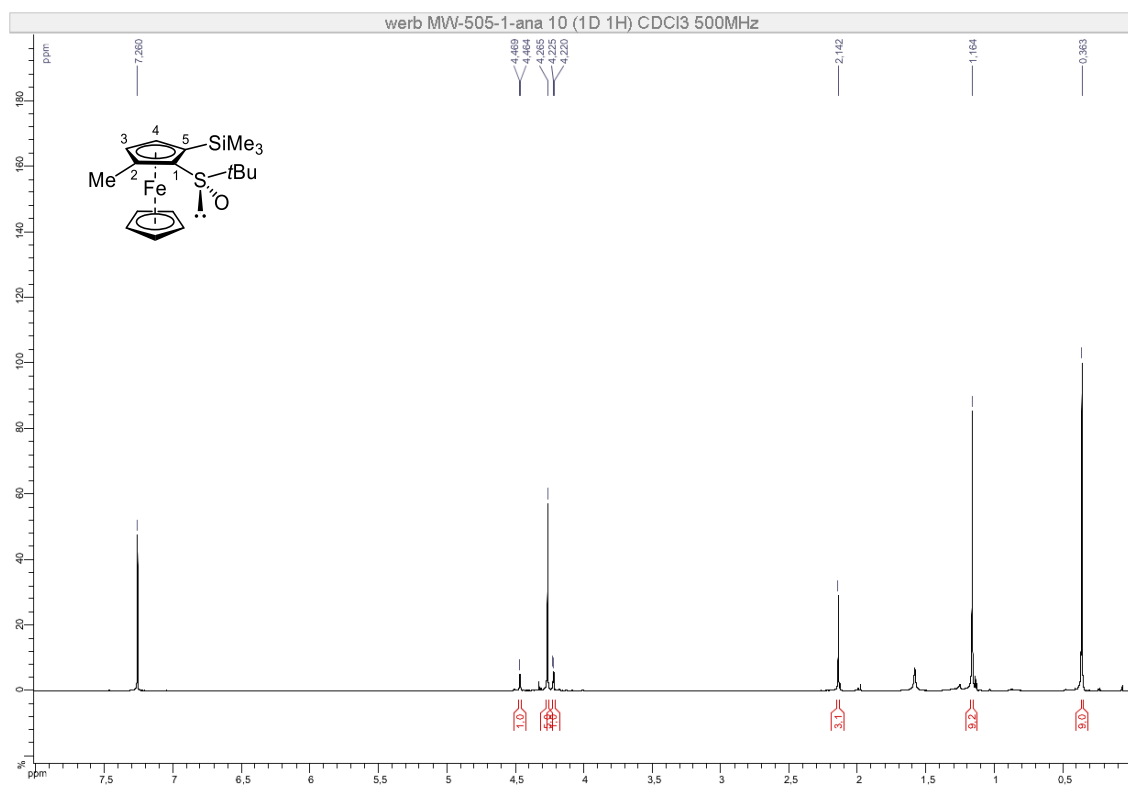
(*S,S*)-*S*-tert-Butyl-2-iodoferrocenesulfoxide (*S,S*-2ab)

^1H NMR (300 MHz, CDCl_3)

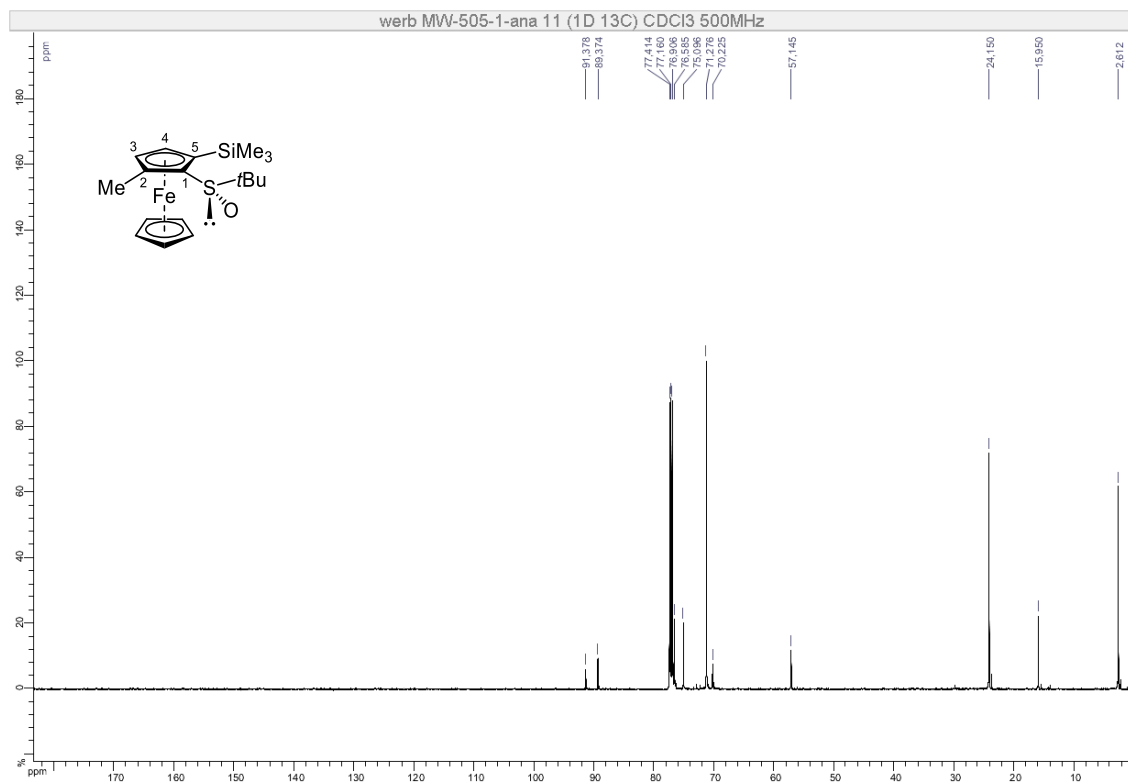


(*S,S*_P)-*S*-*tert*-Butyl-2-methyl-5-(trimethylsilyl)ferrocenesulfoxide (*S,S*_P-2ad)

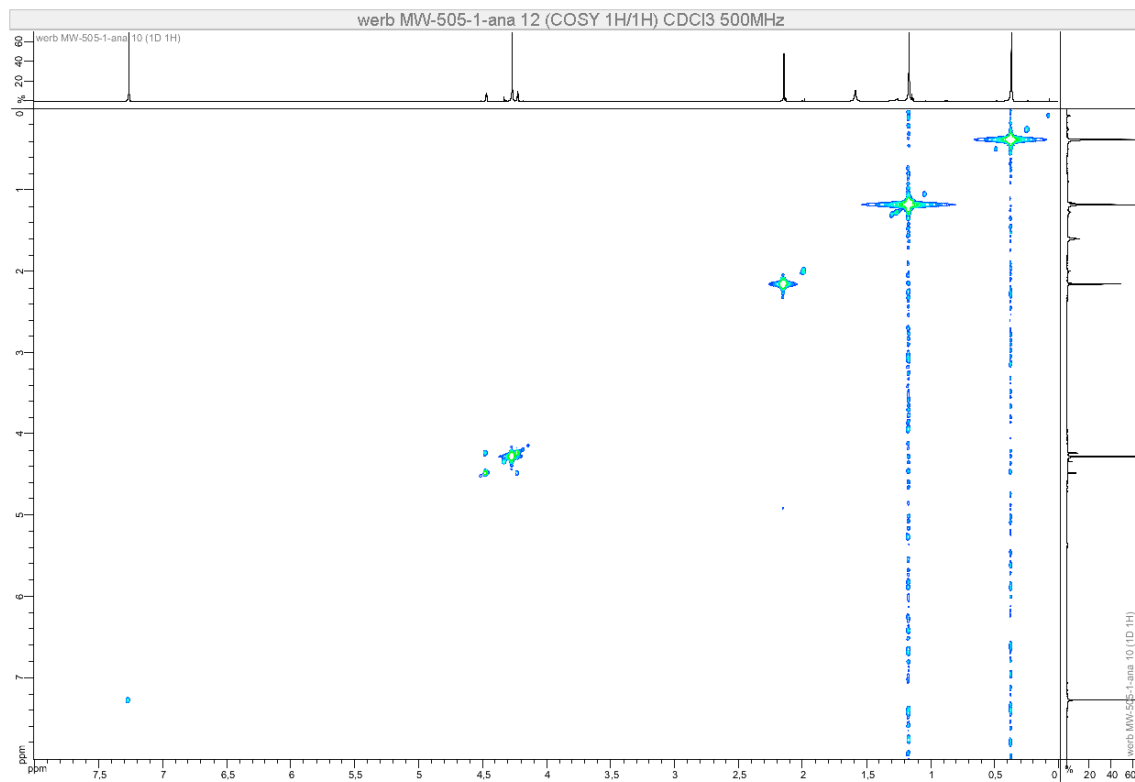
¹H NMR (500 MHz, CDCl₃)



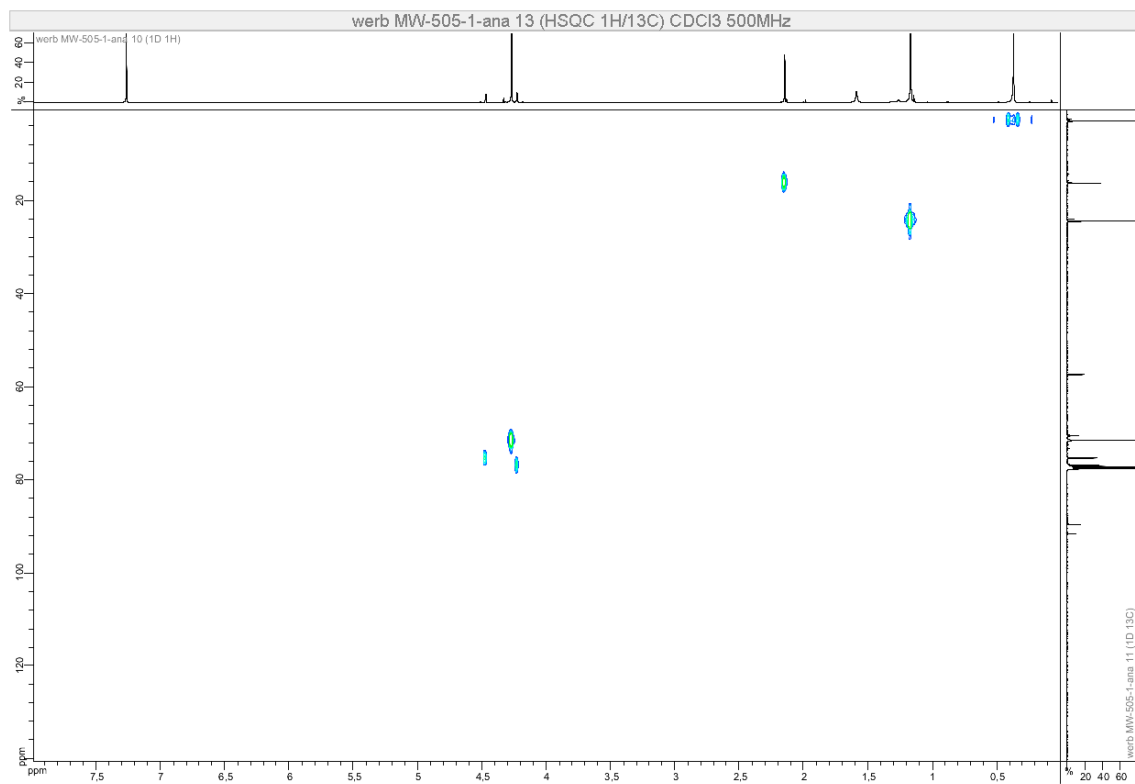
¹³C NMR (126 MHz, CDCl₃)



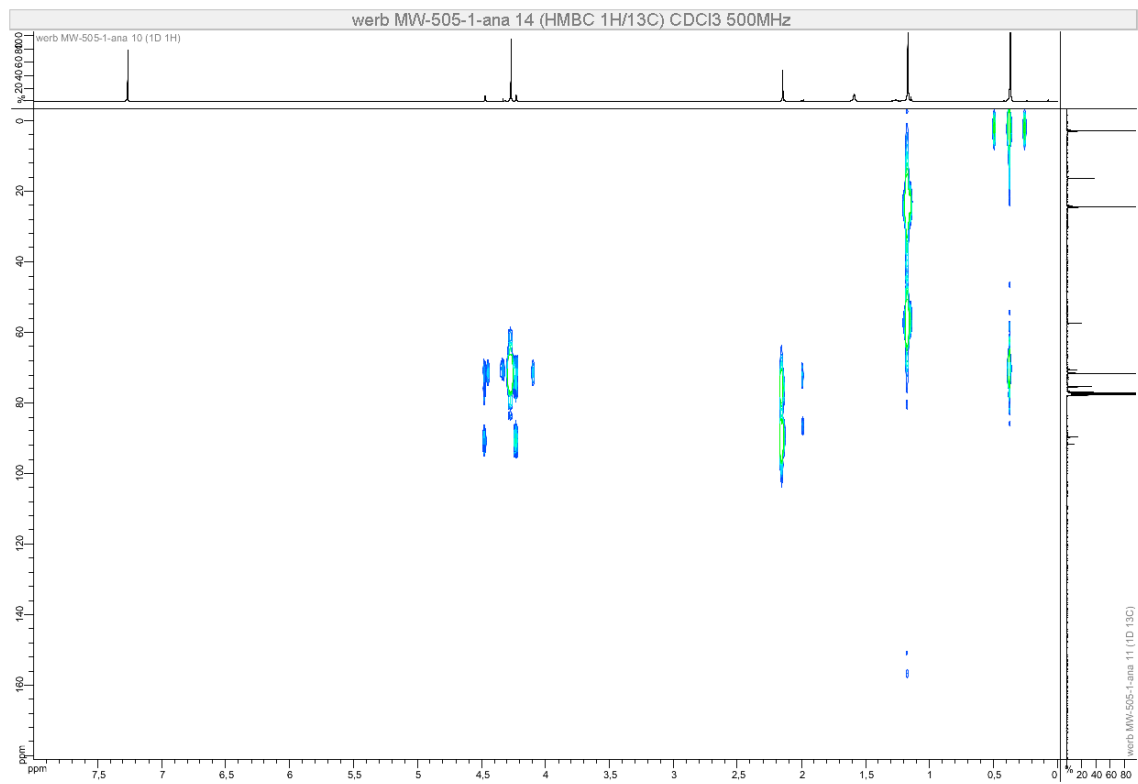
COSY (500 MHz, CDCl₃)



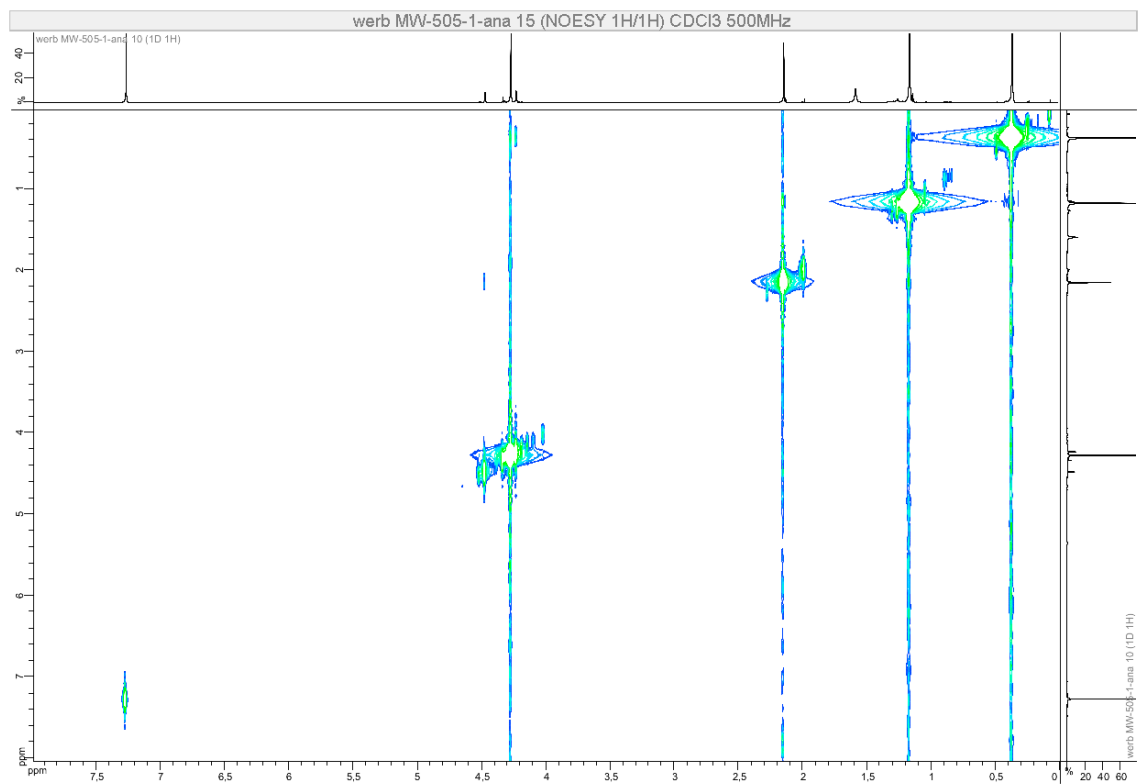
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

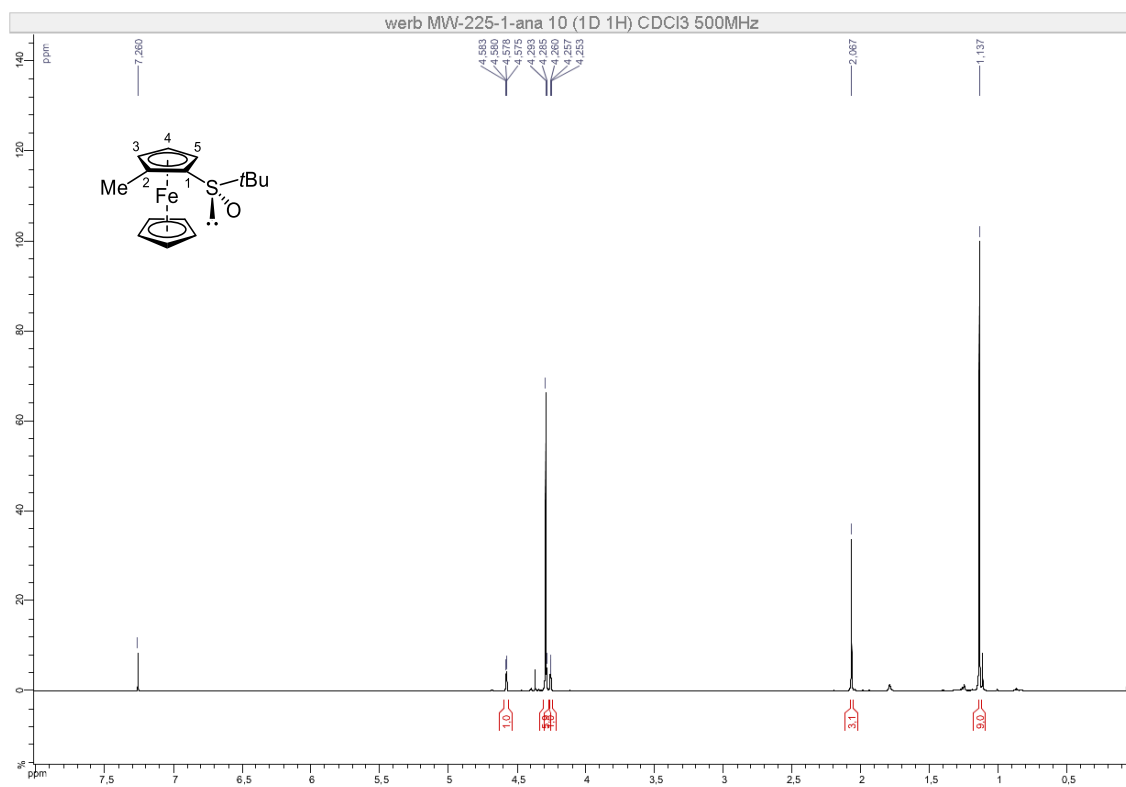


NOESY (500 MHz, CDCl₃)

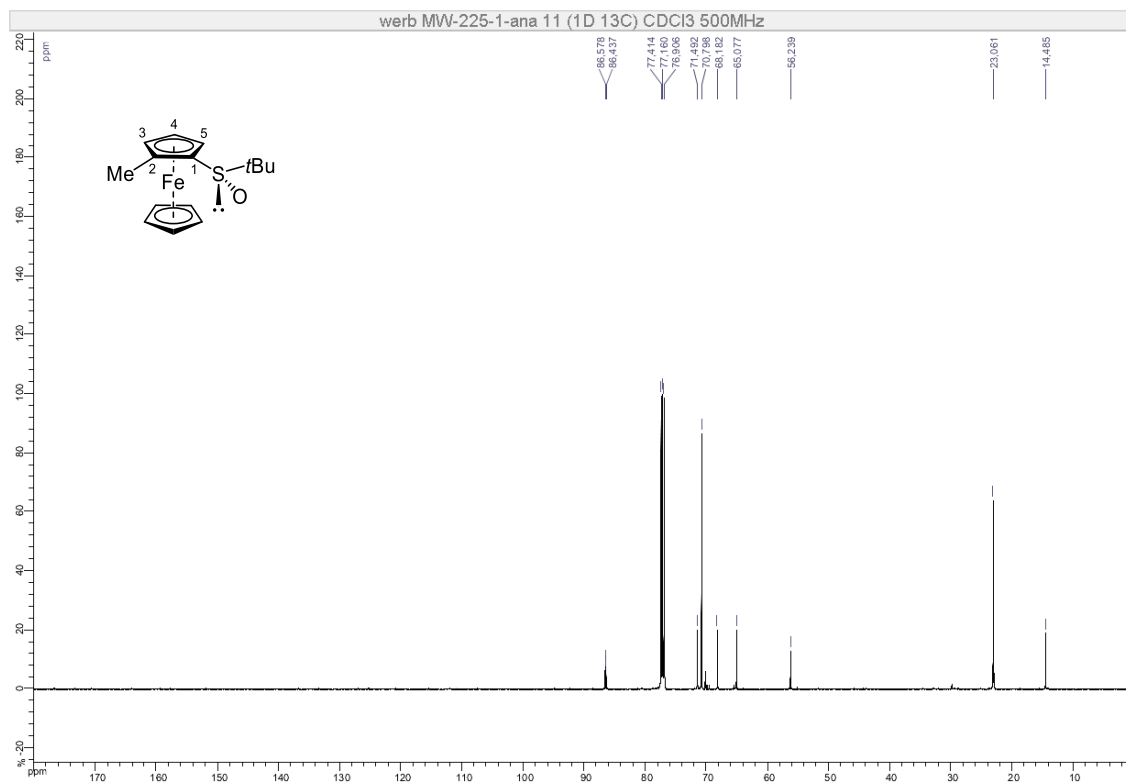


(*S,R_P*)-*S*-tert-Butyl-2-methylferrocenesulfoxide (*S,R_P*-1d)

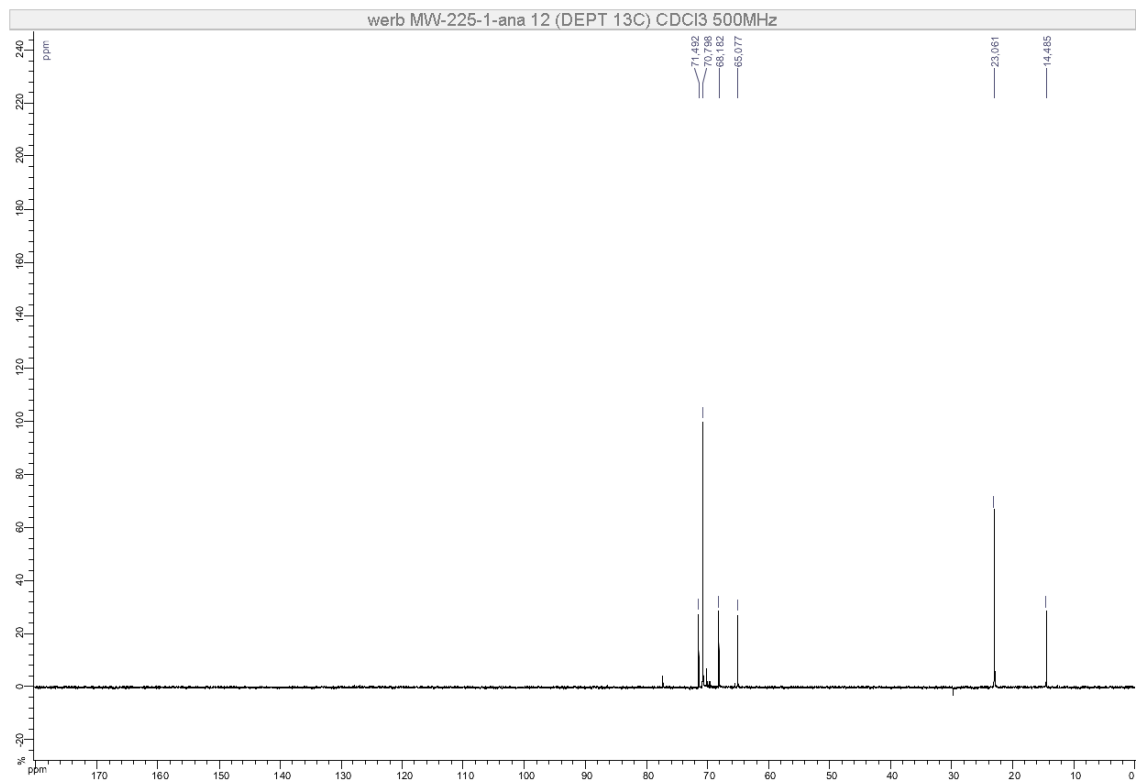
^1H NMR (500 MHz, CDCl_3)



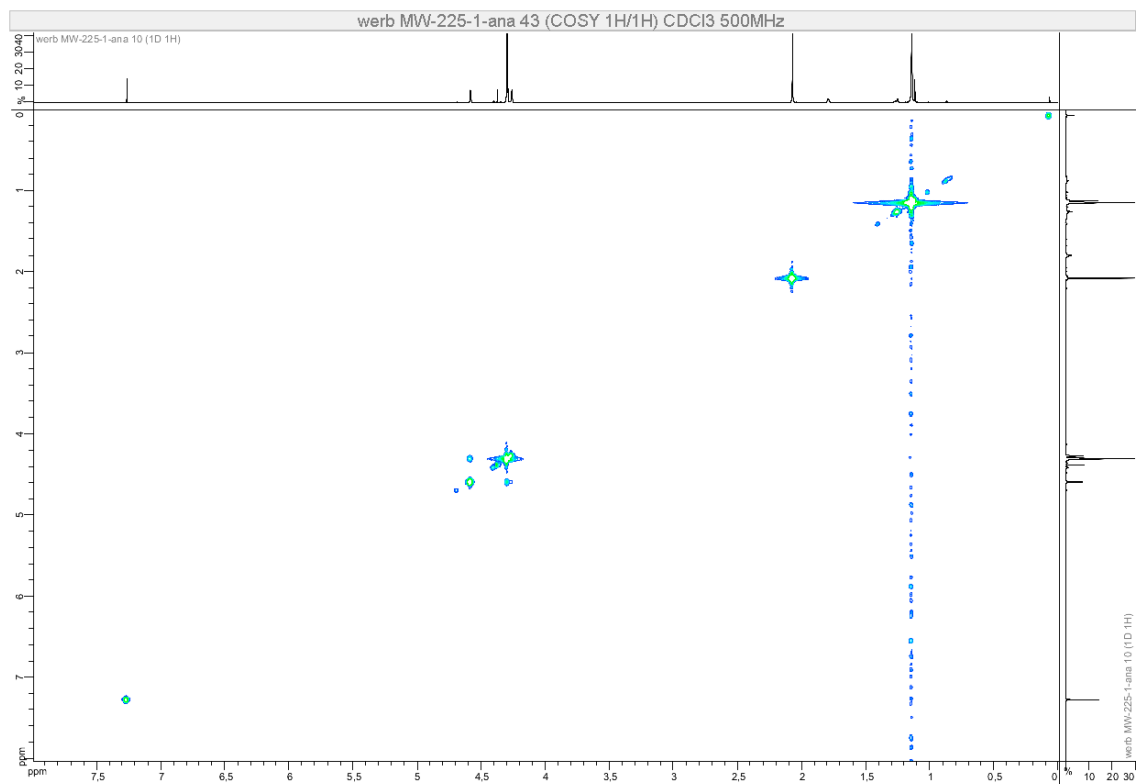
^{13}C NMR (126 MHz, CDCl_3)



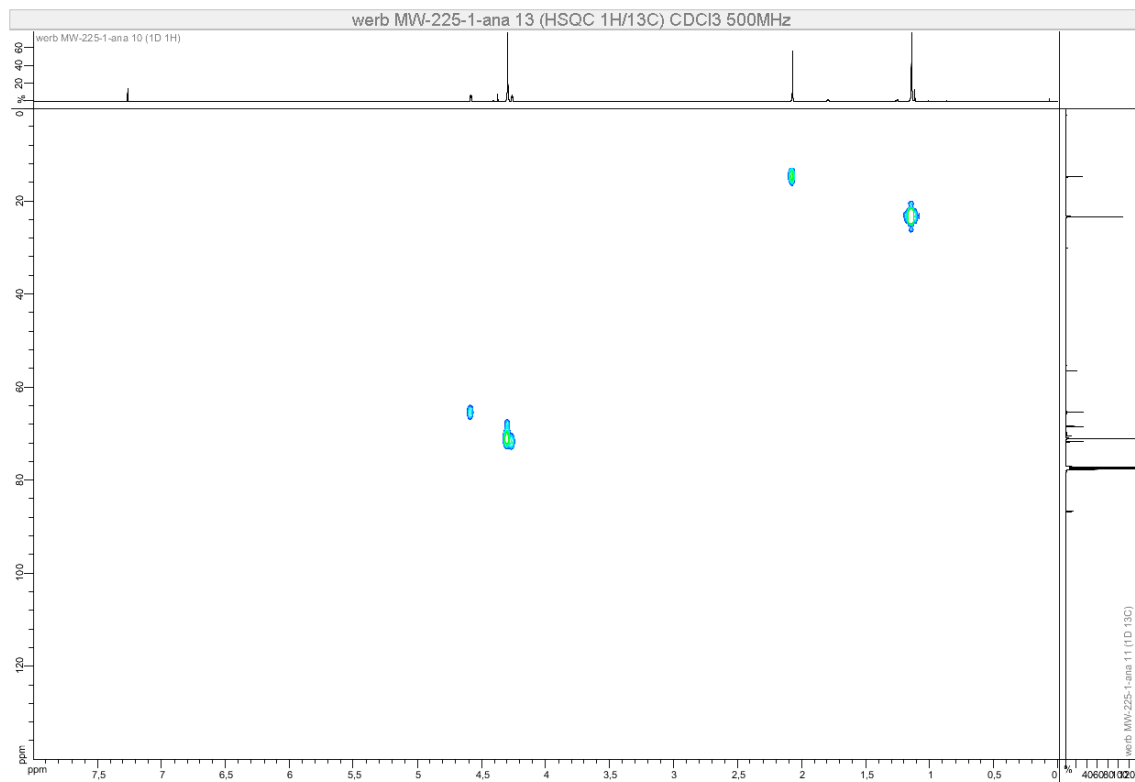
DEPT 135 (126 MHz, CDCl₃)



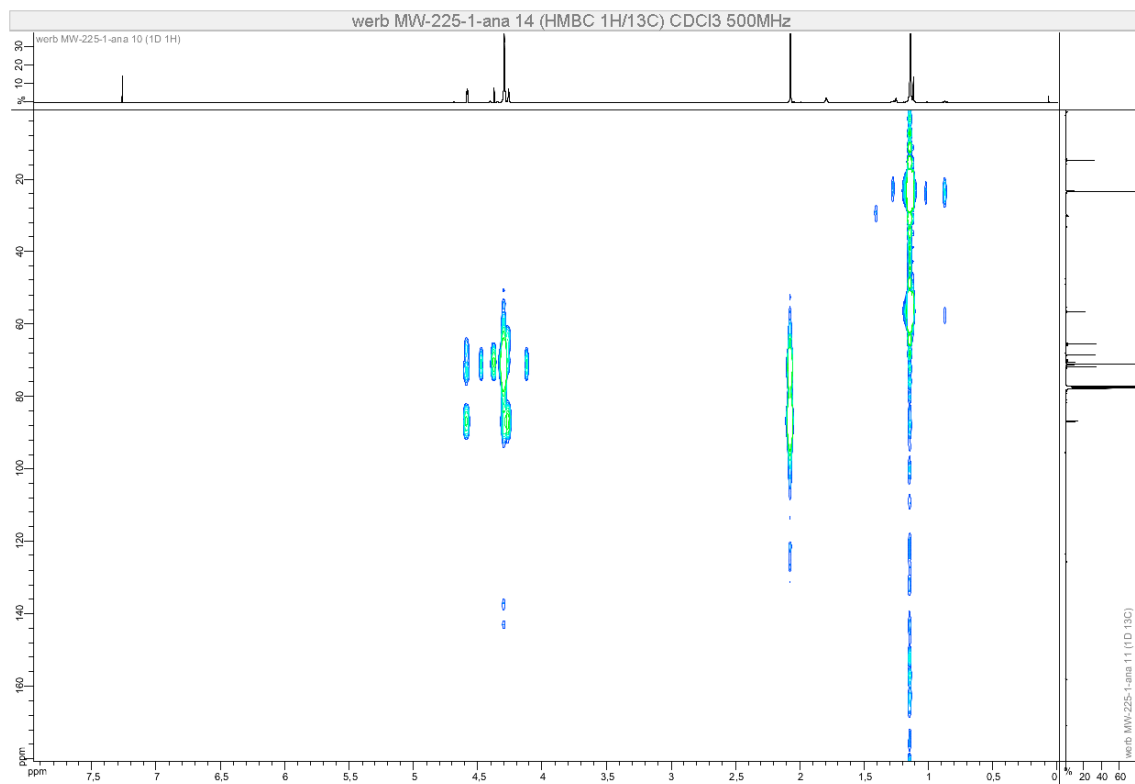
COSY (500 MHz, CDCl₃)



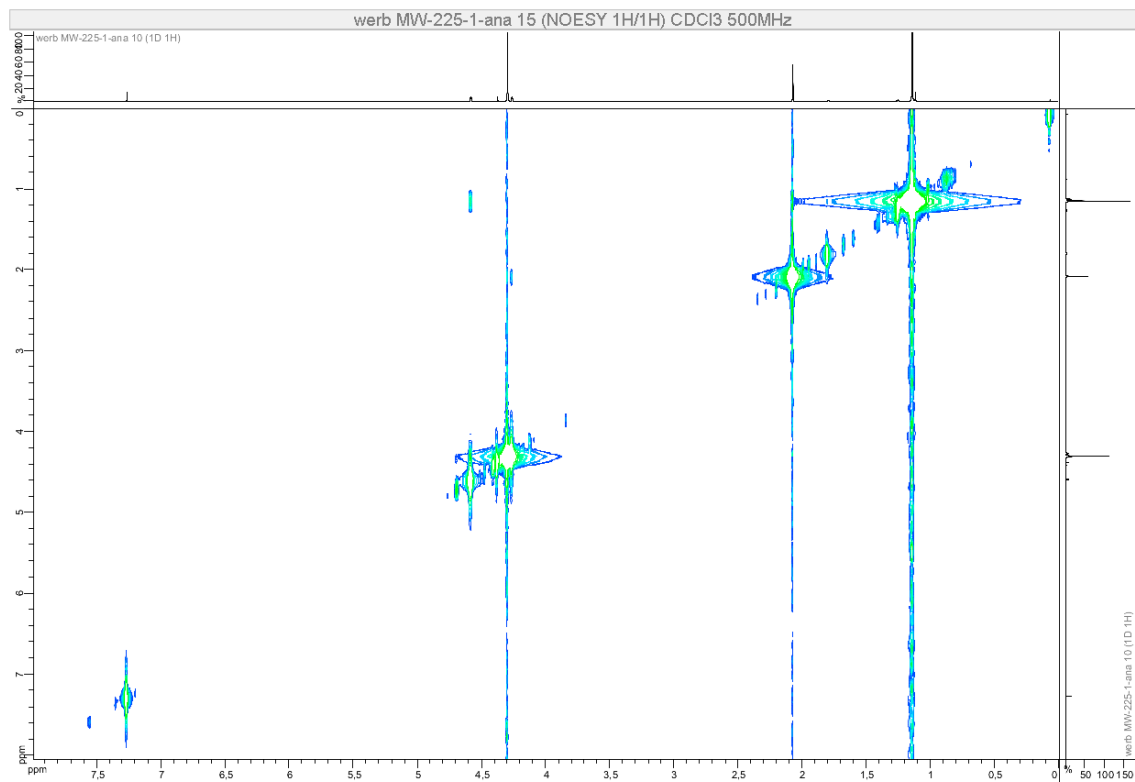
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

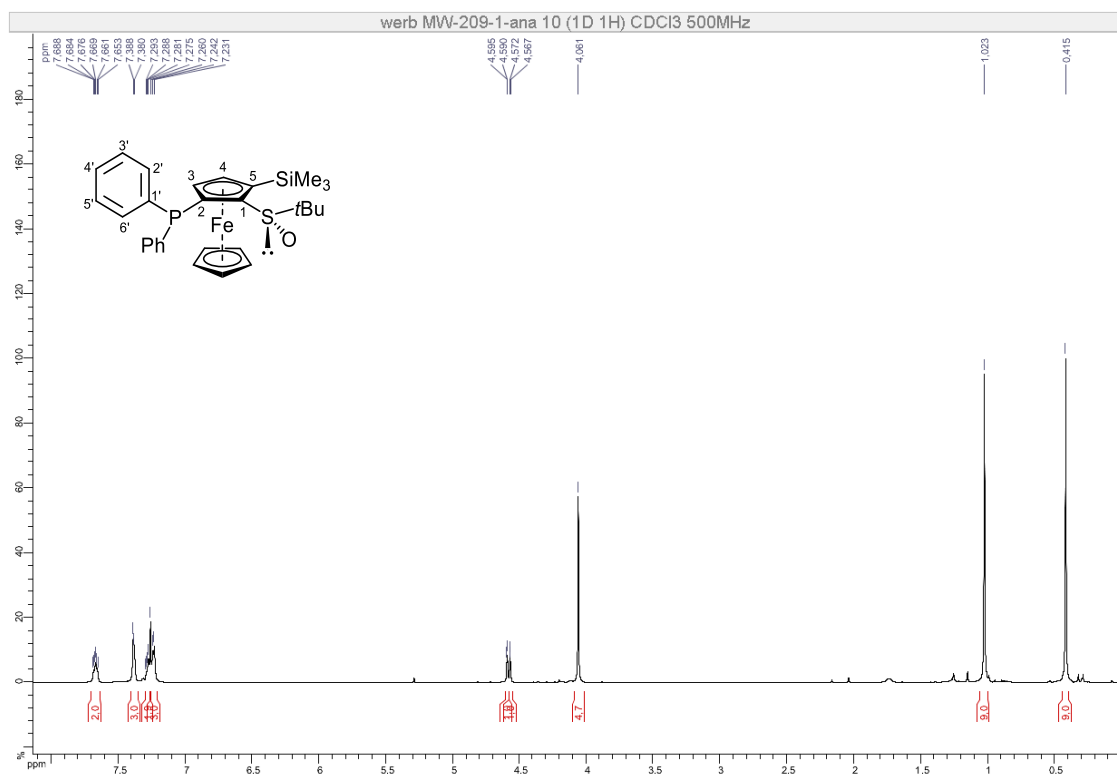


NOESY (500 MHz, CDCl₃)

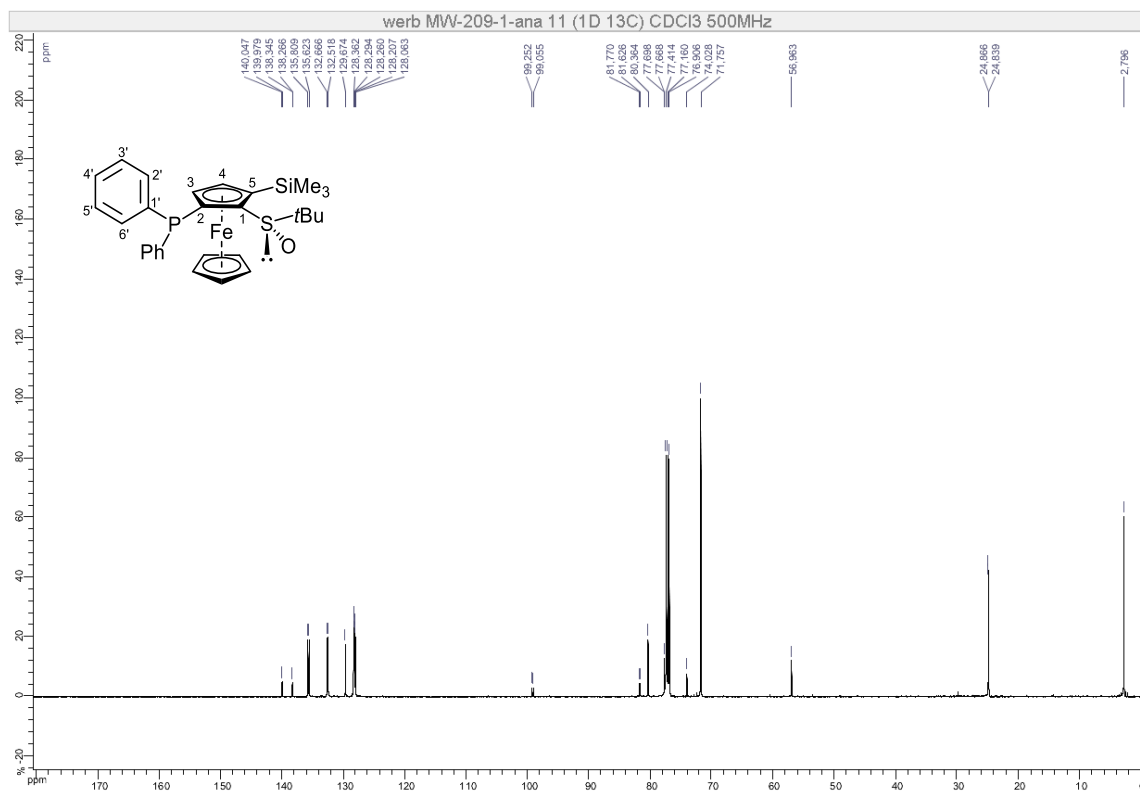


(*S,R_P*)-*S*-tert-Butyl-2-(diphenylphosphino)-5-(trimethylsilyl)ferrocenesulfoxide (*S,R_P*-2ae)

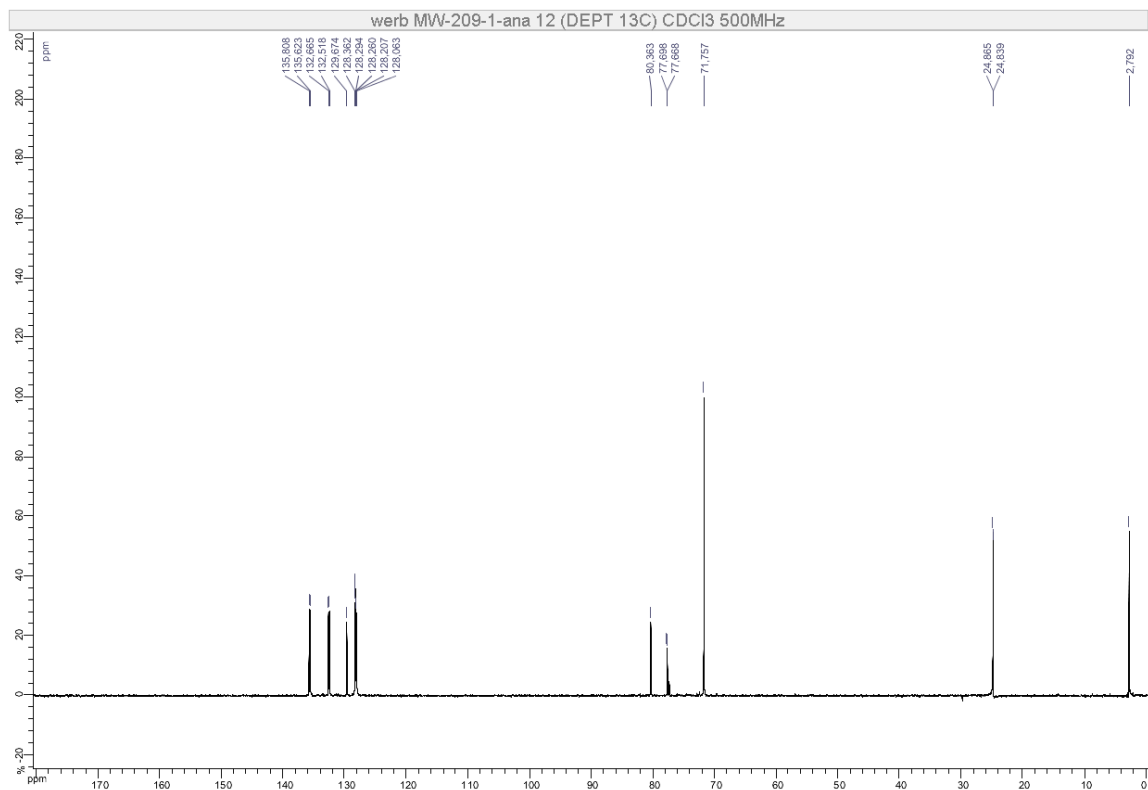
^1H NMR (500 MHz, CDCl_3)



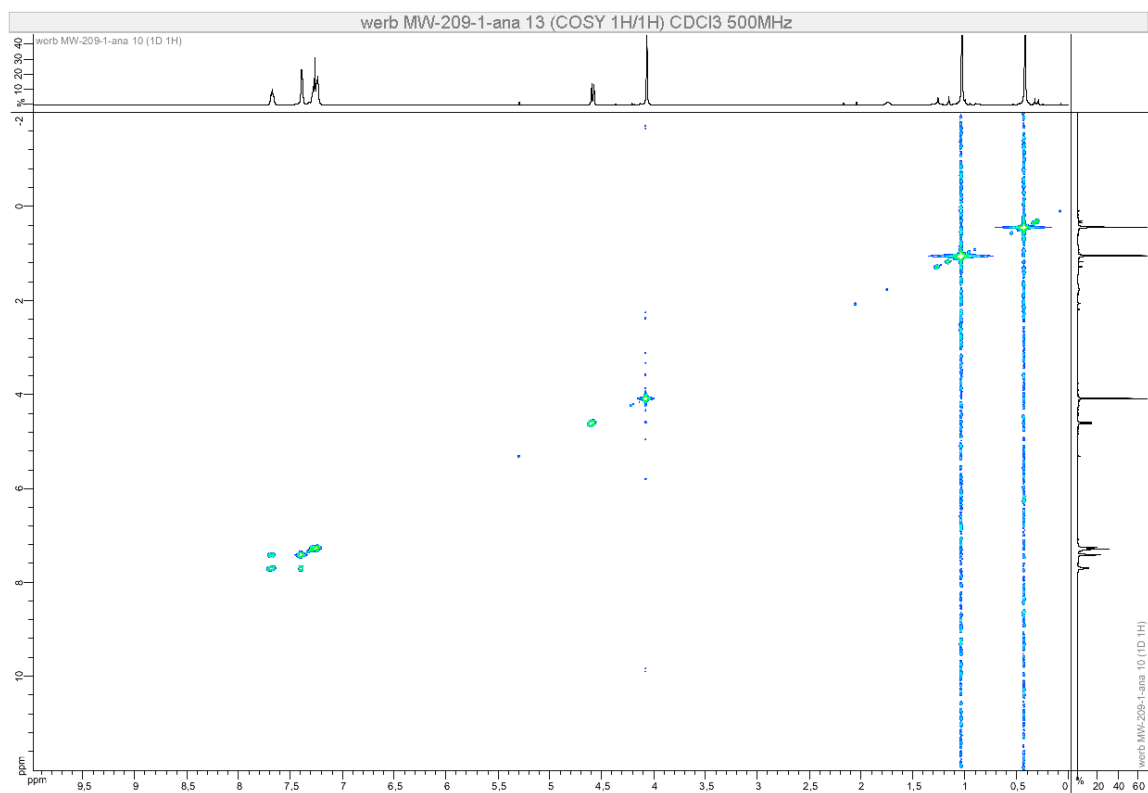
^{13}C NMR (126 MHz, CDCl_3)



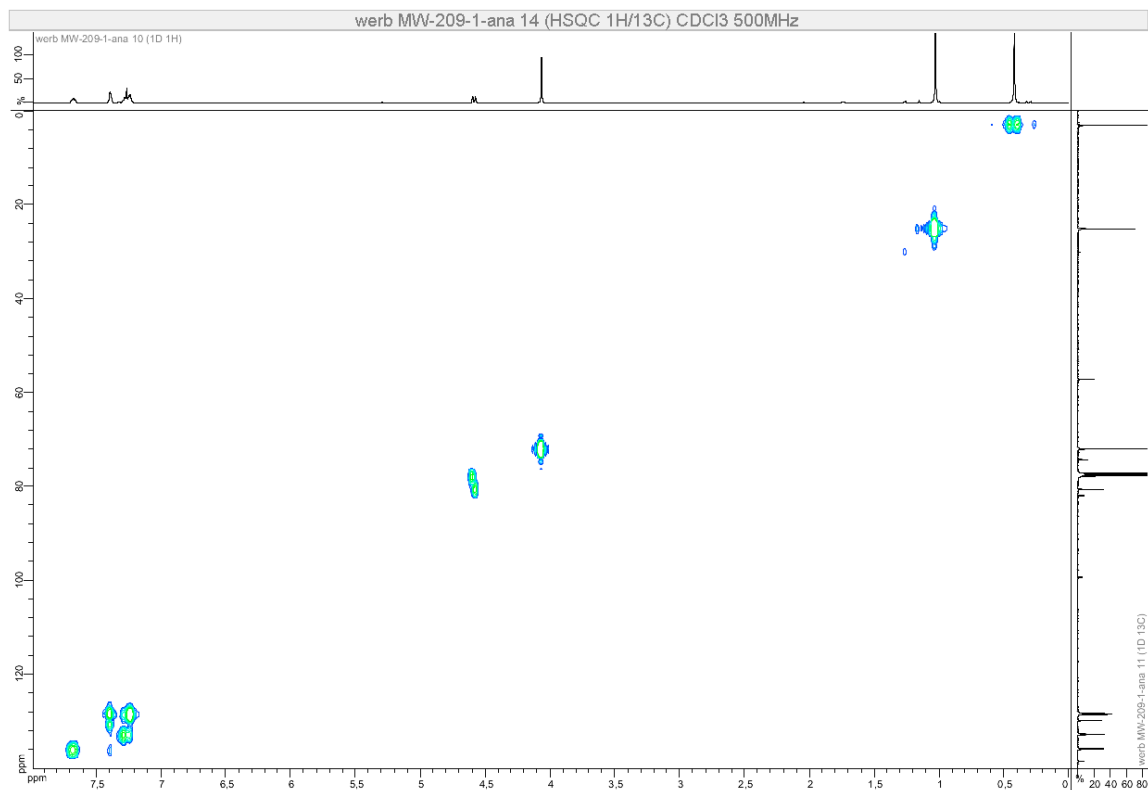
DEPT 135 (126 MHz, CDCl₃)



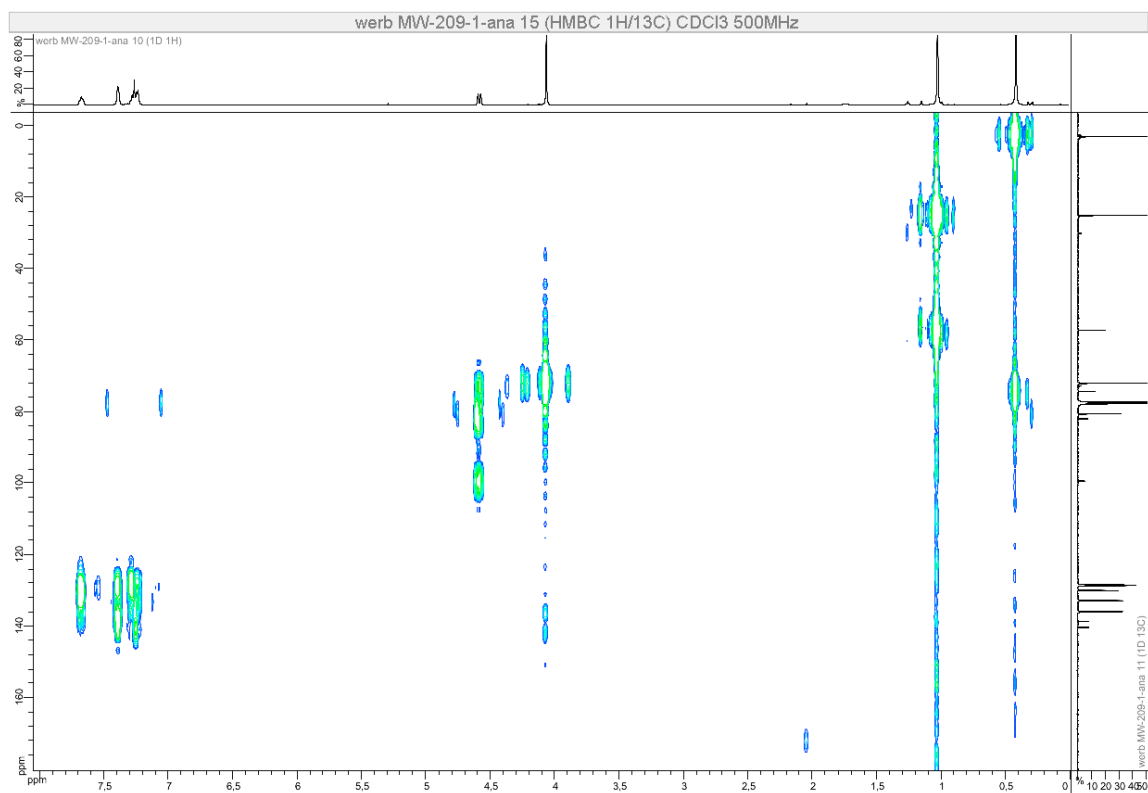
COSY (500 MHz, CDCl₃)



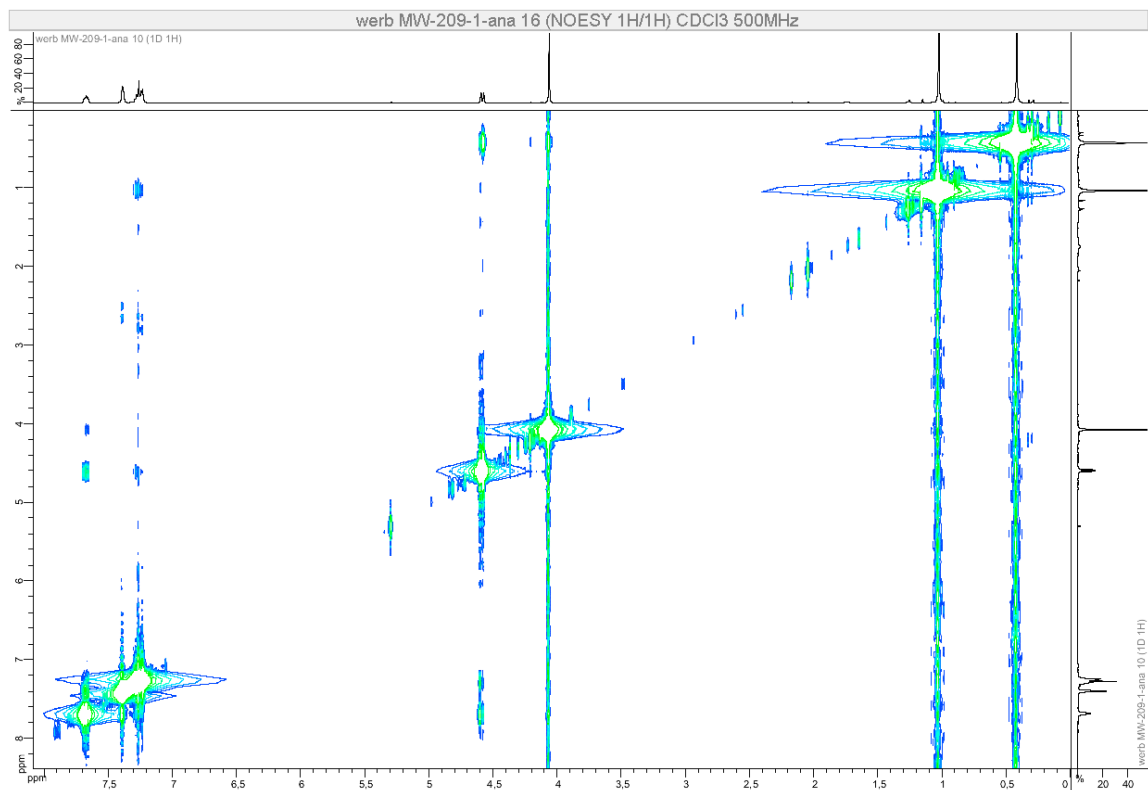
HSQC (500 MHz, CDCl₃)



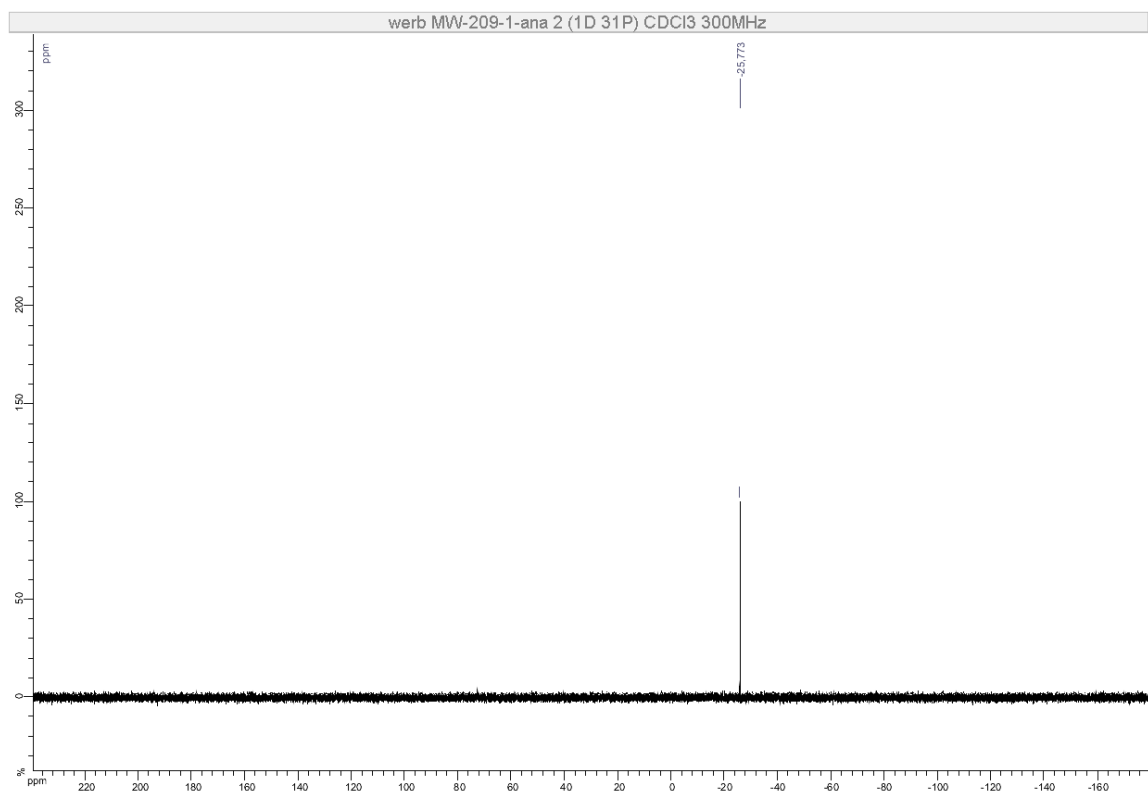
HMBC (500 MHz, CDCl₃)



NOESY (500 MHz, CDCl₃)

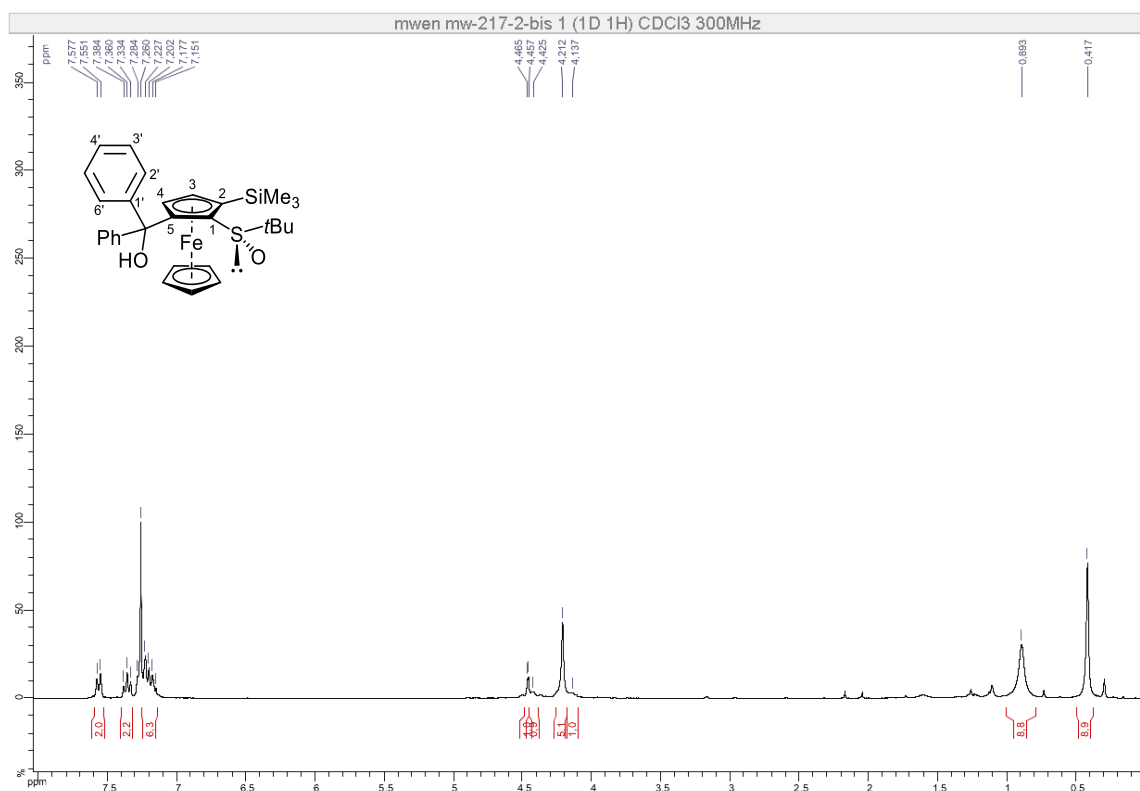


³¹P NMR (121 MHz, CDCl₃)



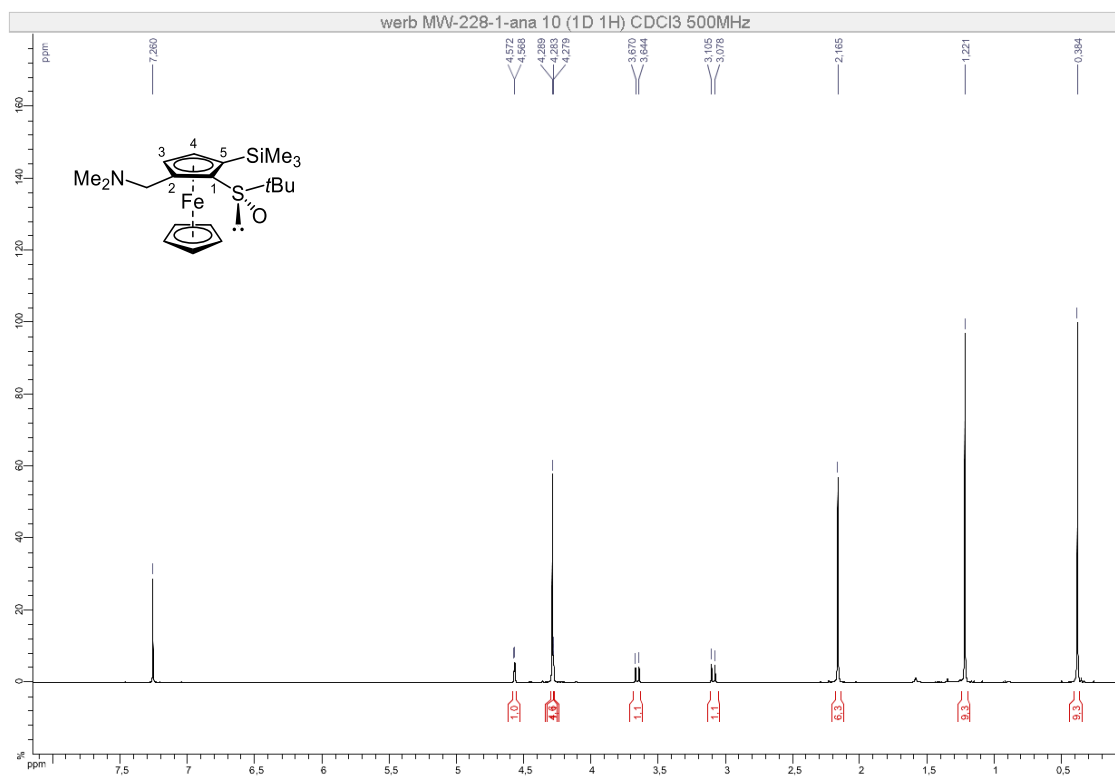
(*S,S*)-*S*-tert-Butyl-2-[(α,α -diphenyl)hydroxymethyl]-5-(trimethylsilyl)ferrocenesulfoxide (*S,S*P-2ag)

^1H NMR (300 MHz, CDCl_3)

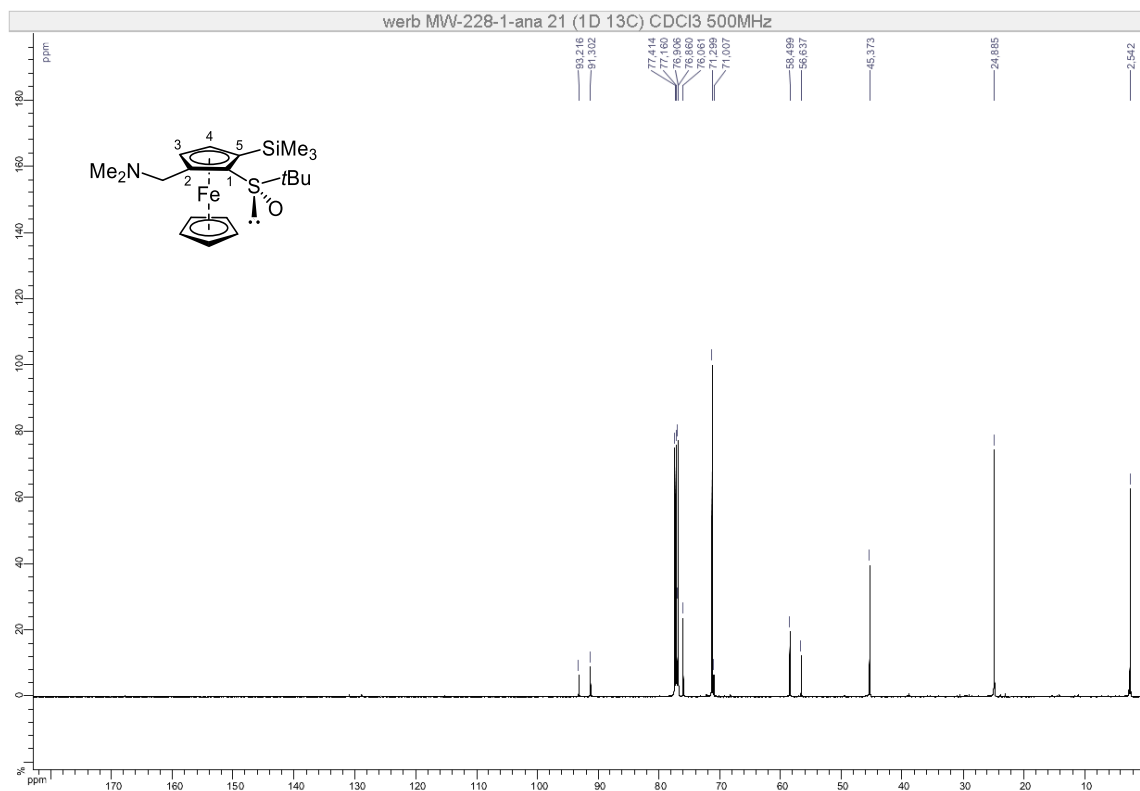


(*S,S_P*)-*S*-tert-Butyl-2-(dimethylaminomethyl)-5-(trimethylsilyl)ferrocenesulfoxide (*S,S_P*-2ah)

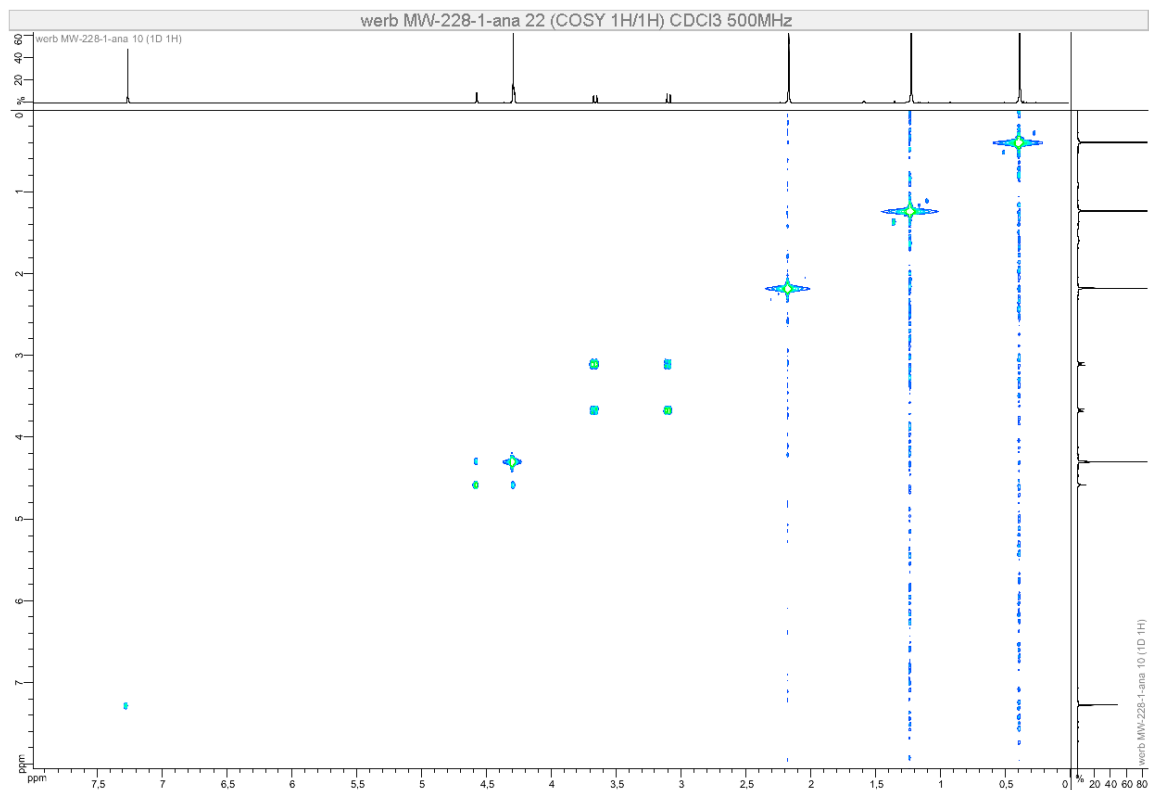
^1H NMR (500 MHz, CDCl_3)



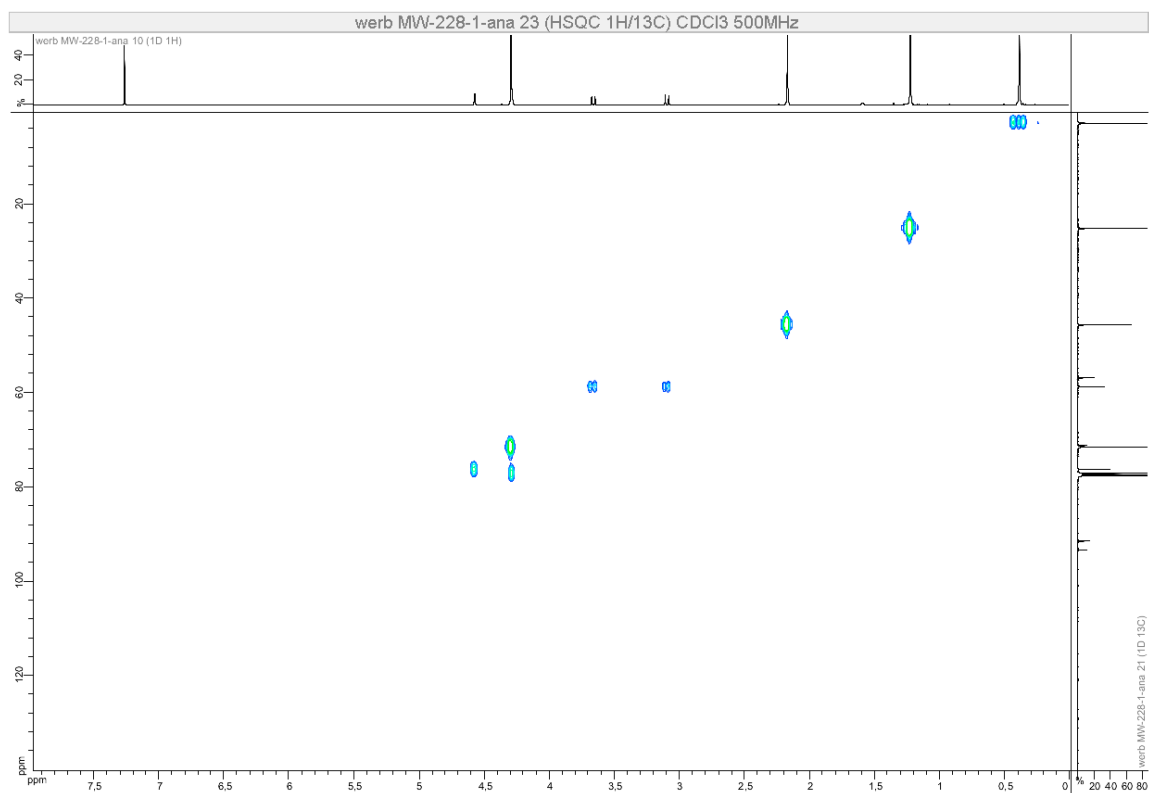
^{13}C NMR (126 MHz, CDCl_3)



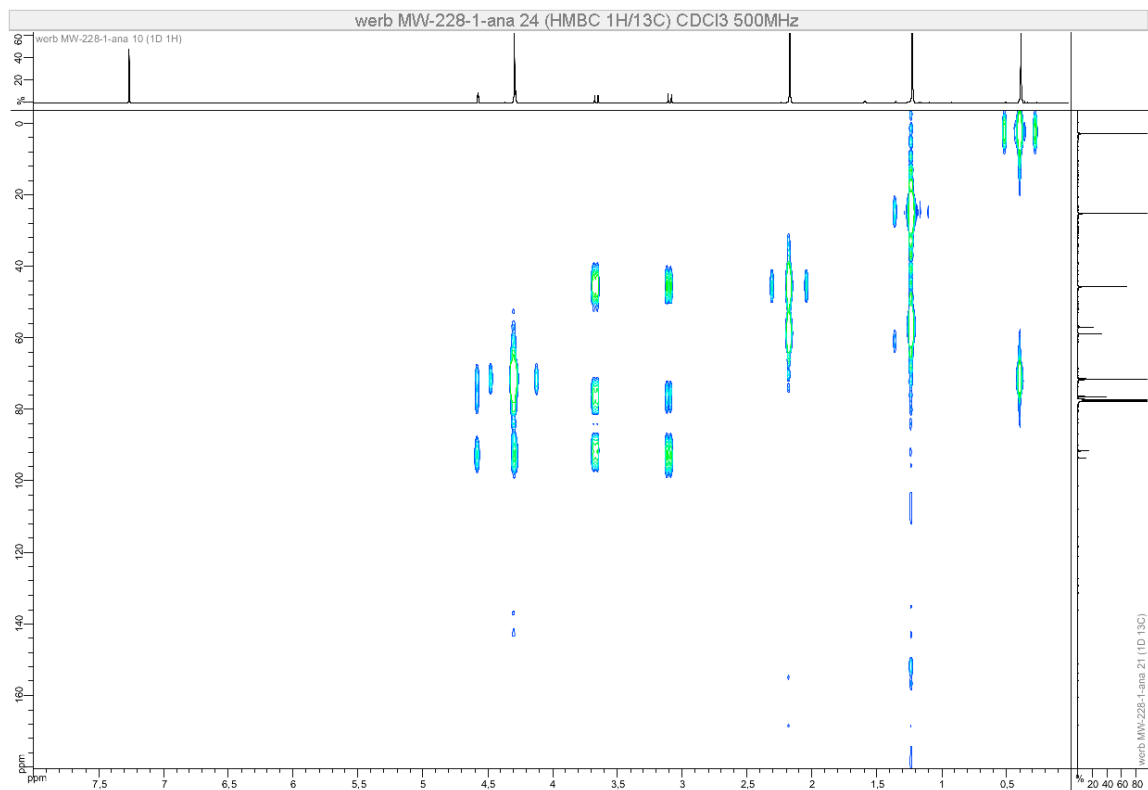
COSY (500 MHz, CDCl₃)



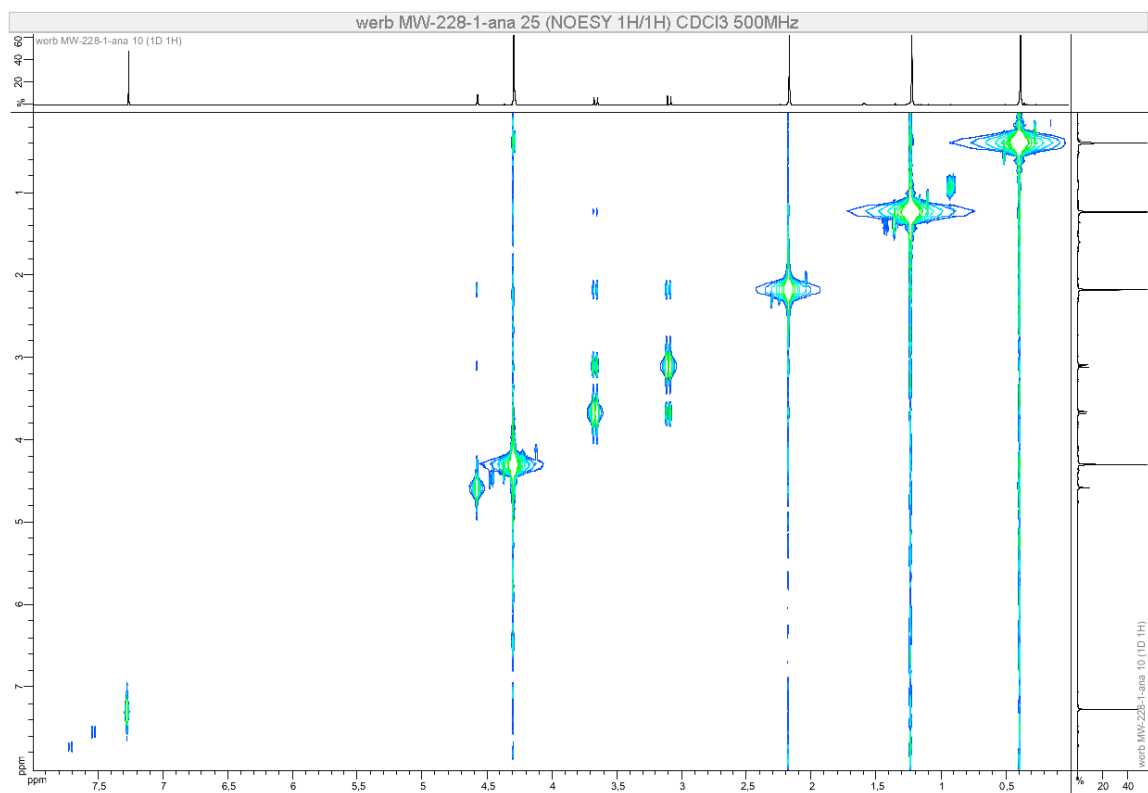
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

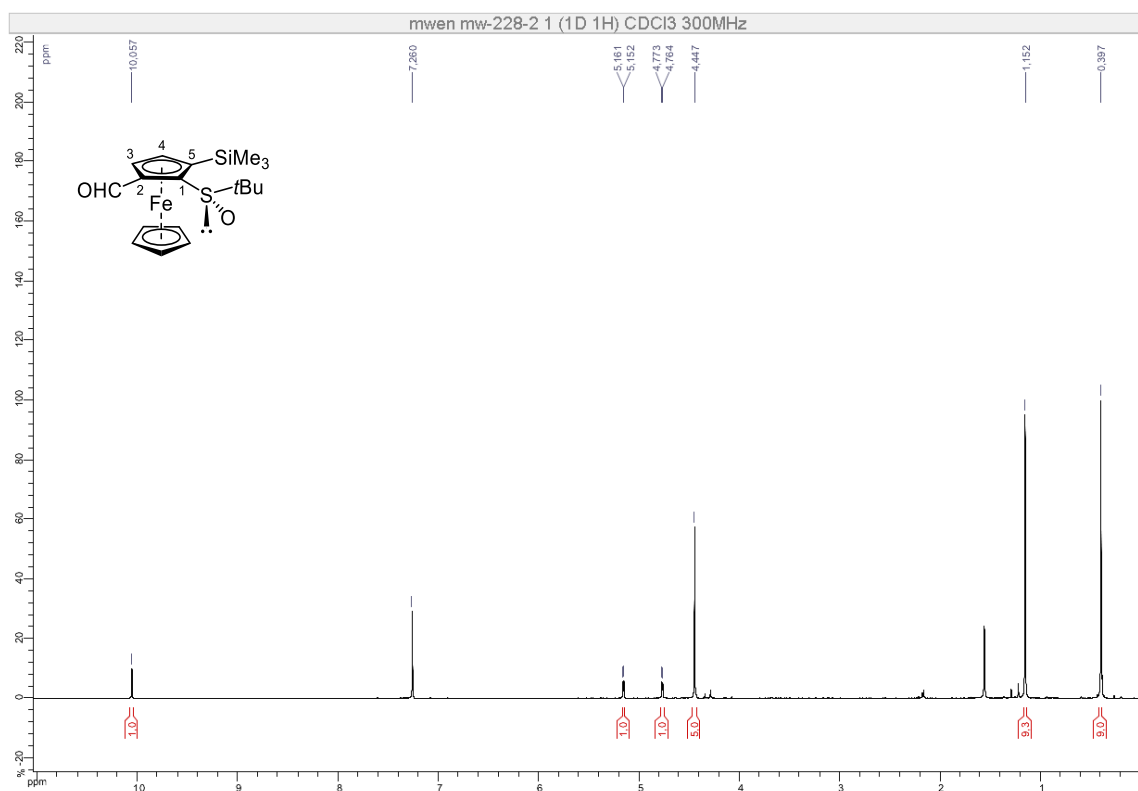


NOESY (500 MHz, CDCl₃)



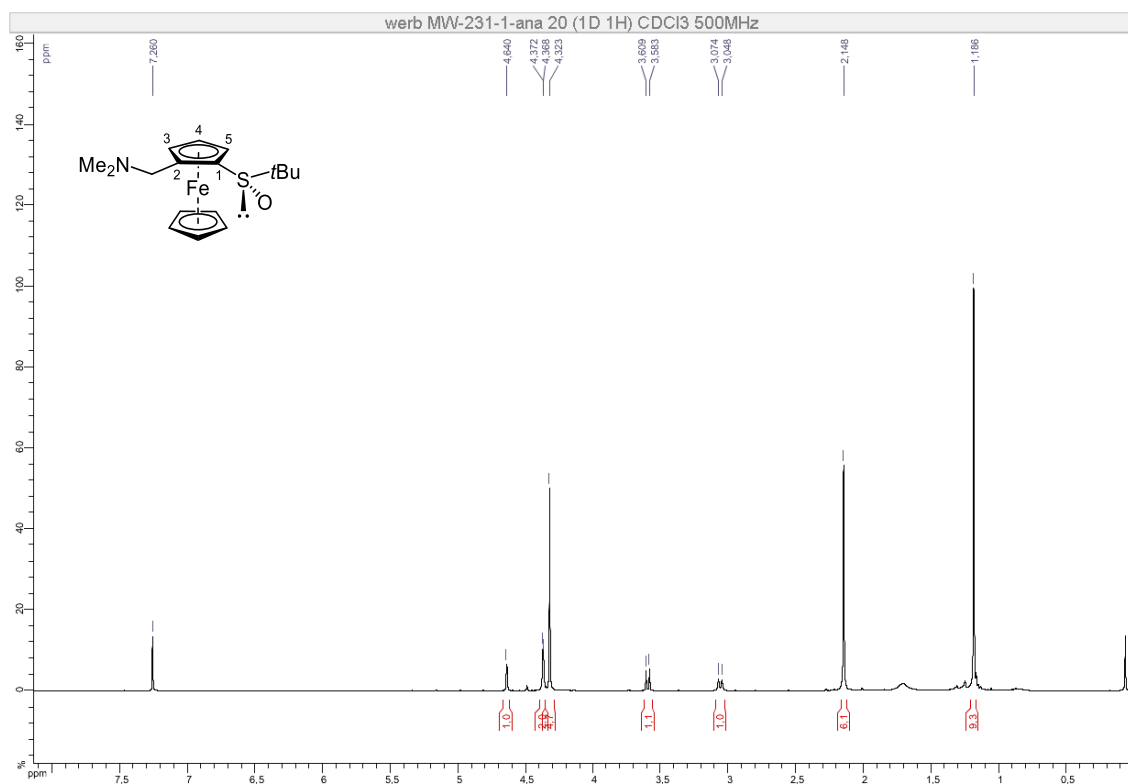
(*S,S*_P)-*S*-tert-Butyl-2-formyl-5-(trimethylsilyl)ferrocenesulfoxide (*S,S*_P-2ah')

¹H NMR (300 MHz, CDCl₃)

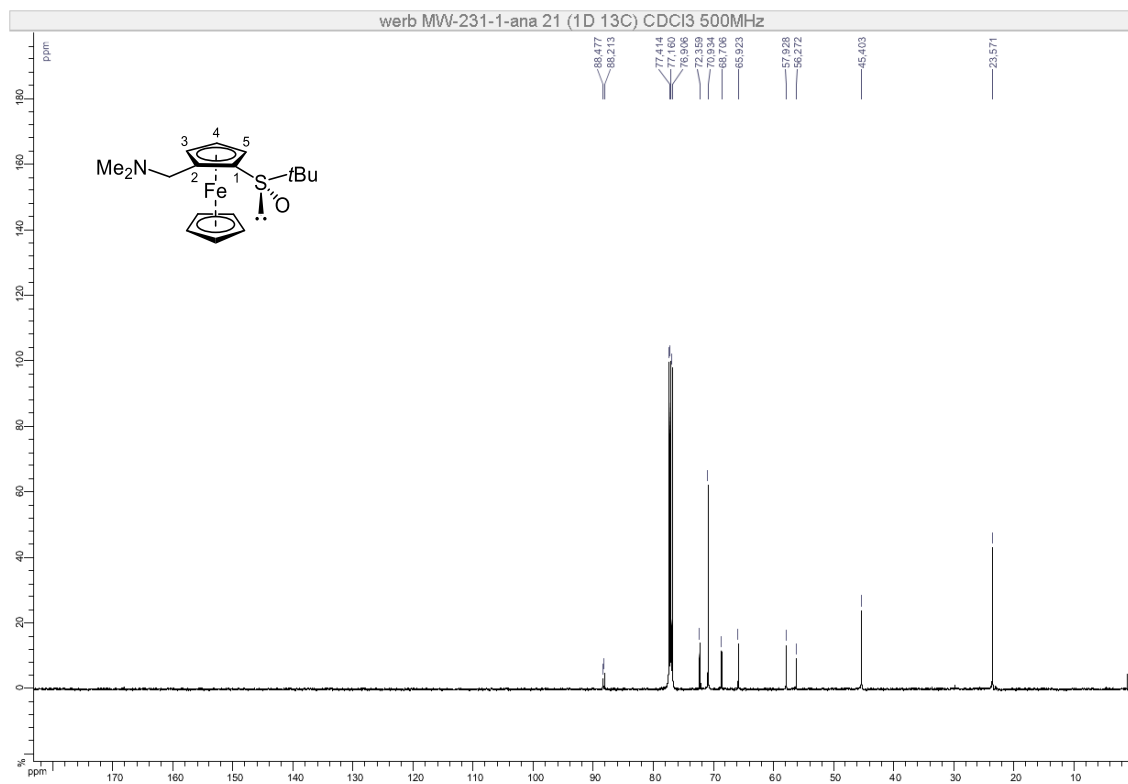


(*S,R_P*)-*S*-tert-Butyl-2-(dimethylaminomethyl)ferrocenesulfoxide (*S,R_P*-1h)

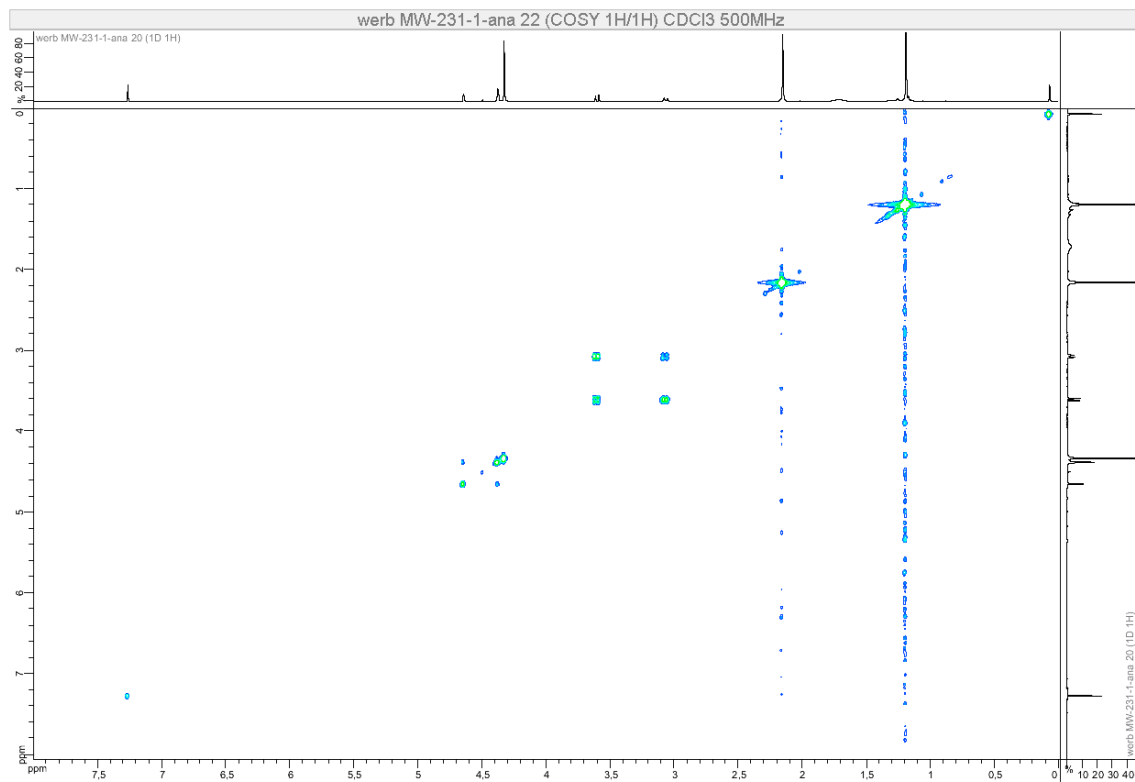
^1H NMR (500 MHz, CDCl_3)



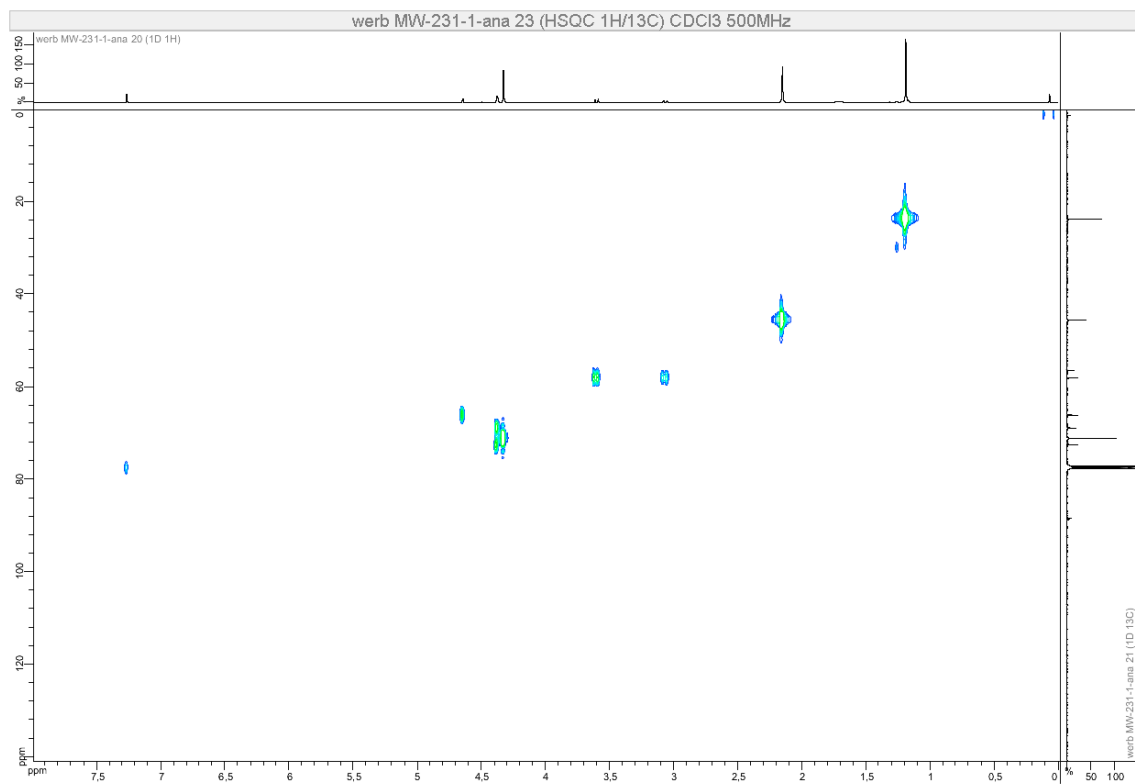
^{13}C NMR (126 MHz, CDCl_3)



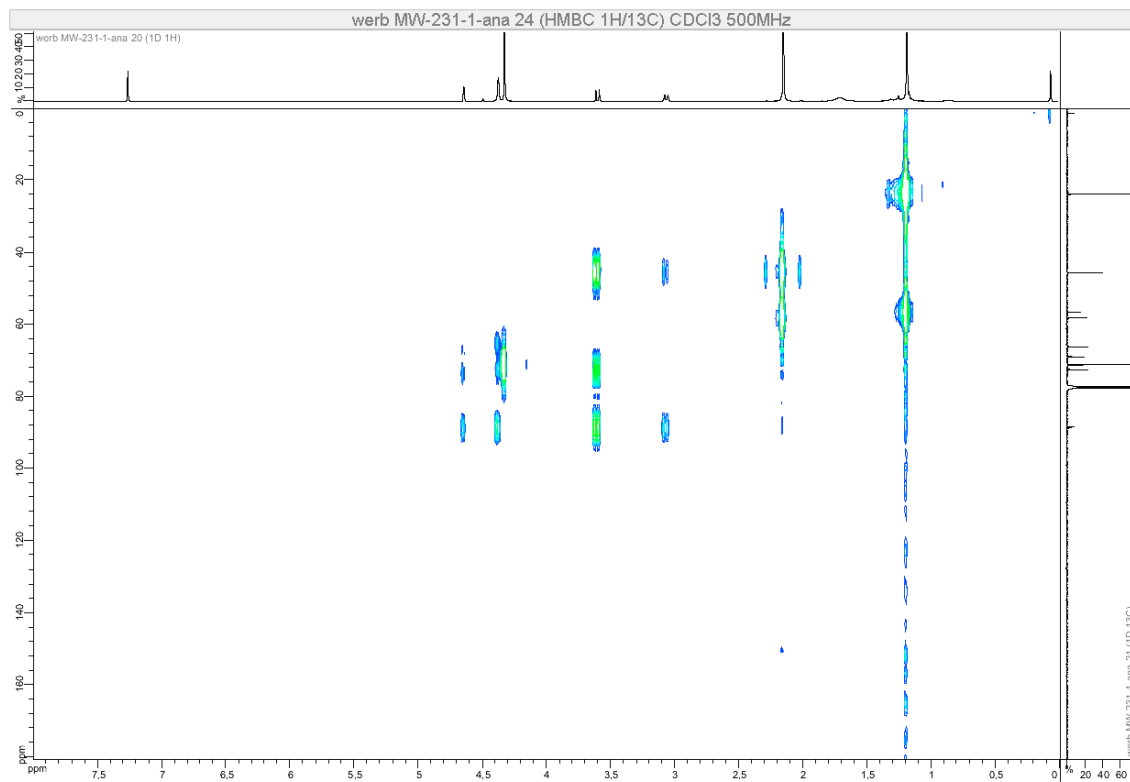
COSY (500 MHz, CDCl₃)



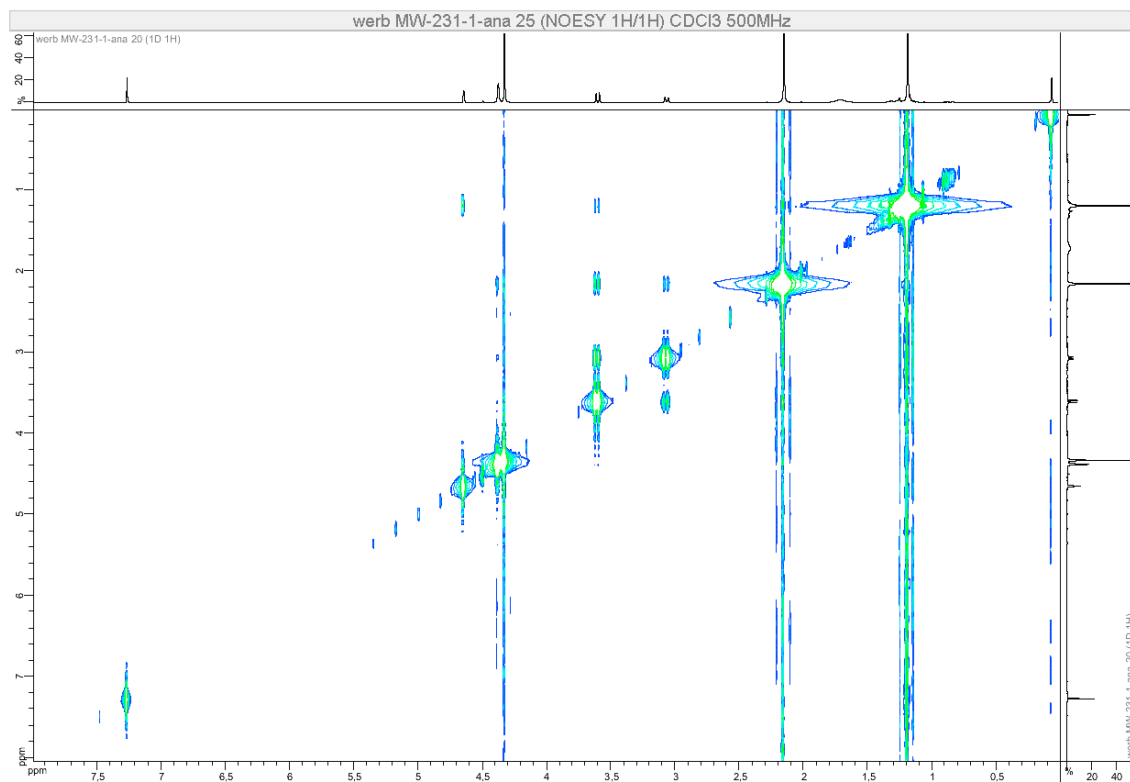
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

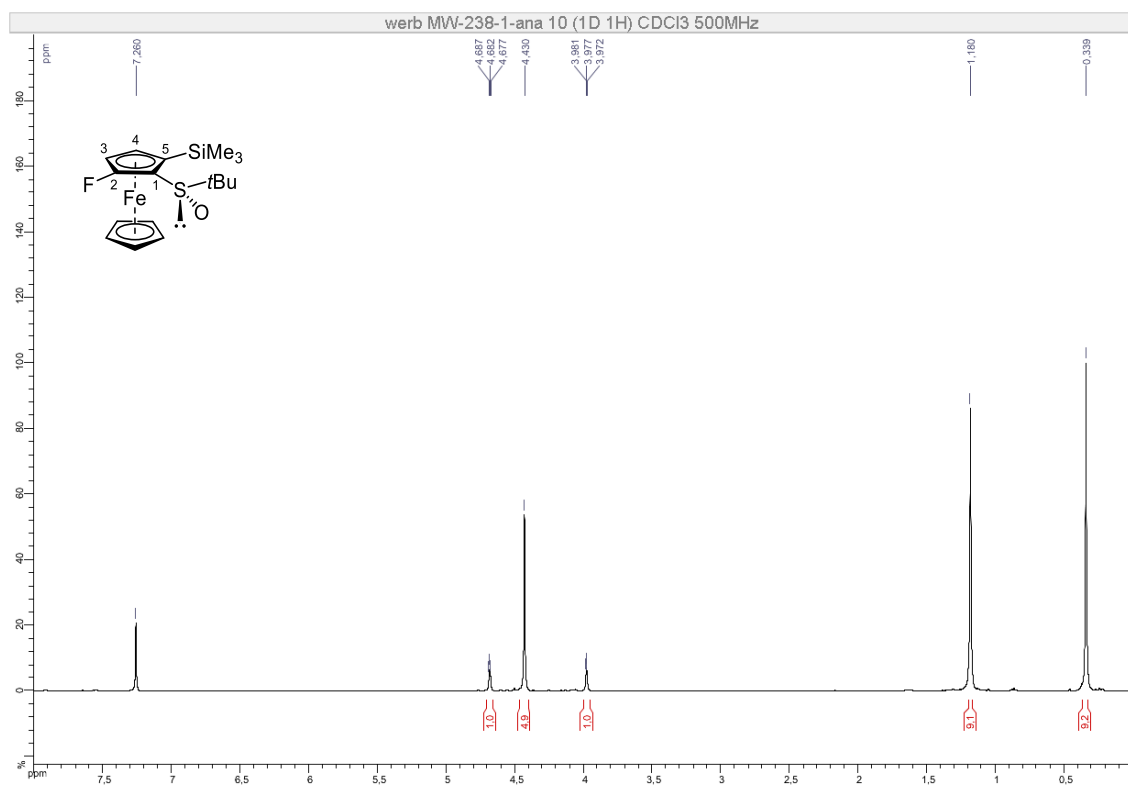


NOESY (500 MHz, CDCl₃)

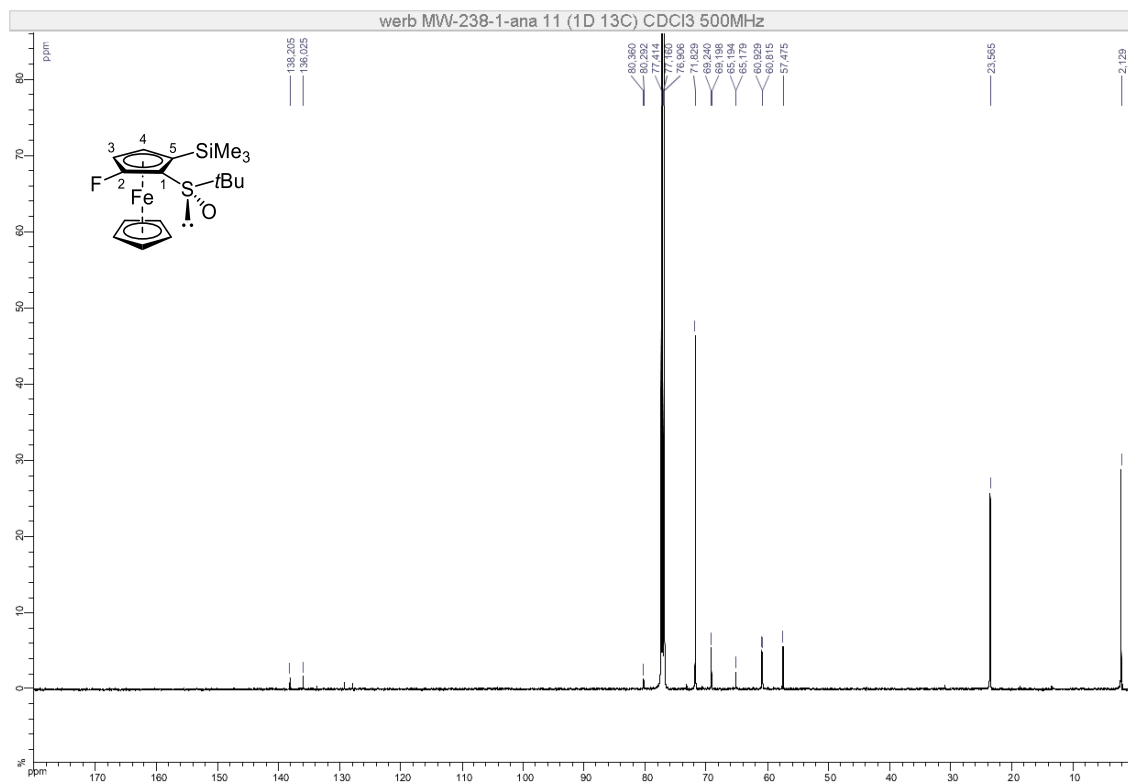


(*S,S*_P)-*S*-tert-Butyl-2-fluoro-5-(trimethylsilyl)ferrocenesulfoxide (*S,S*_P-2ai)

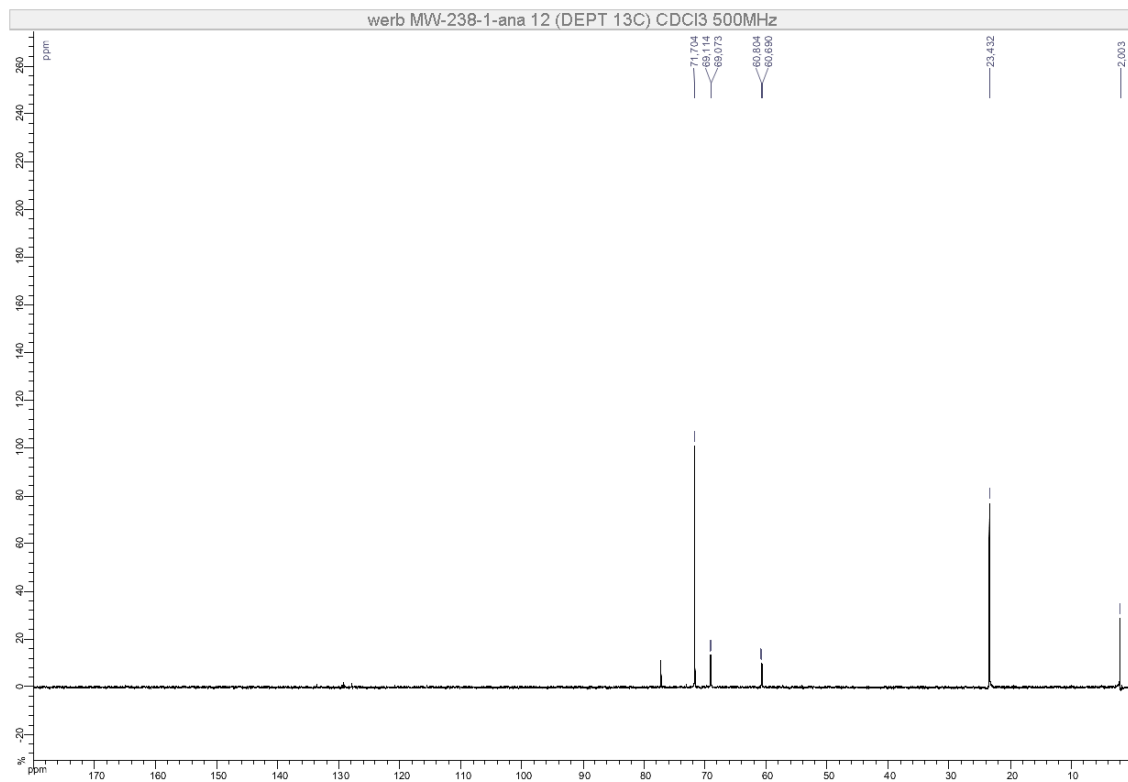
¹H NMR (500 MHz, CDCl₃)



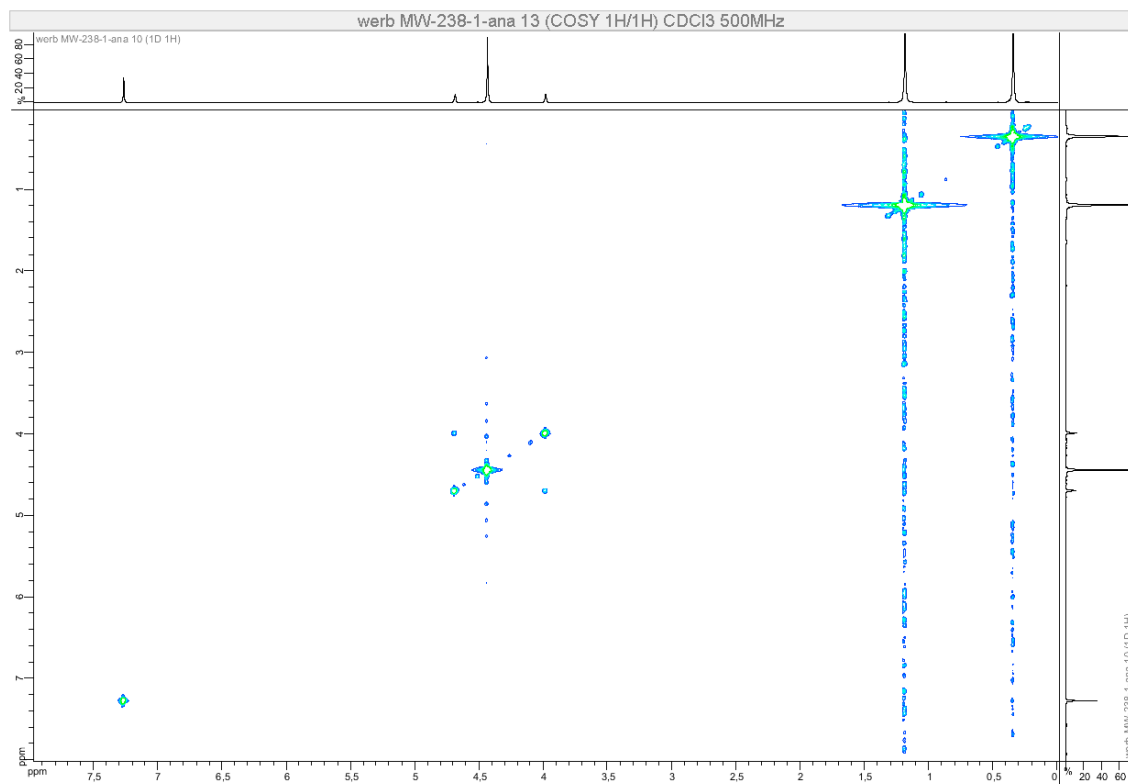
¹³C NMR (126 MHz, CDCl₃)



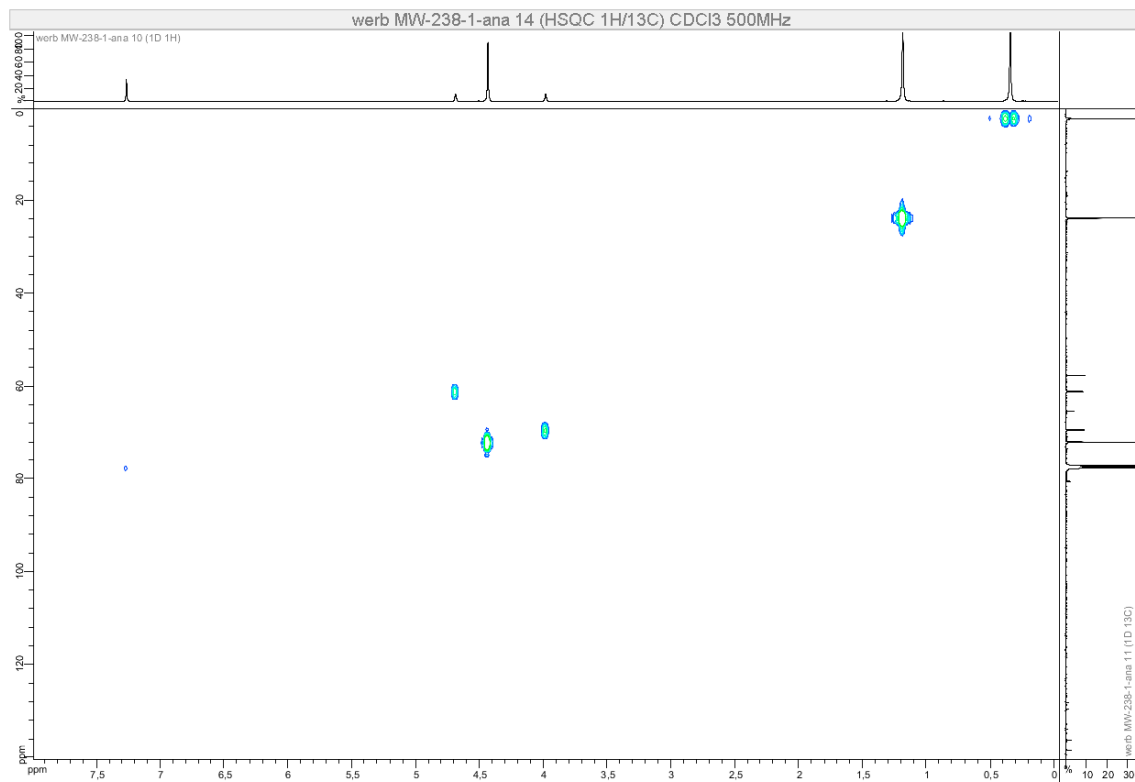
DEPT 135 (126 MHz, CDCl₃)



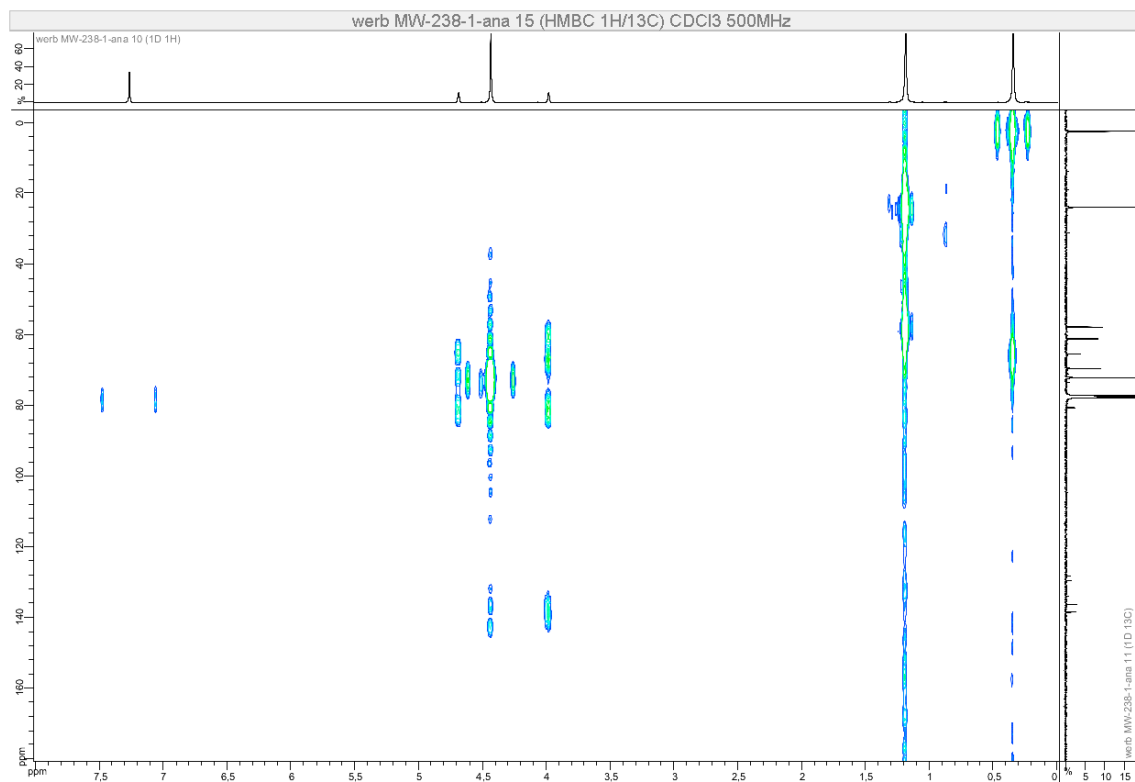
COSY (500 MHz, CDCl₃)



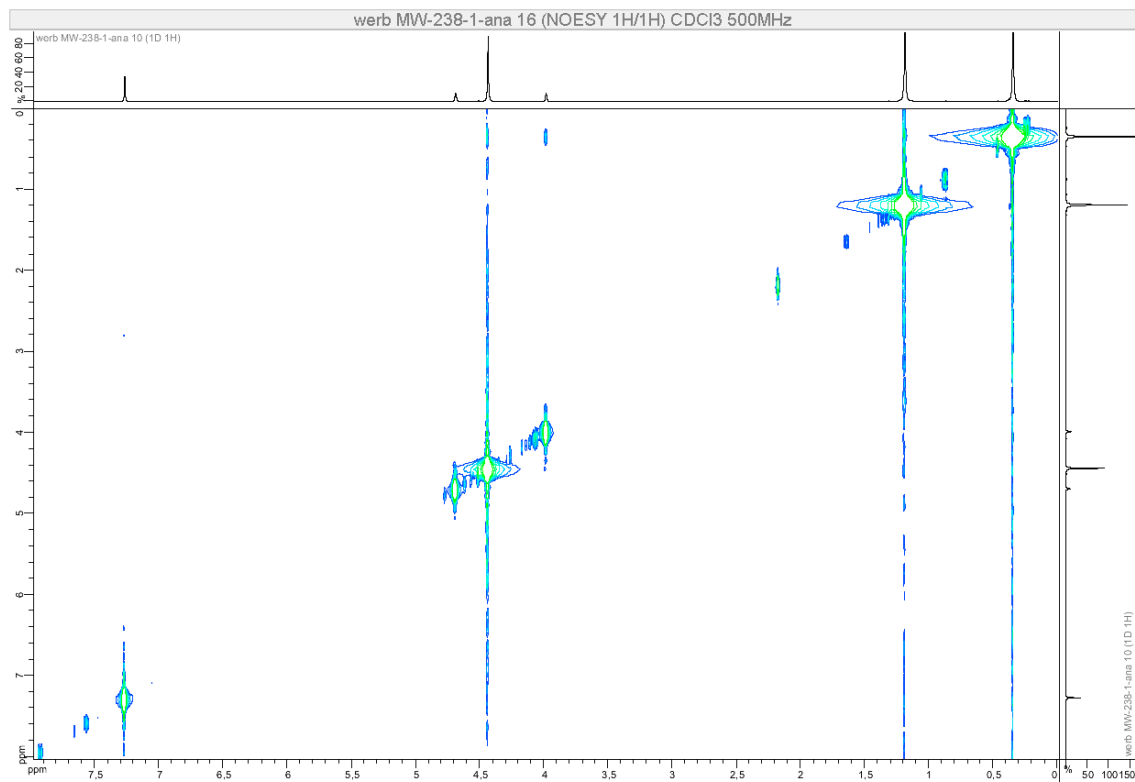
HSQC (500 MHz, CDCl₃)



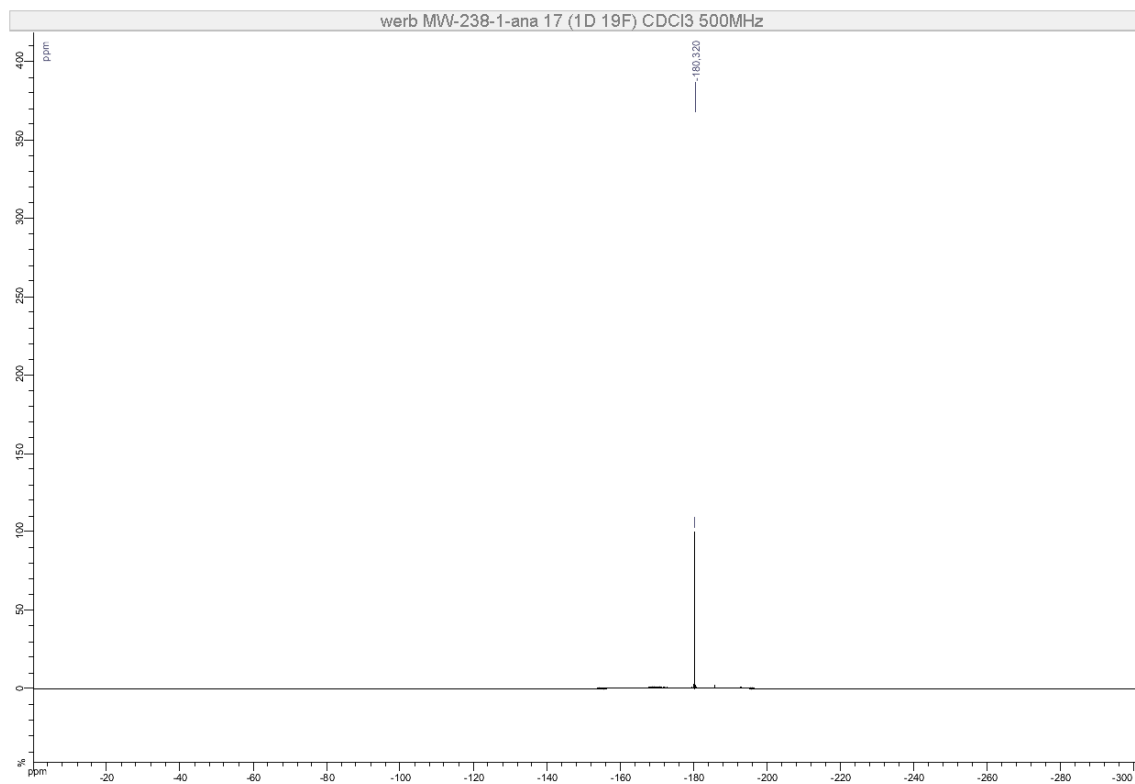
HMBC (500 MHz, CDCl₃)



NOESY (500 MHz, CDCl₃)

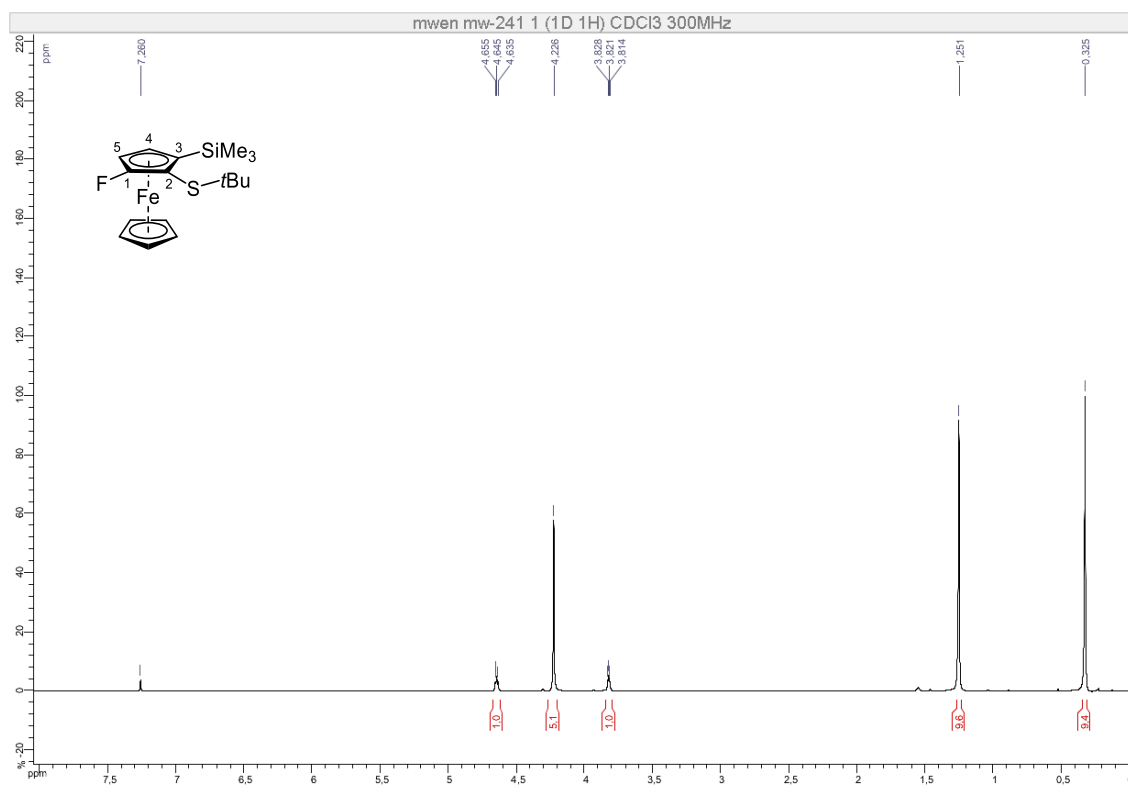


¹⁹F NMR (471 MHz, CDCl₃)



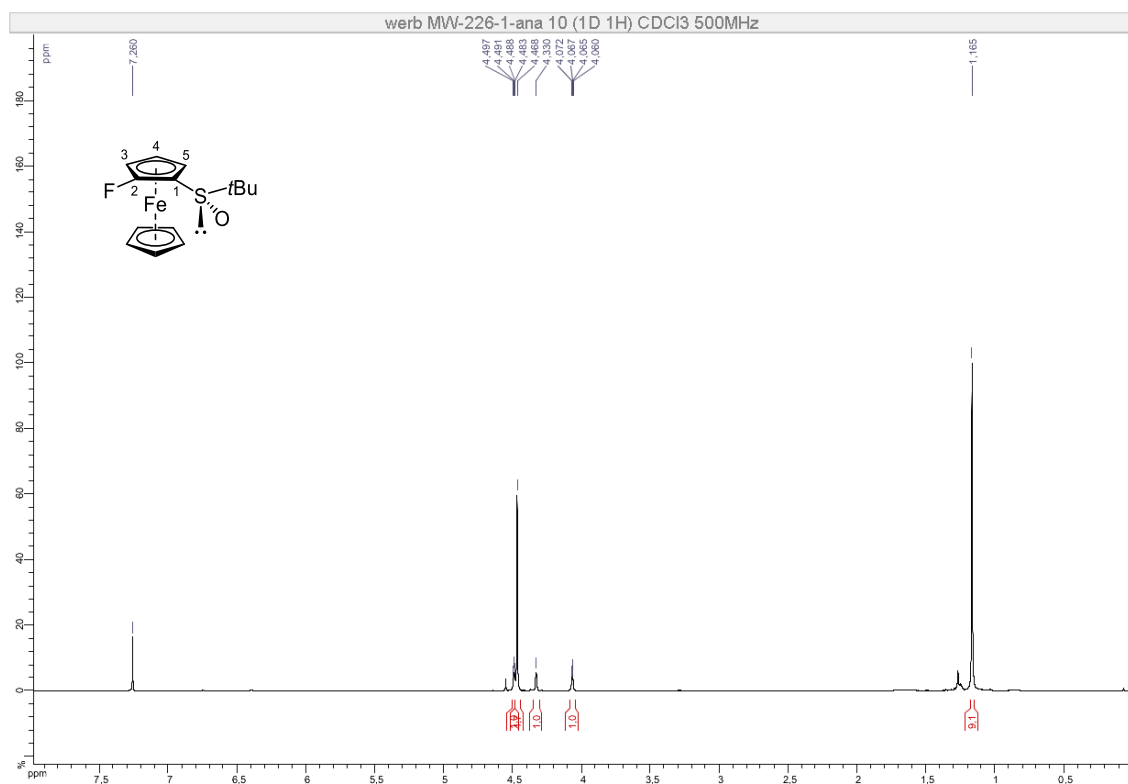
(*S_P*)-2-(*tert*-Butylthio)-1-fluoro-3-(trimethylsilyl)ferrocene (*S_P*-8ai)

¹H NMR (300 MHz, CDCl₃)

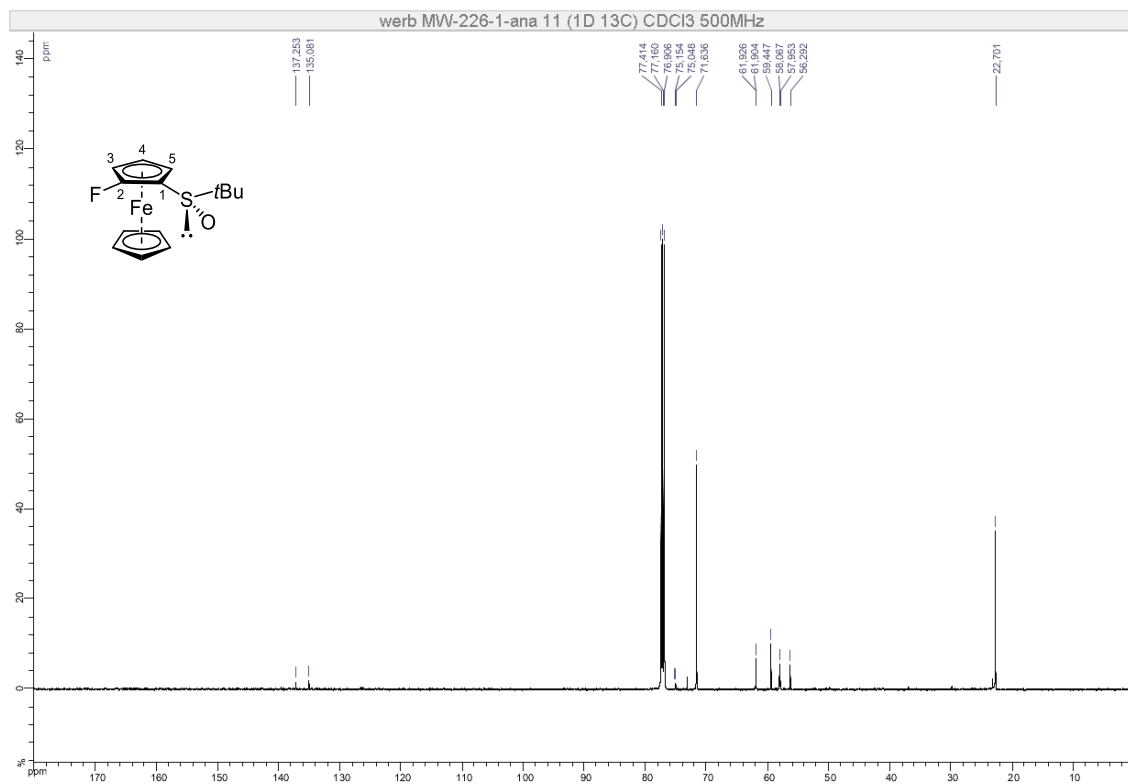


(*S,R_P*)-*S*-tert-Butyl-2-fluoroferrocenenesulfoxide (*S,R_P*-1i)

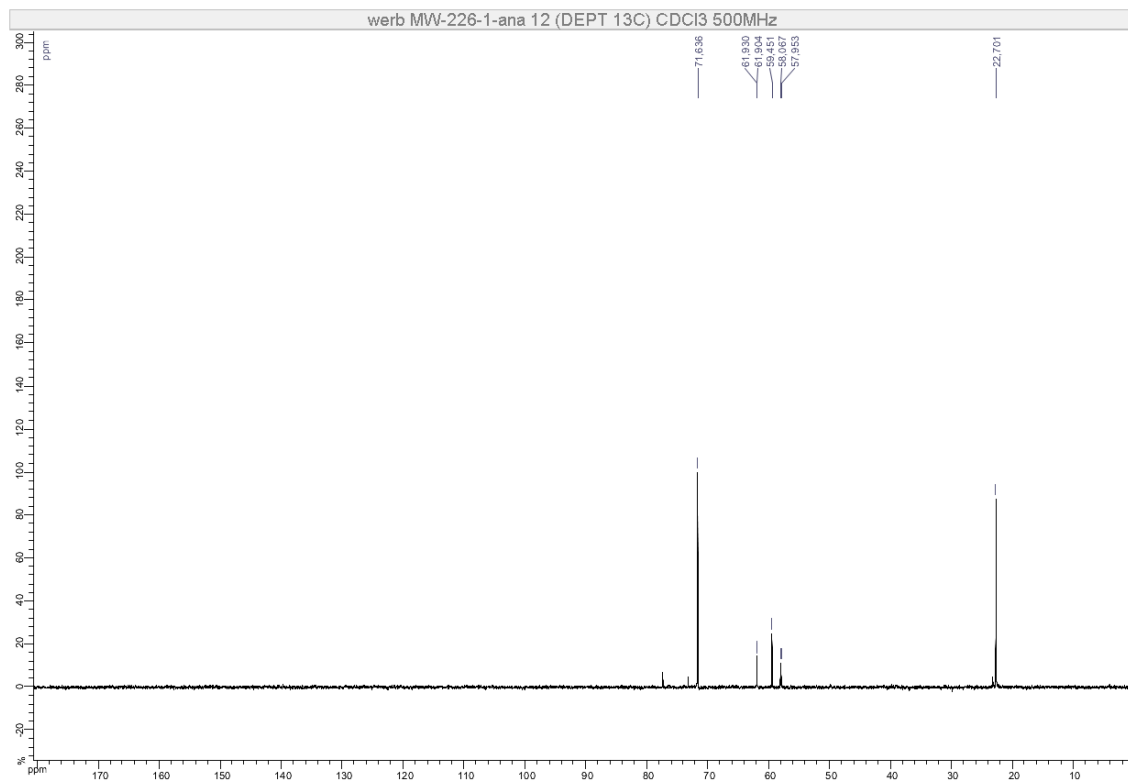
^1H NMR (500 MHz, CDCl_3)



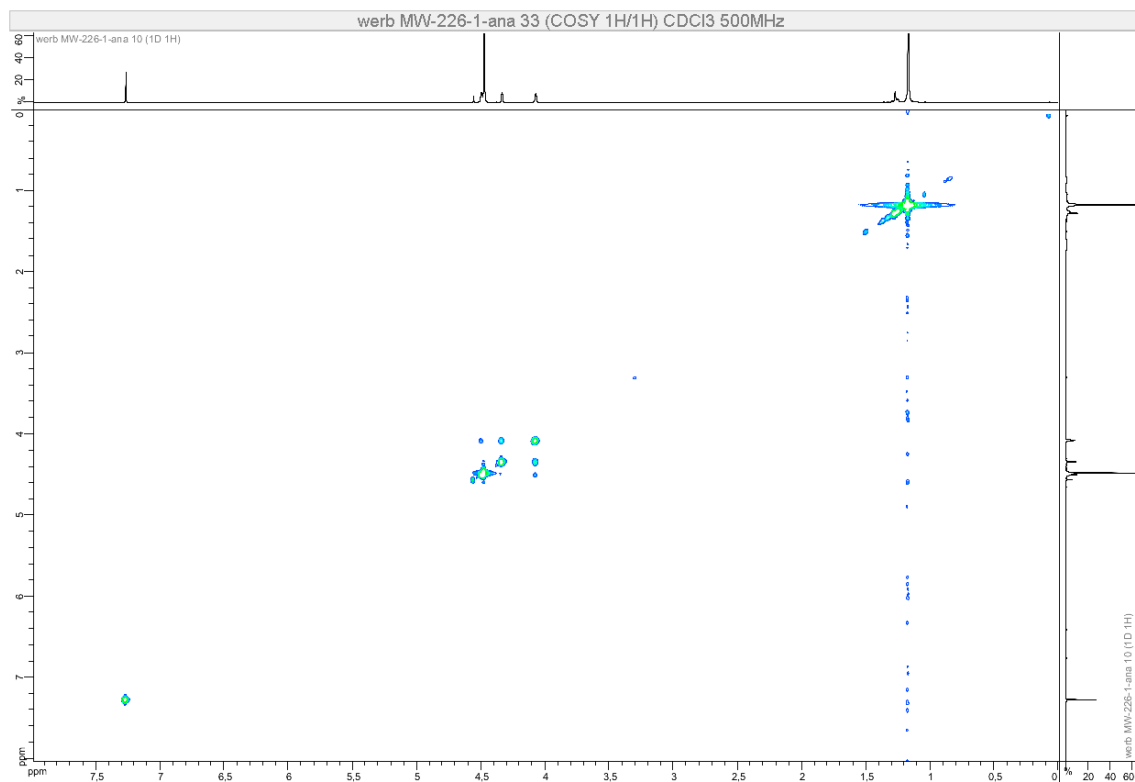
^{13}C NMR (126 MHz, CDCl_3)



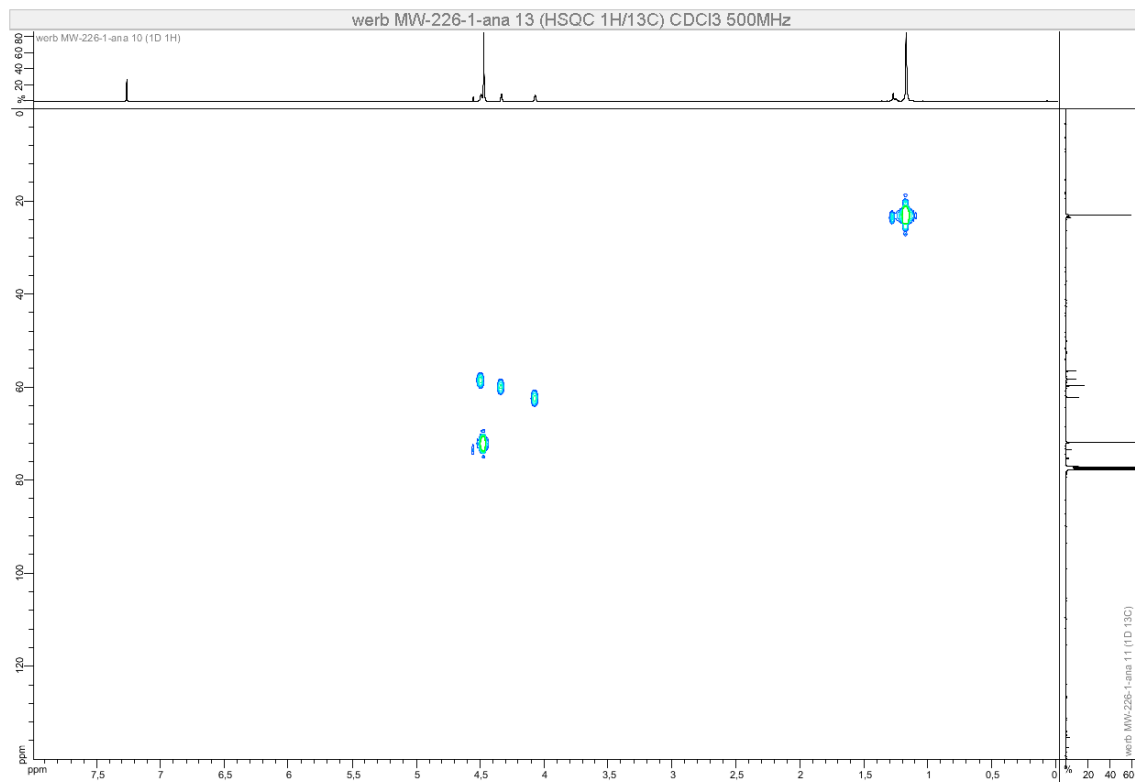
DEPT 135 (126 MHz, CDCl₃)



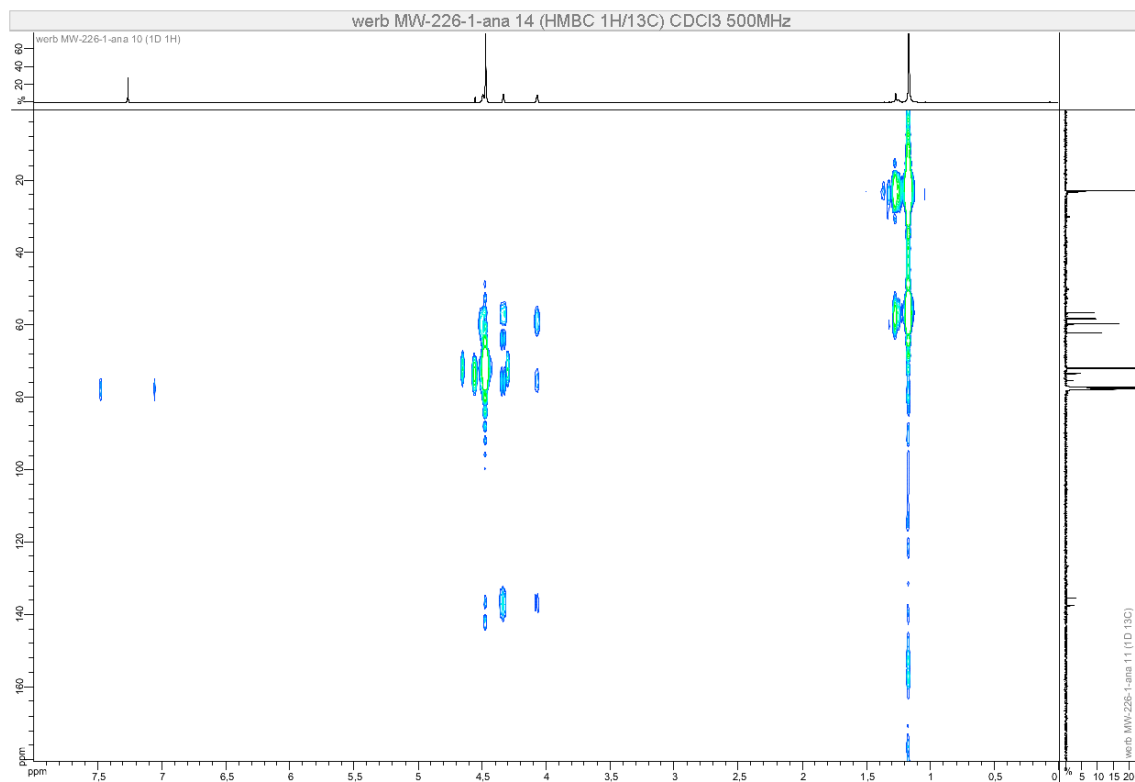
COSY (500 MHz, CDCl₃)



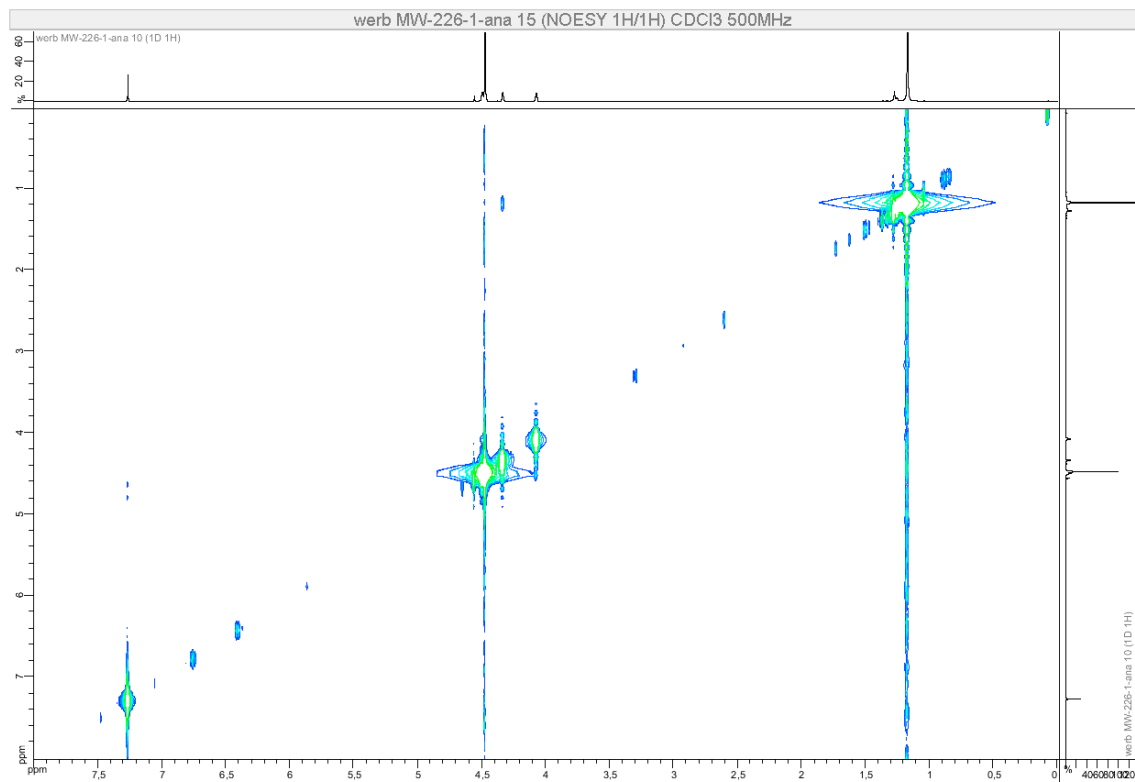
HSQC (500 MHz, CDCl₃)



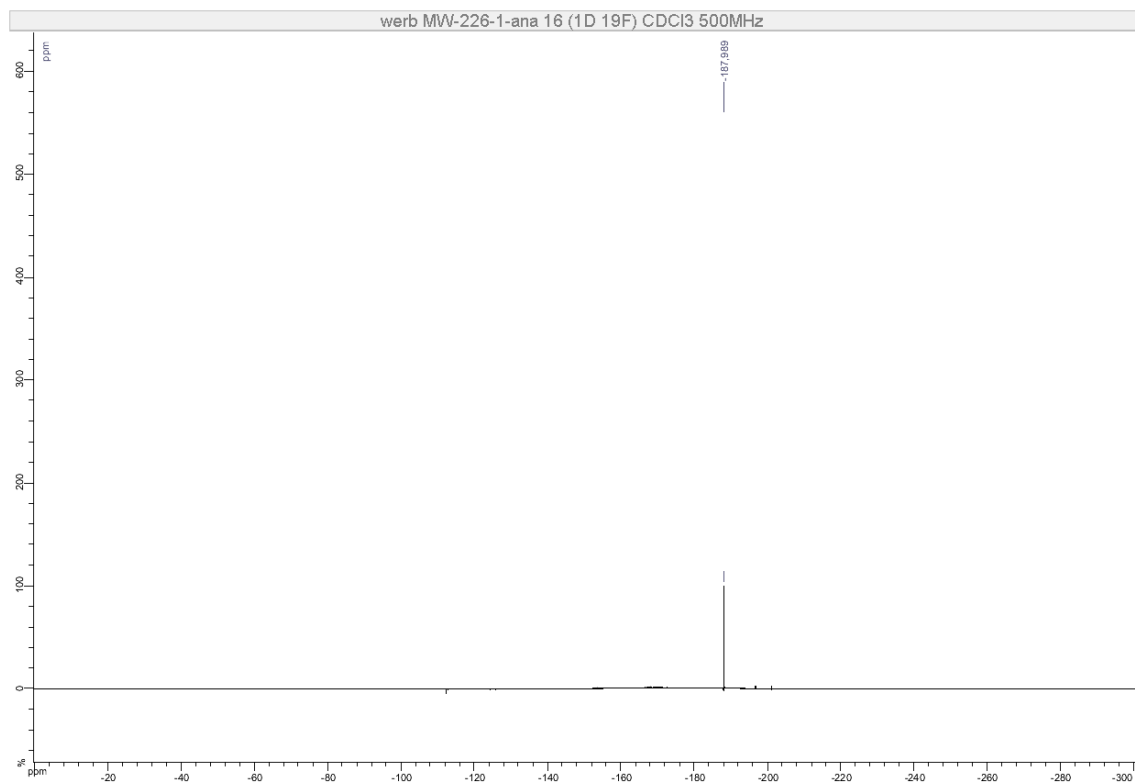
HMBC (500 MHz, CDCl₃)



NOESY (500 MHz, CDCl₃)

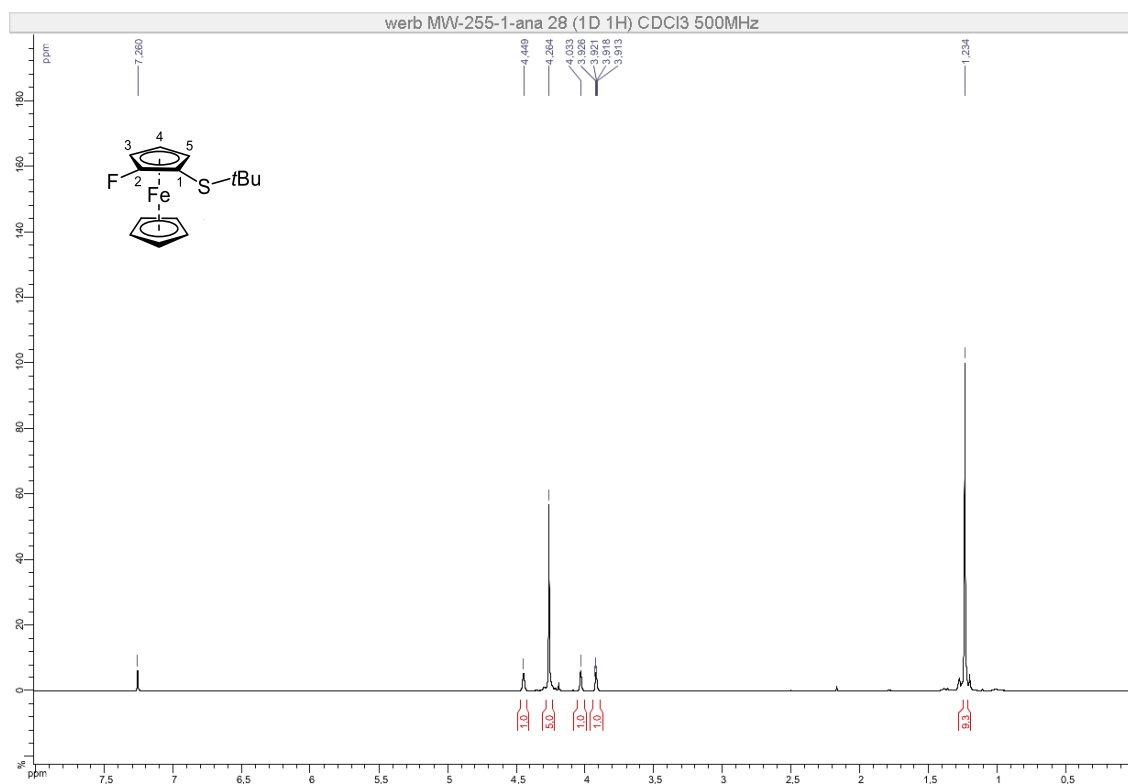


¹⁹F NMR (471 MHz, CDCl₃)

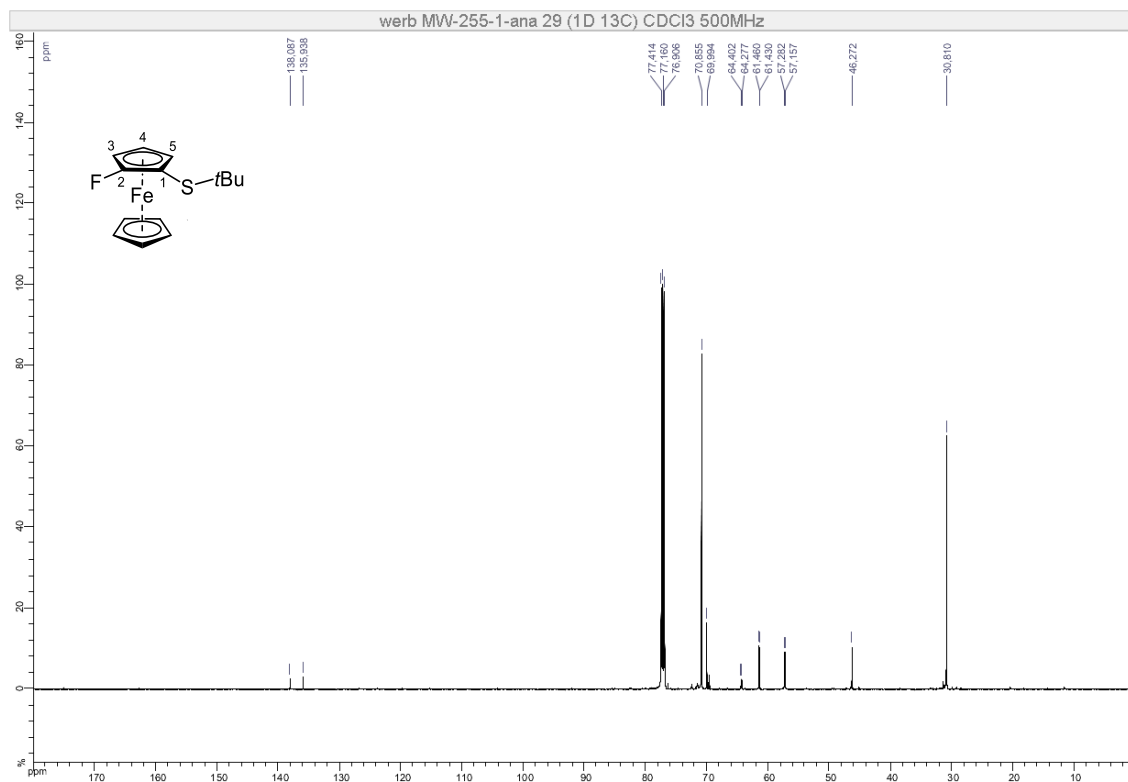


(*R_P*)-1-(*tert*-Butylthio)-2-fluoroferrocene (*R_P*-8i)

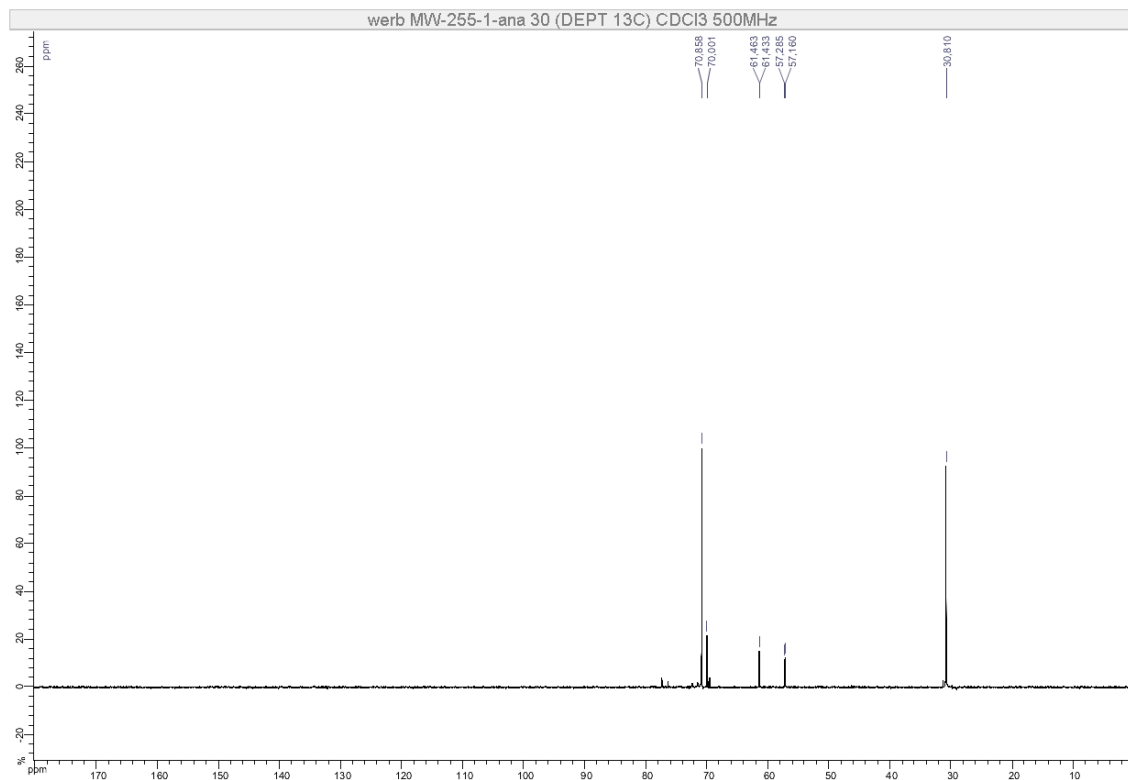
¹H NMR (500 MHz, CDCl₃)



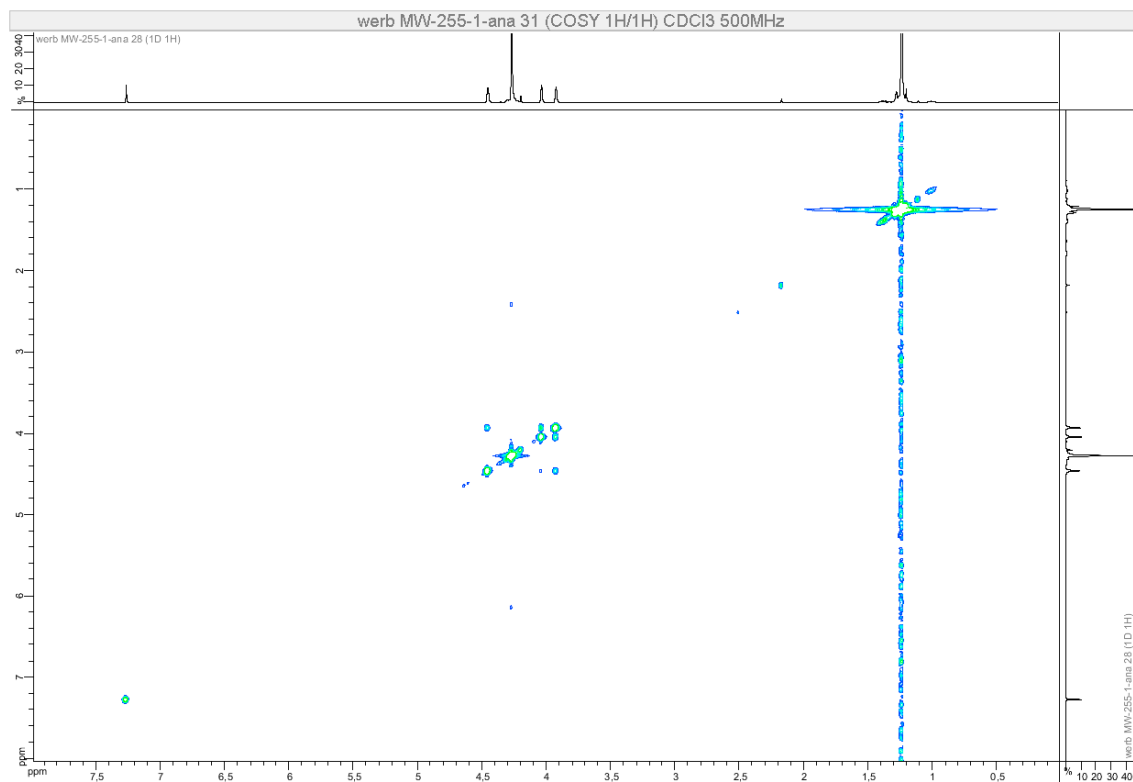
¹³C NMR (126 MHz, CDCl₃)



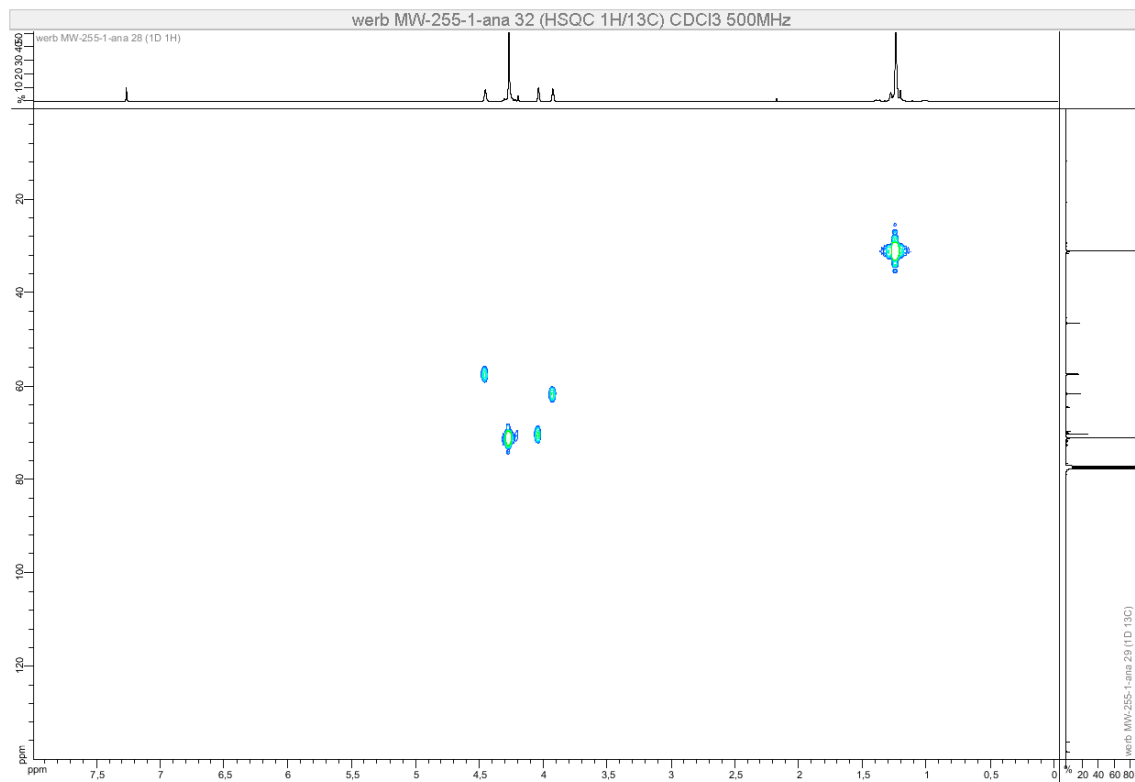
DEPT 135 (126 MHz, CDCl₃)



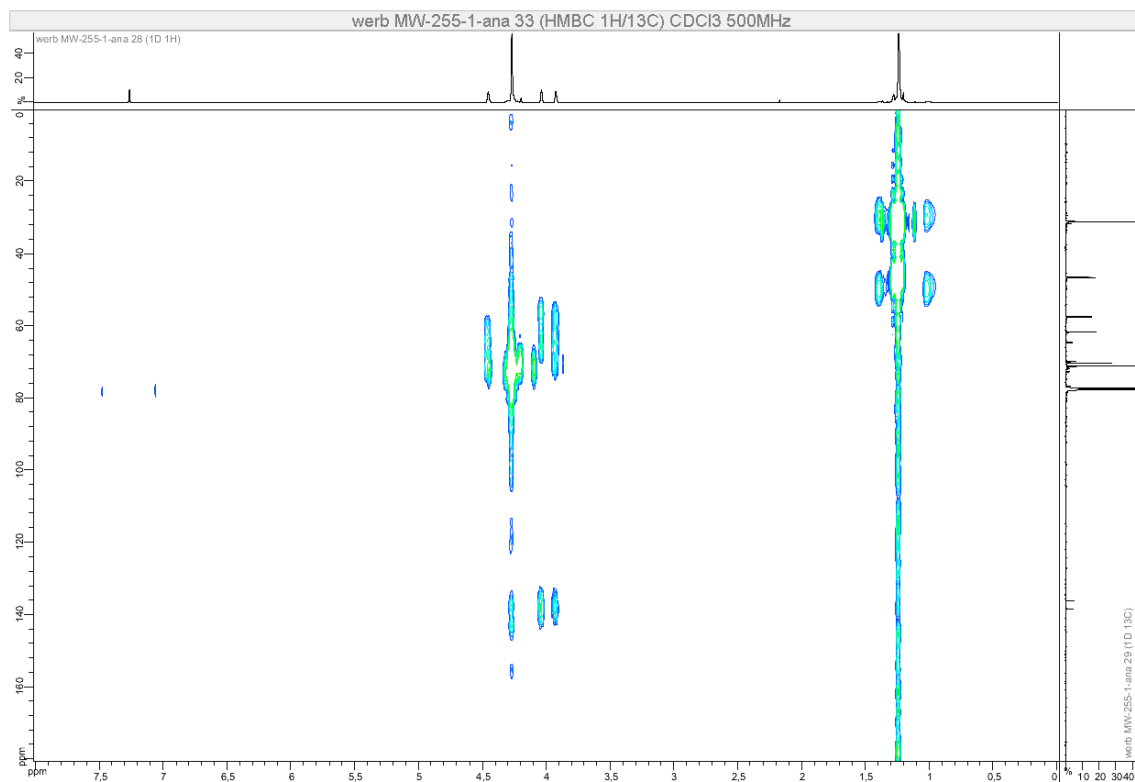
COSY (500 MHz, CDCl₃)



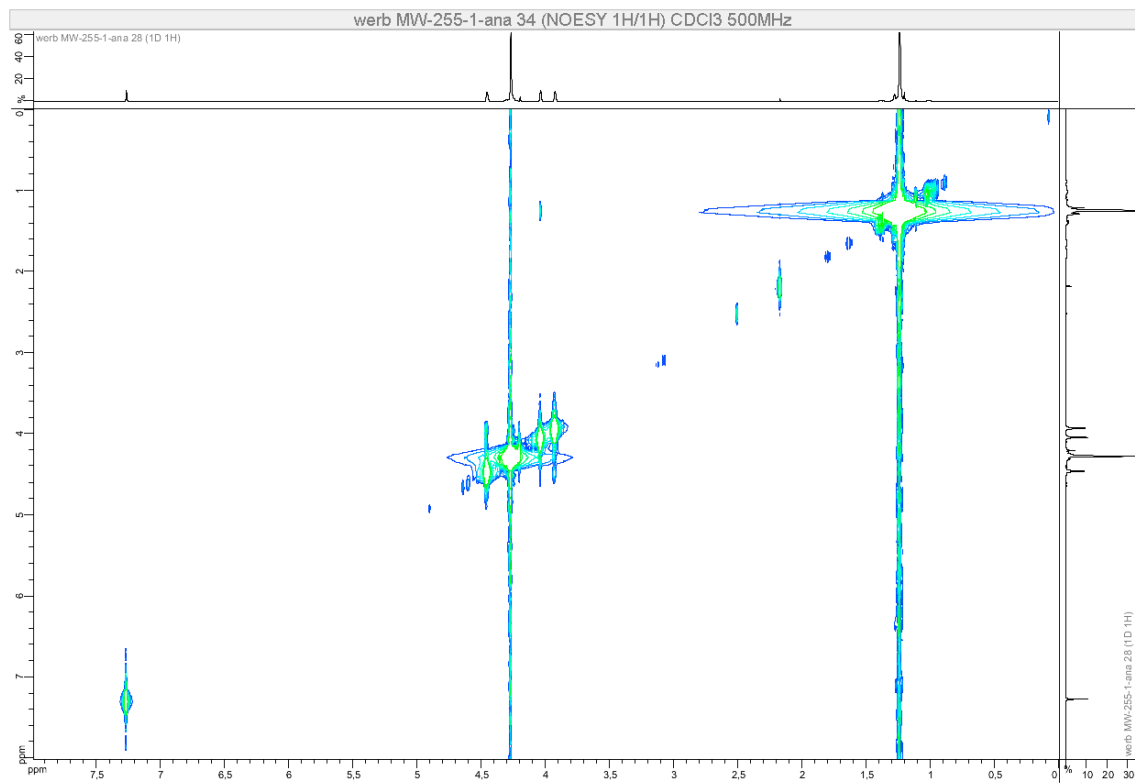
HSQC (500 MHz, CDCl₃)



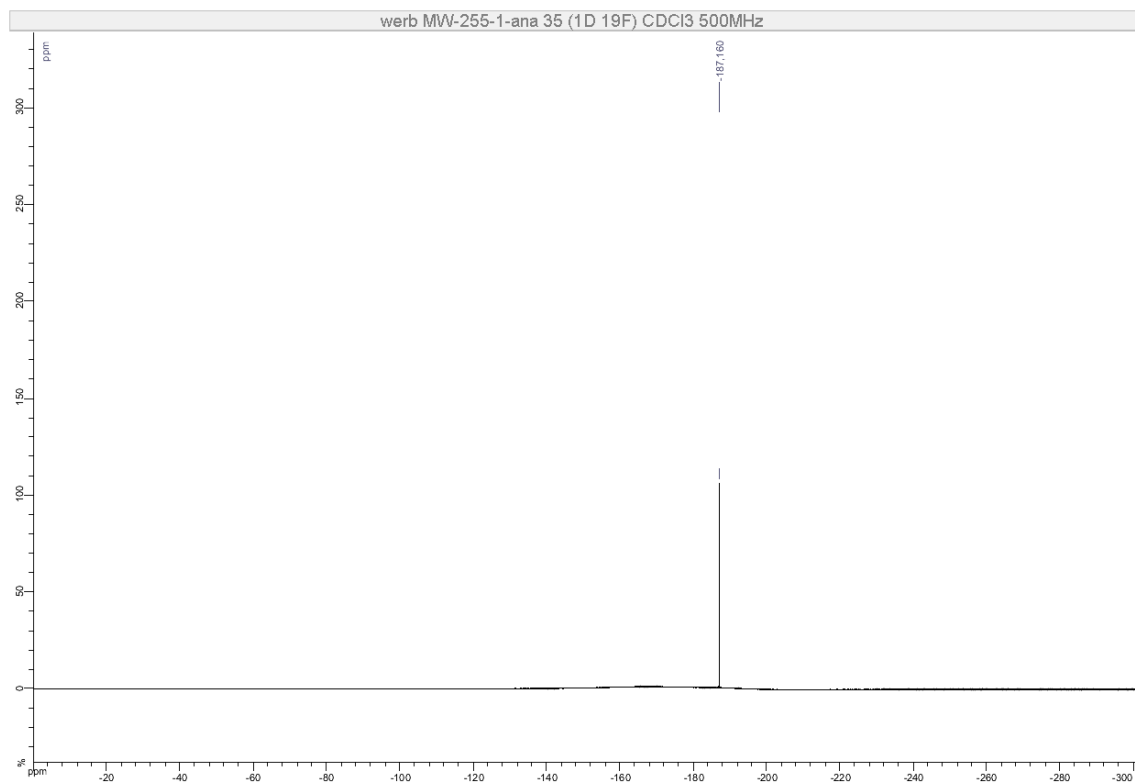
HMBC (500 MHz, CDCl₃)



NOESY (500 MHz, CDCl₃)

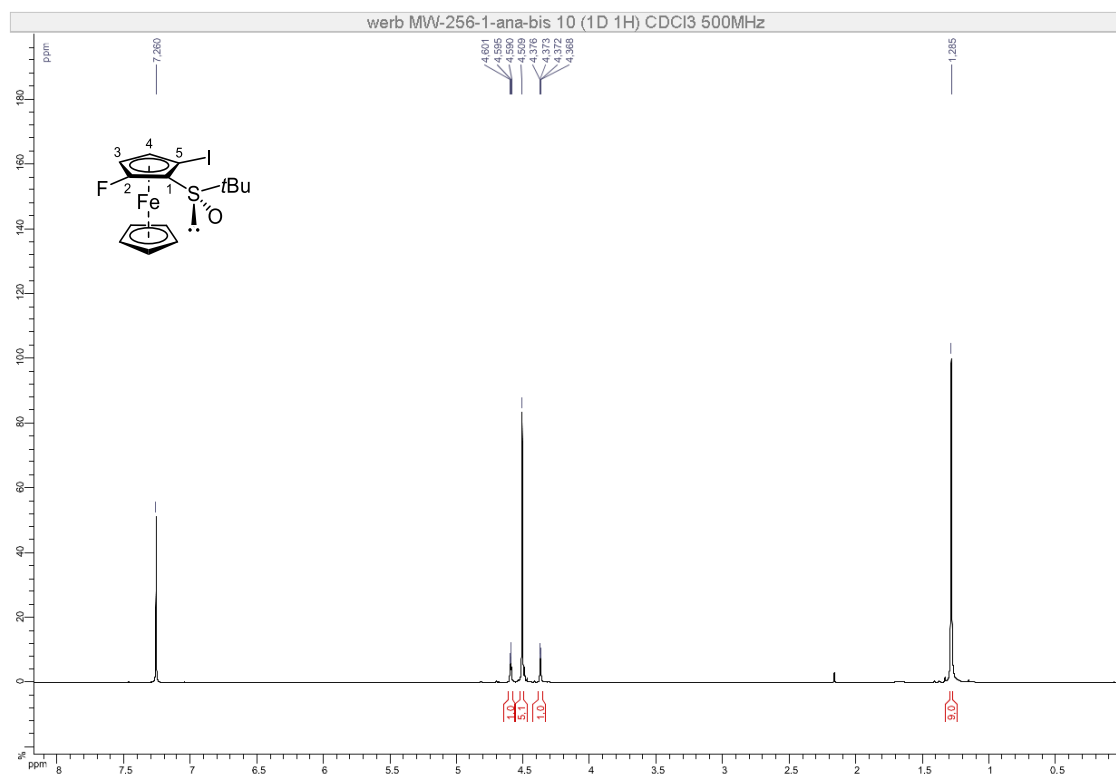


¹⁹F NMR (471 MHz, CDCl₃)

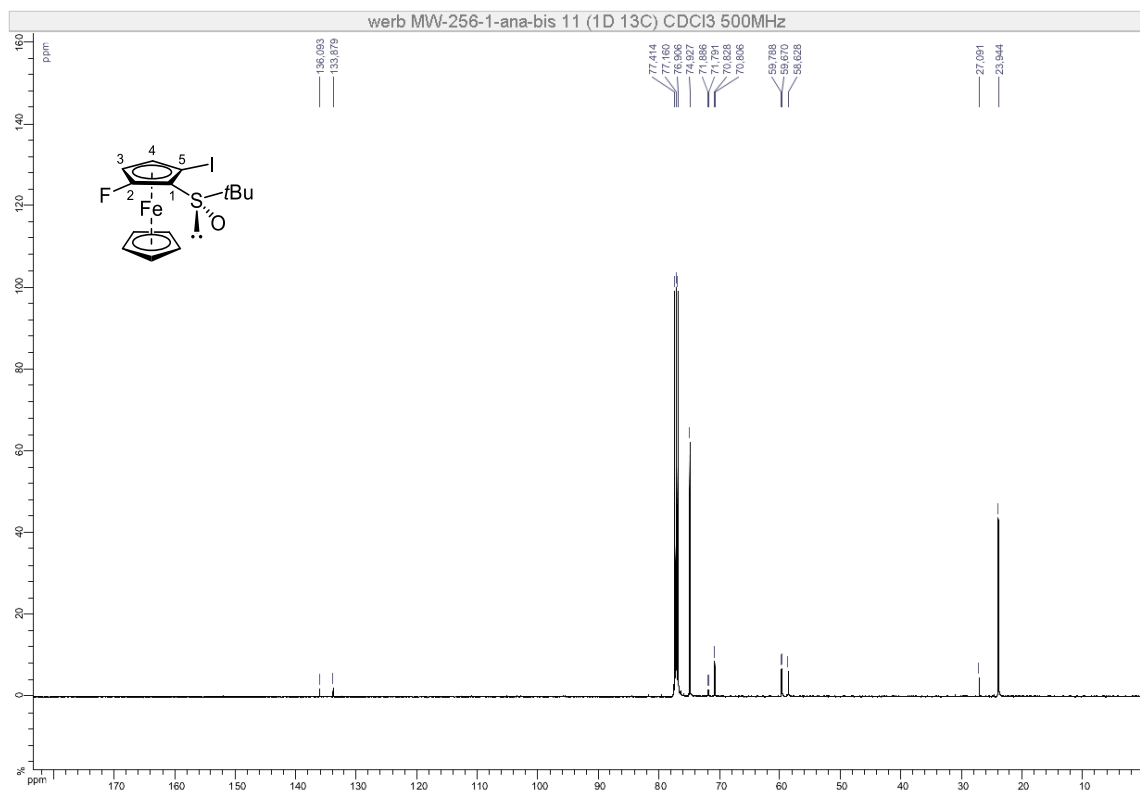


(*S,R_P*)-*S*-tert-Butyl-2-fluoro-5-iodoferrocenesulfoxide (*S,R_P*-2bi)

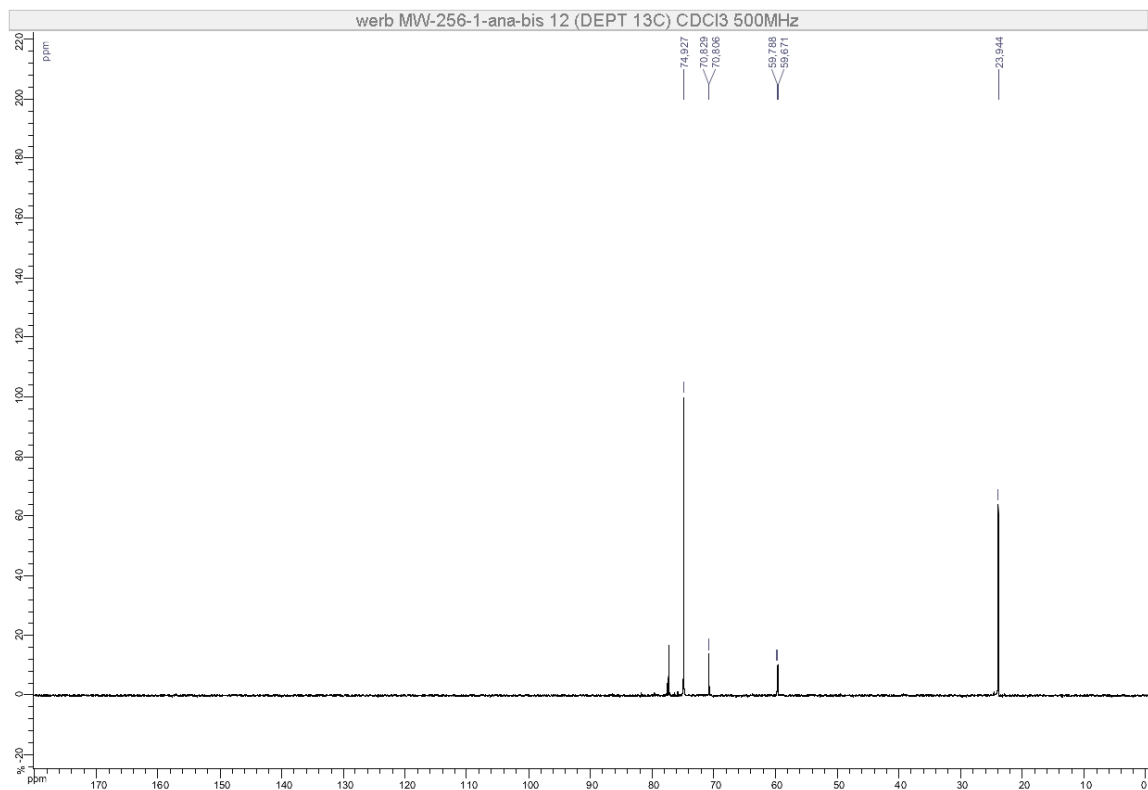
^1H NMR (500 MHz, CDCl_3)



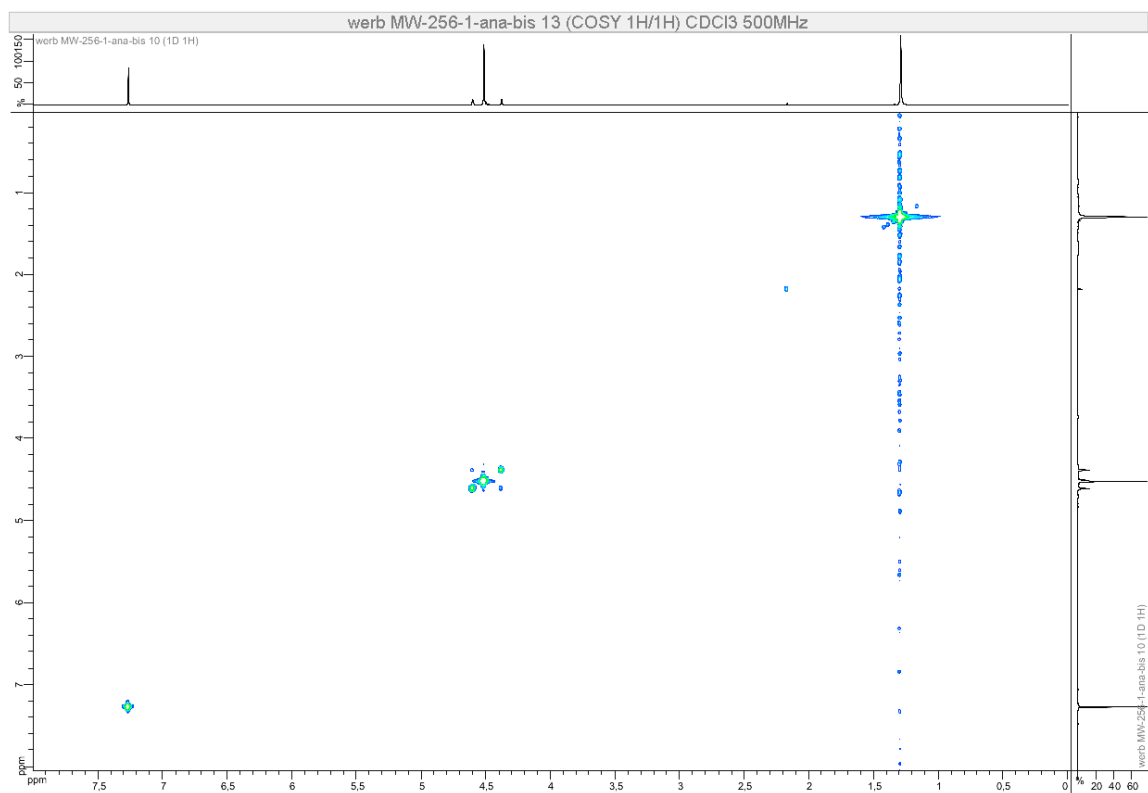
^{13}C NMR (126 MHz, CDCl_3)



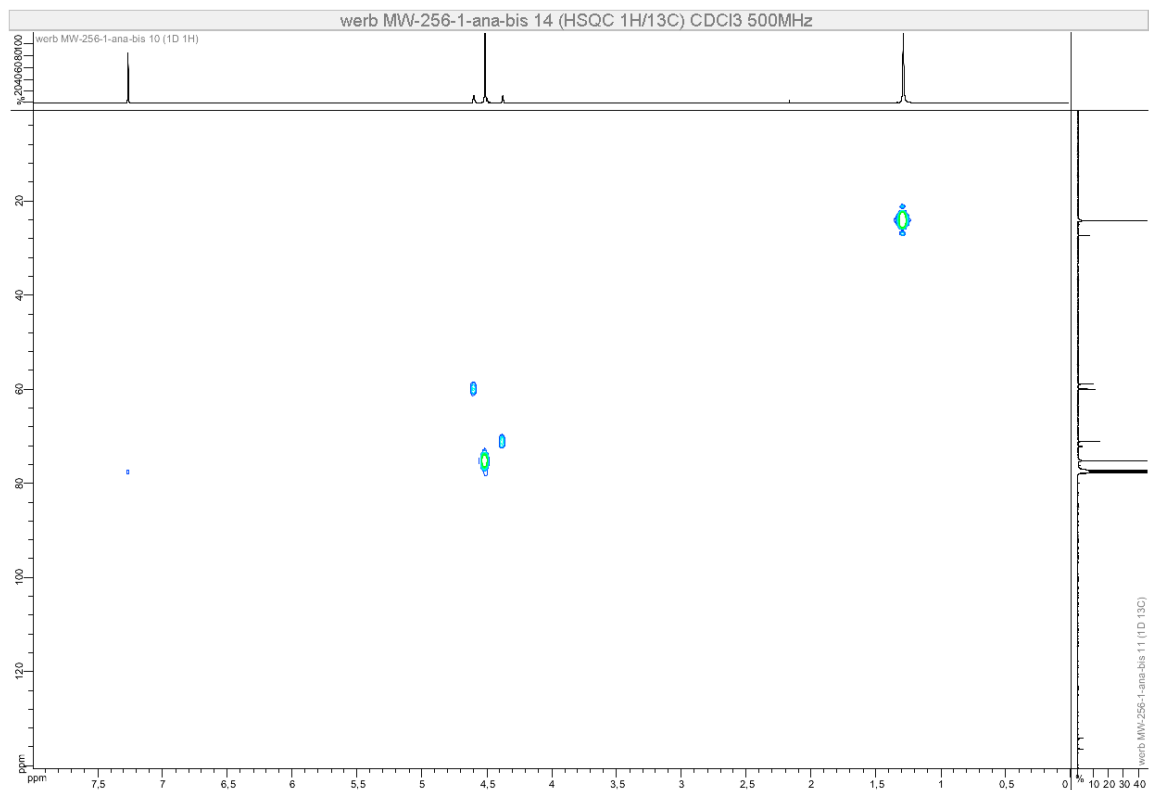
DEPT 135 (126 MHz, CDCl₃)



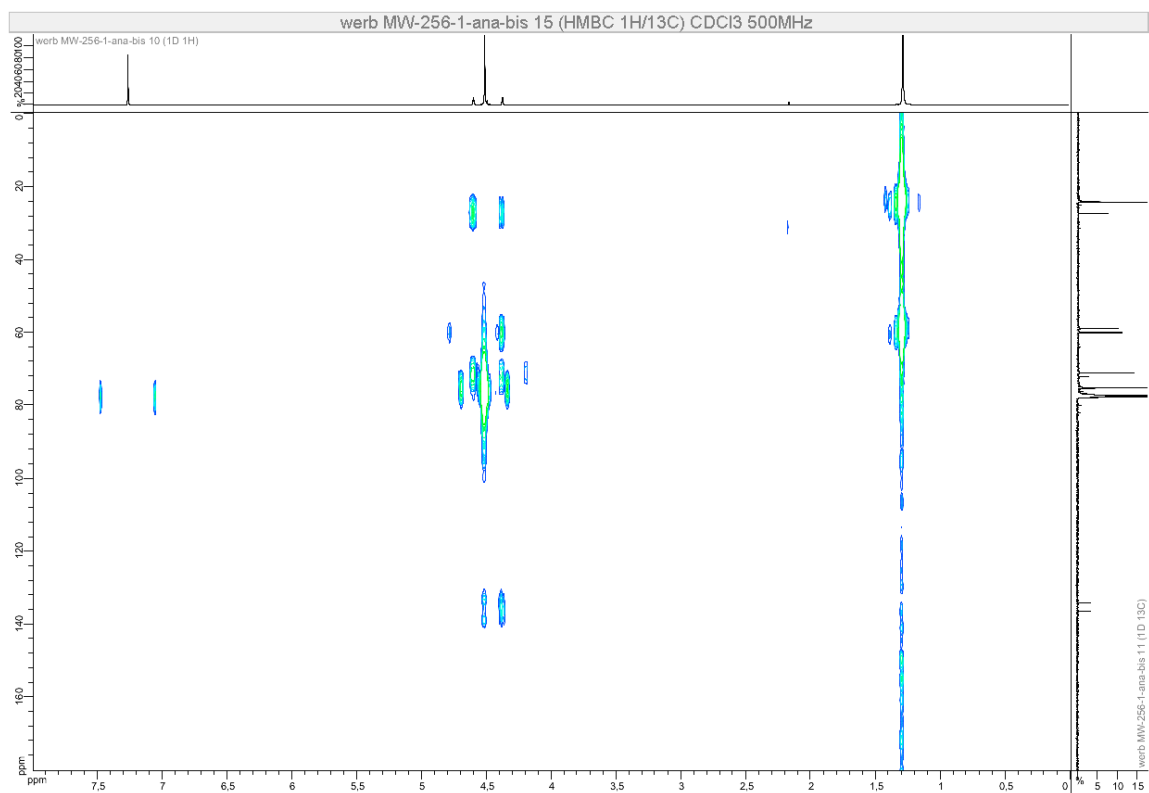
COSY (500 MHz, CDCl₃)



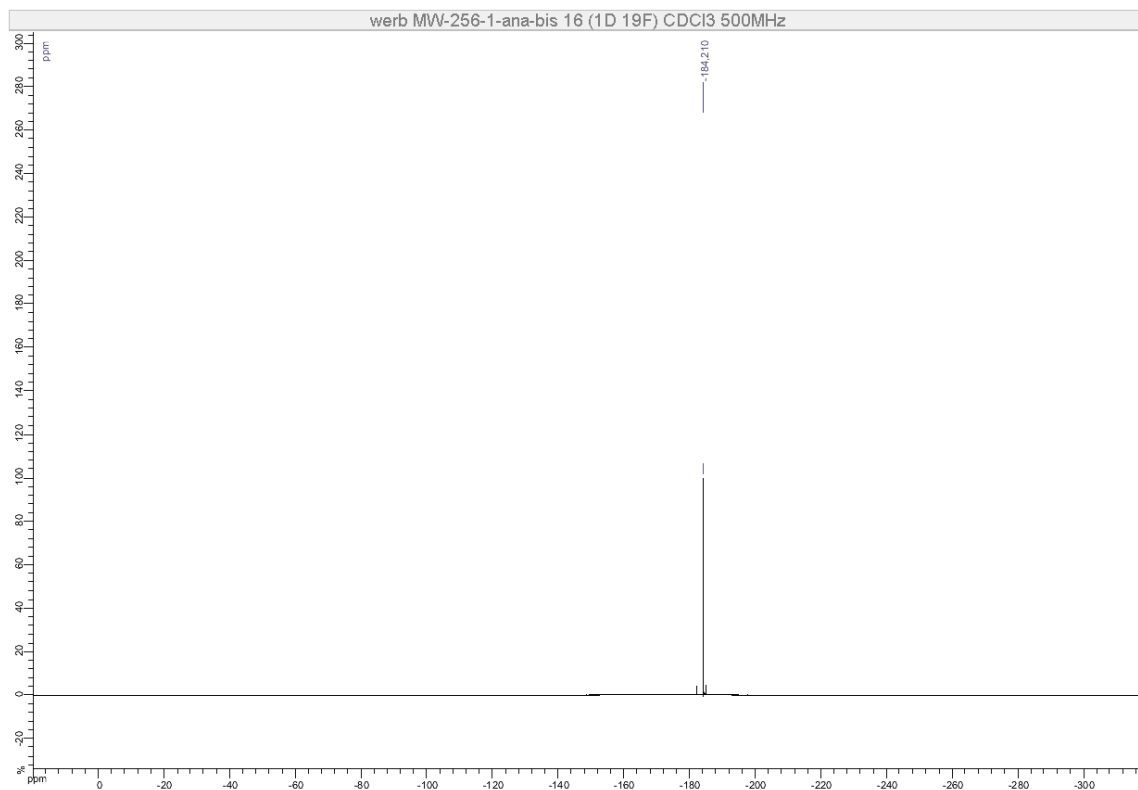
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

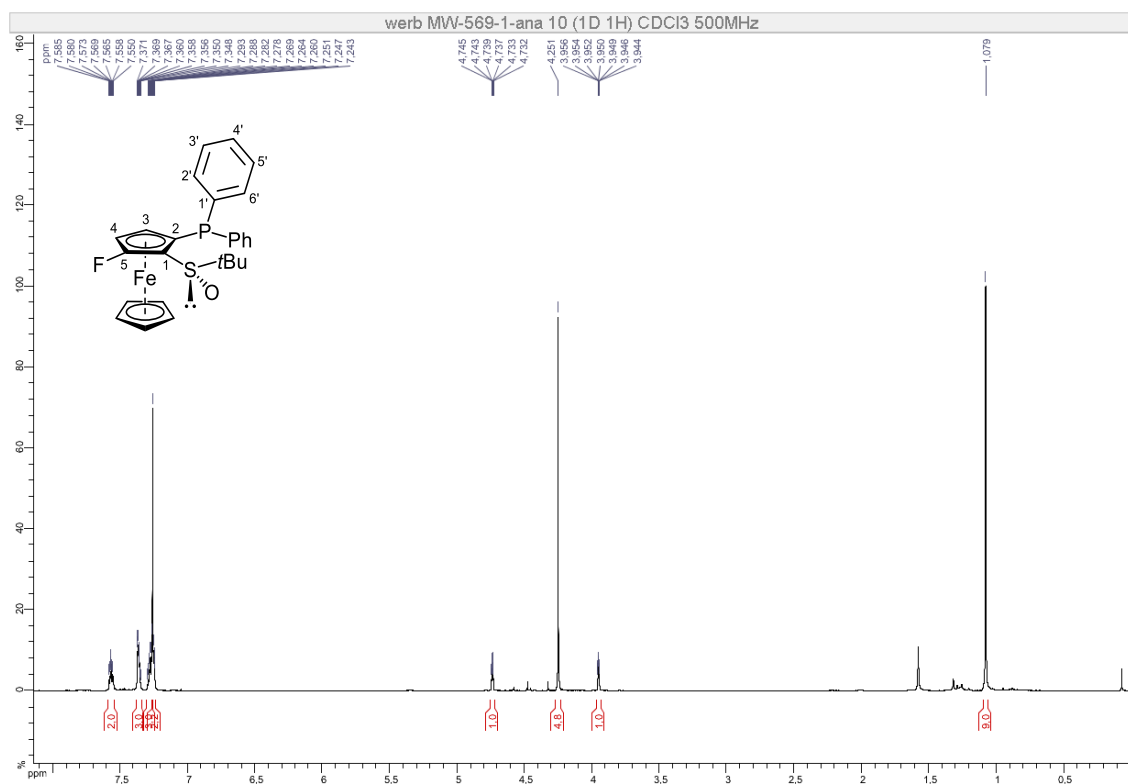


^{19}F NMR (471 MHz, CDCl_3)

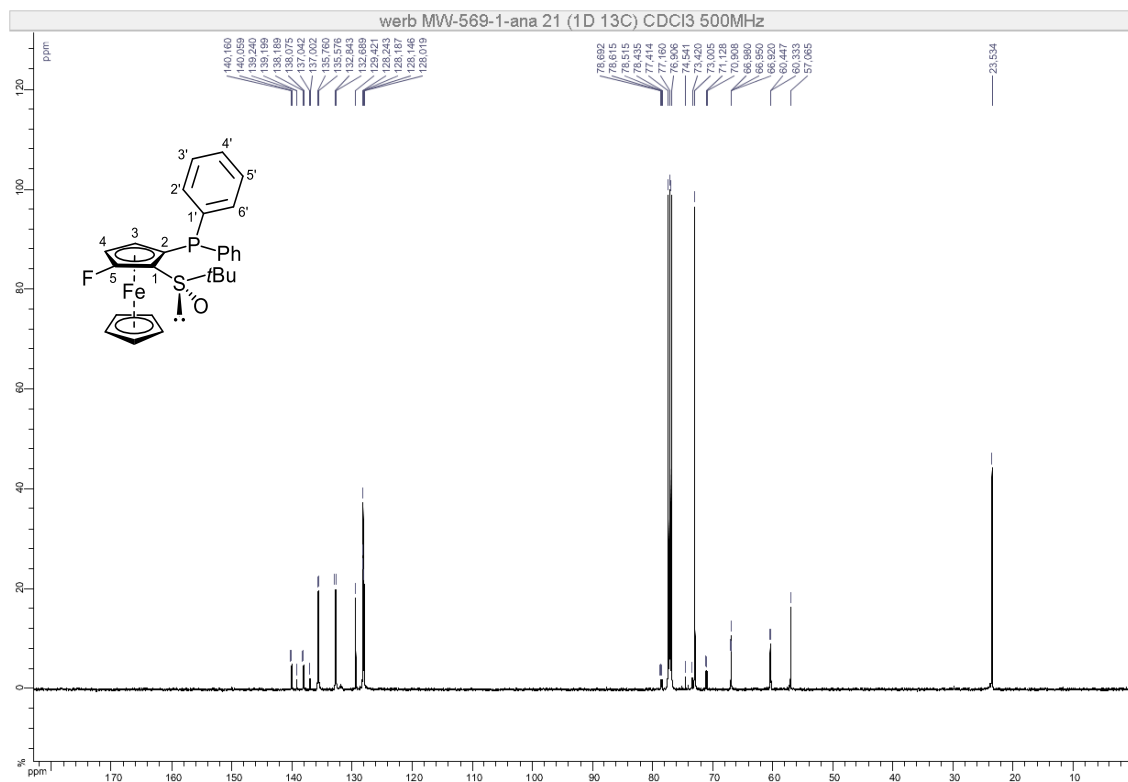


(*S,S*_P)-*S*-tert-Butyl-2-(diphenylphosphino)-5-fluoroferrocenenesulfoxide (*S,S*_P-2ei)

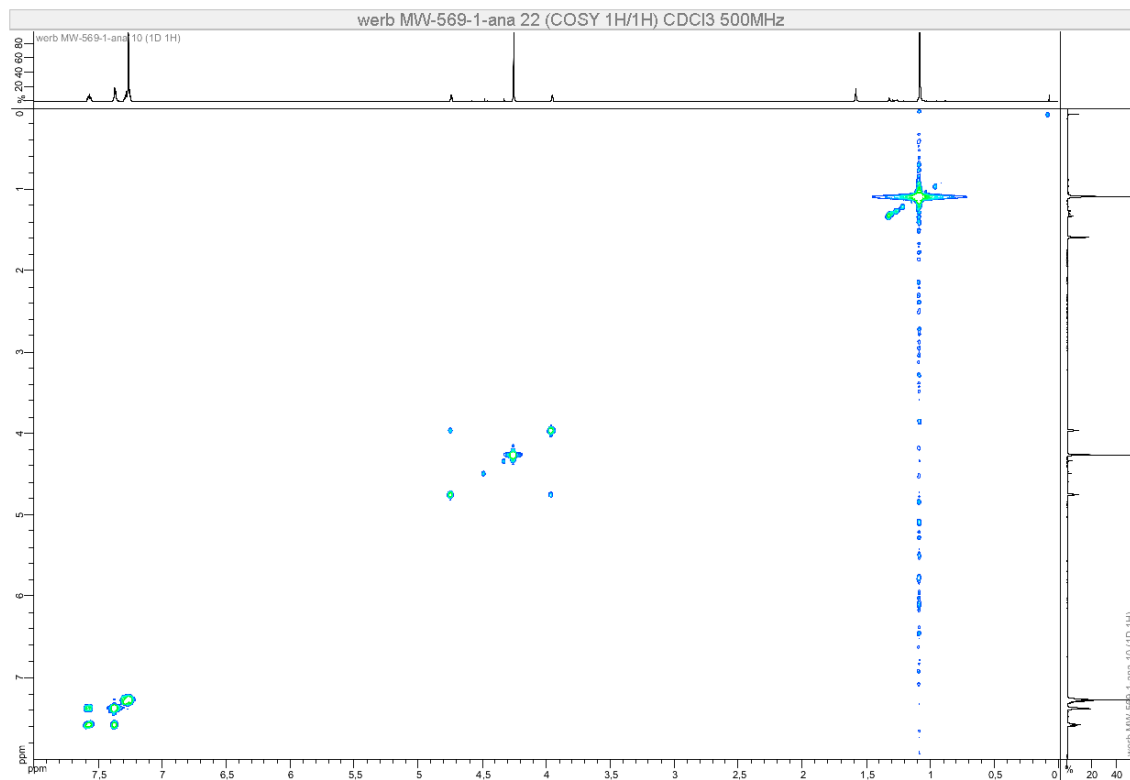
¹H NMR (500 MHz, CDCl₃)



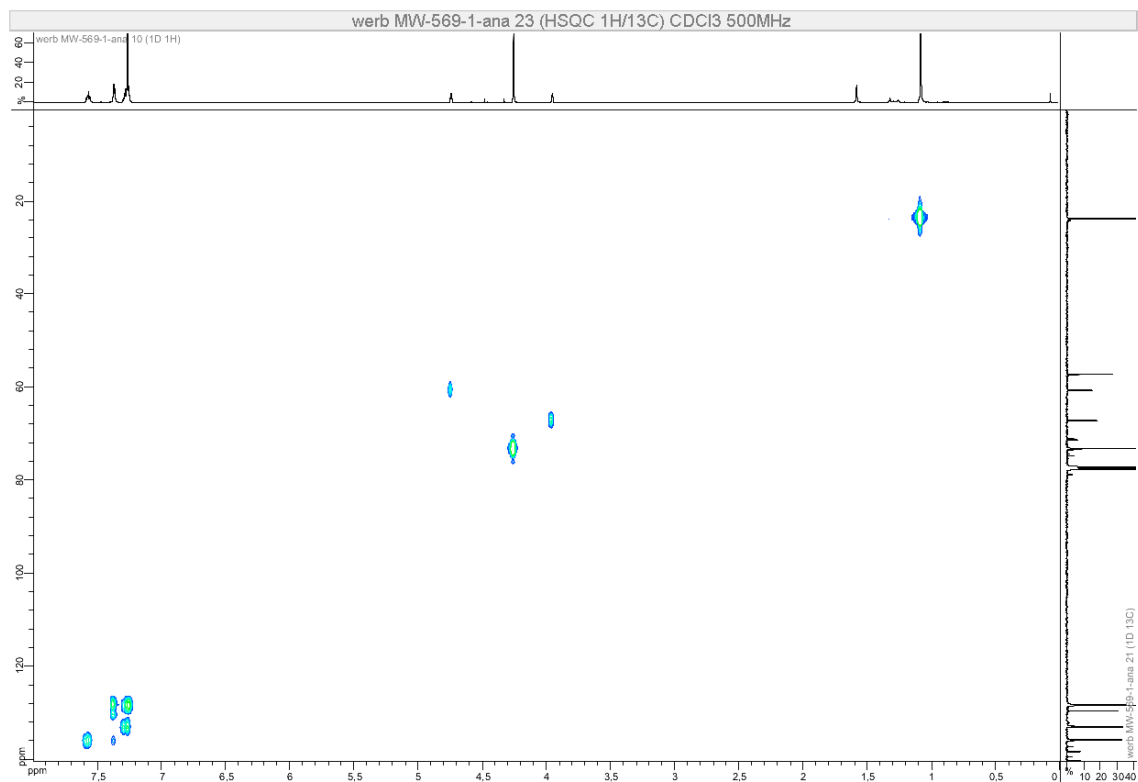
¹³C NMR (126 MHz, CDCl₃)



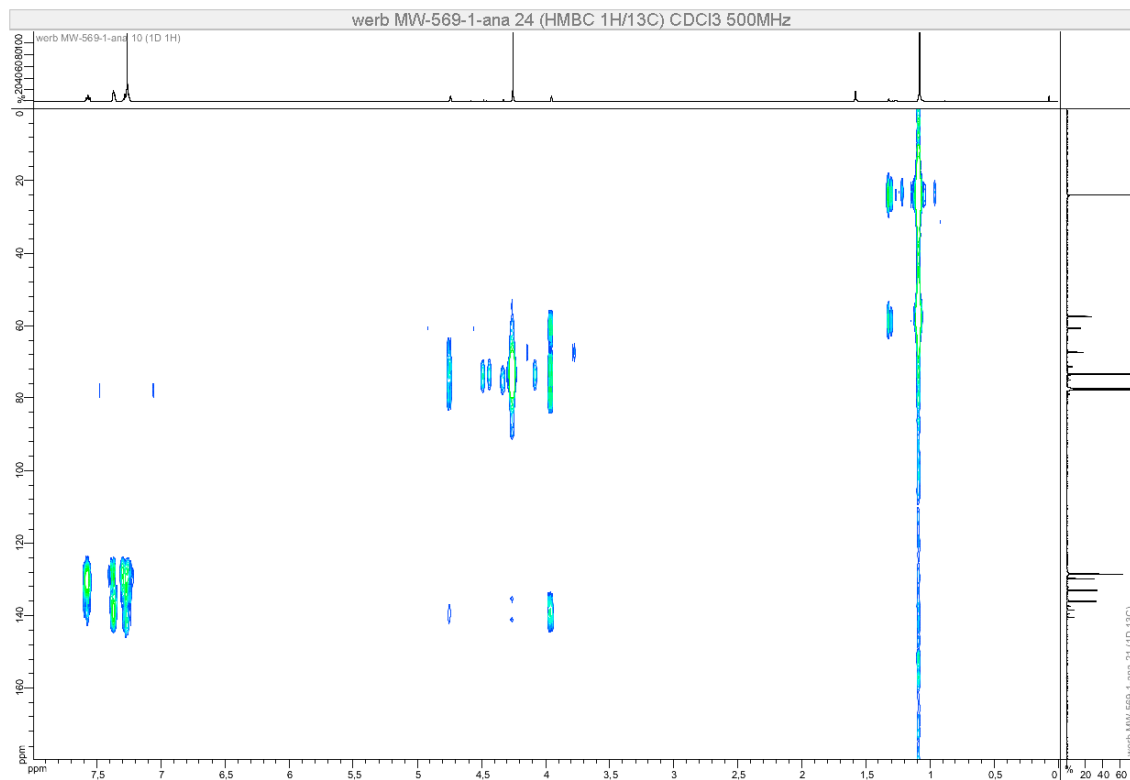
COSY (500 MHz, CDCl₃)



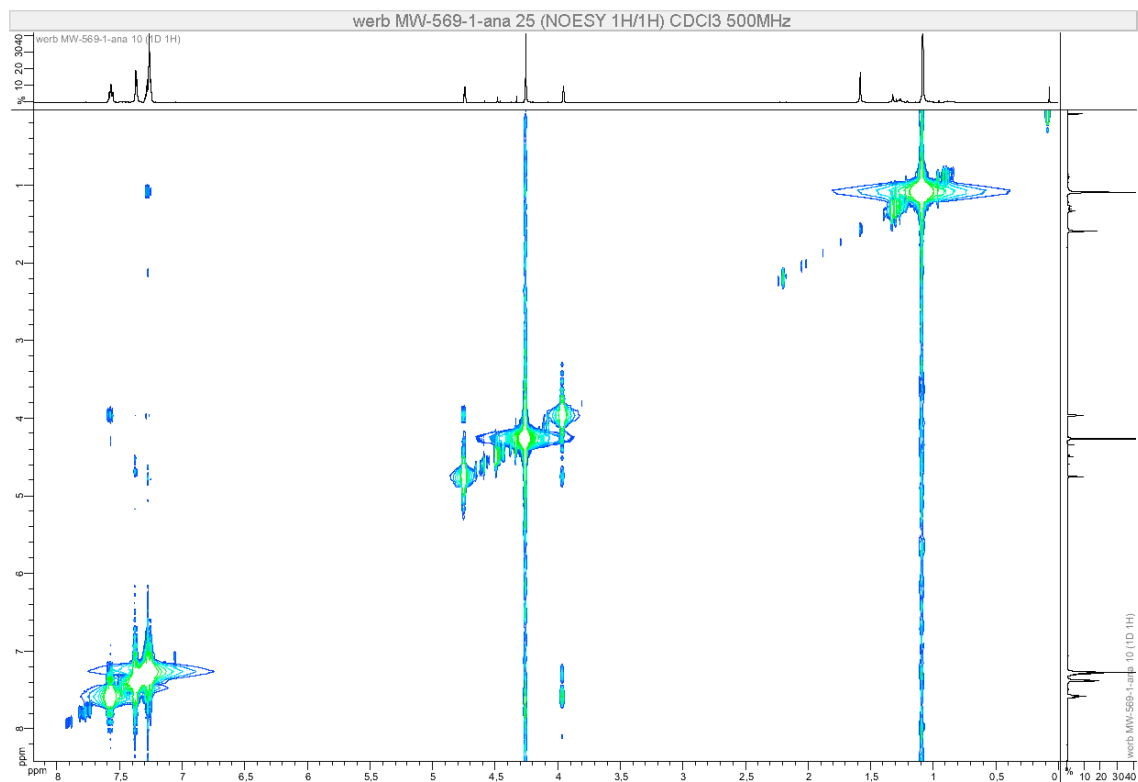
HSQC (500 MHz, CDCl₃)



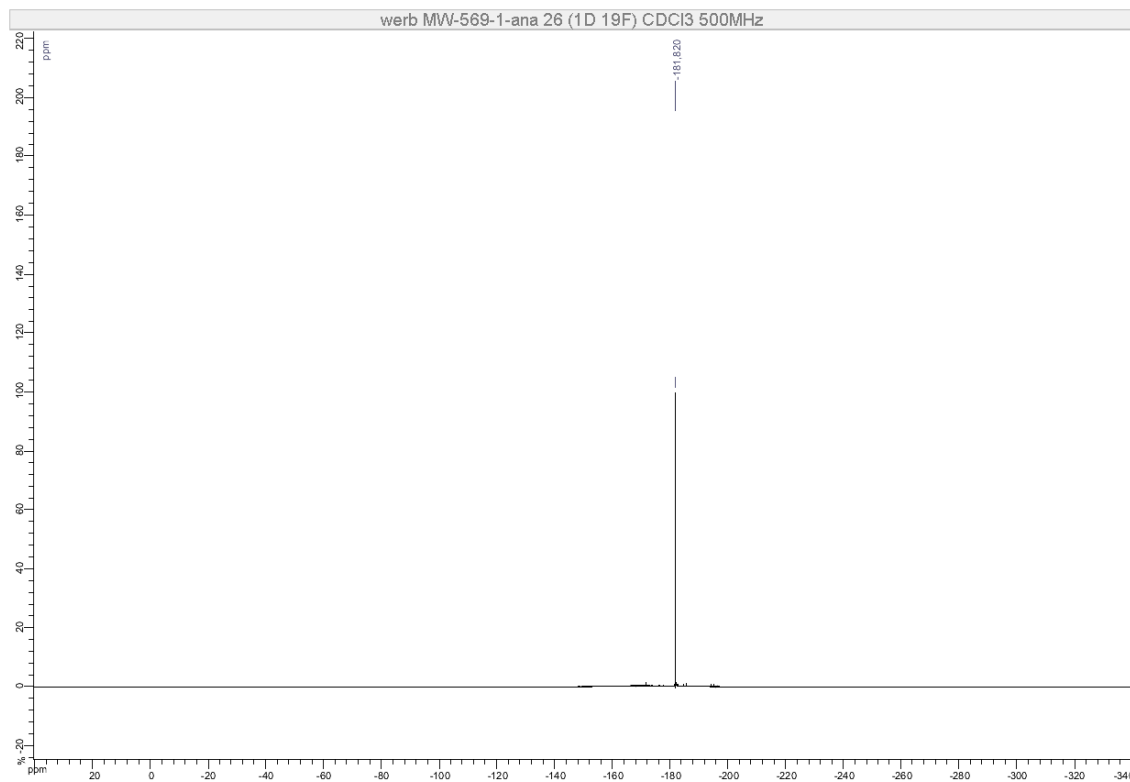
HMBC (500 MHz, CDCl₃)



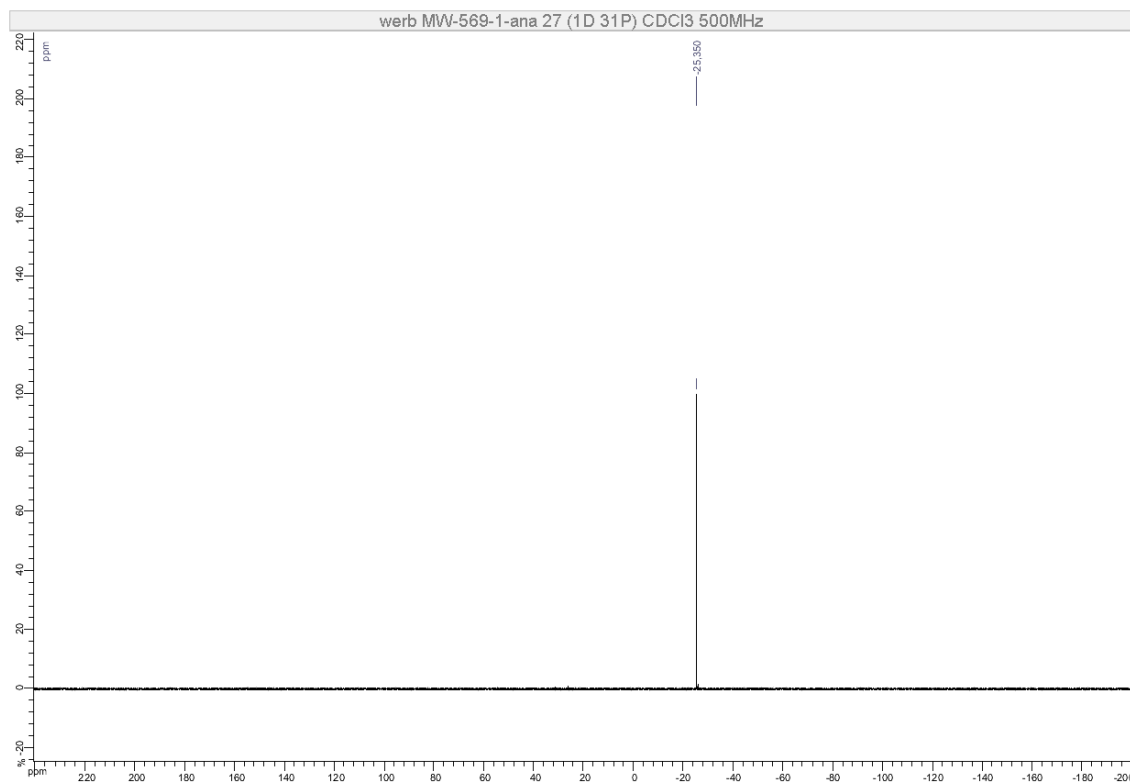
NOESY (500 MHz, CDCl₃)



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

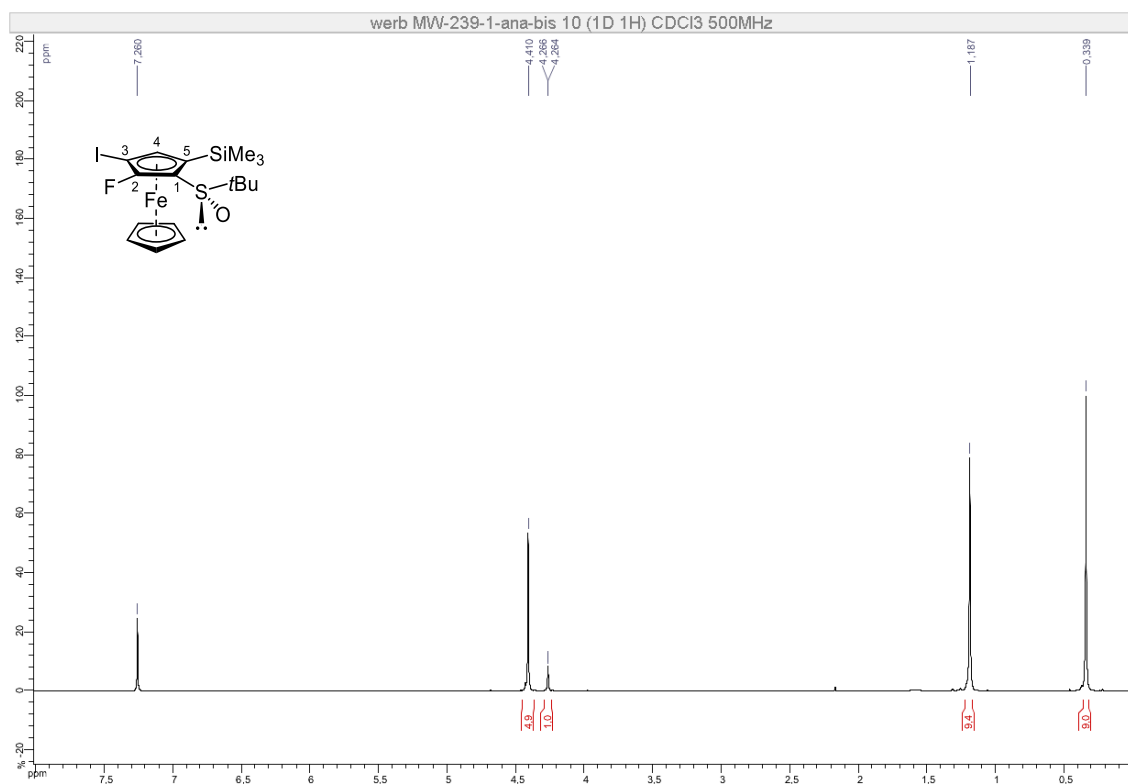


^{31}P NMR (202 MHz, CDCl_3)

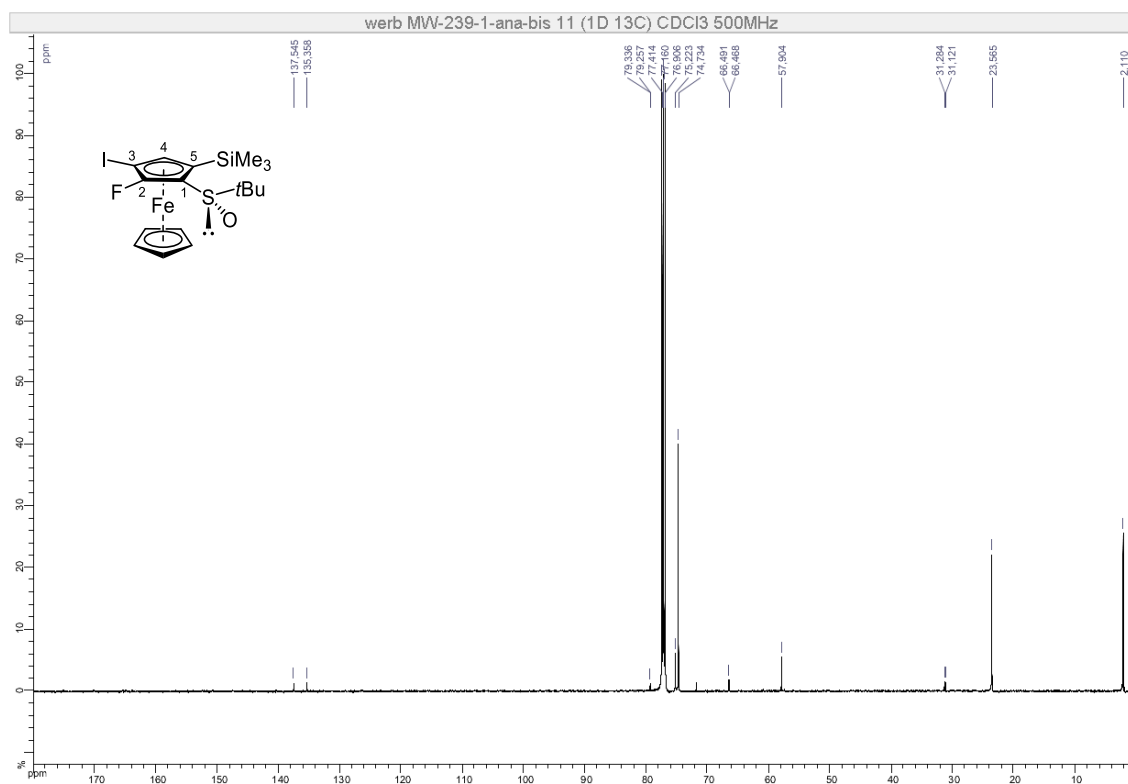


(*S,S*)-*S*-tert-Butyl-2-fluoro-3-iodo-5-(trimethylsilyl)ferrocenesulfoxide (*S,S*-9b)

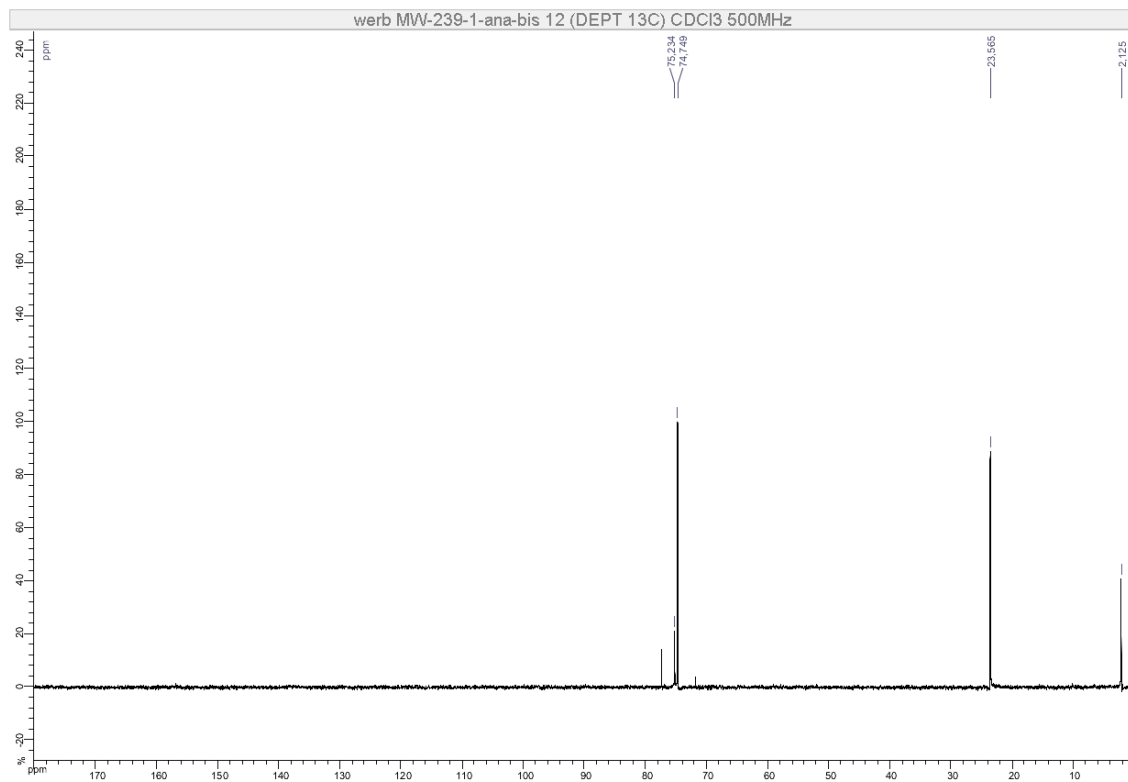
^1H NMR (500 MHz, CDCl_3)



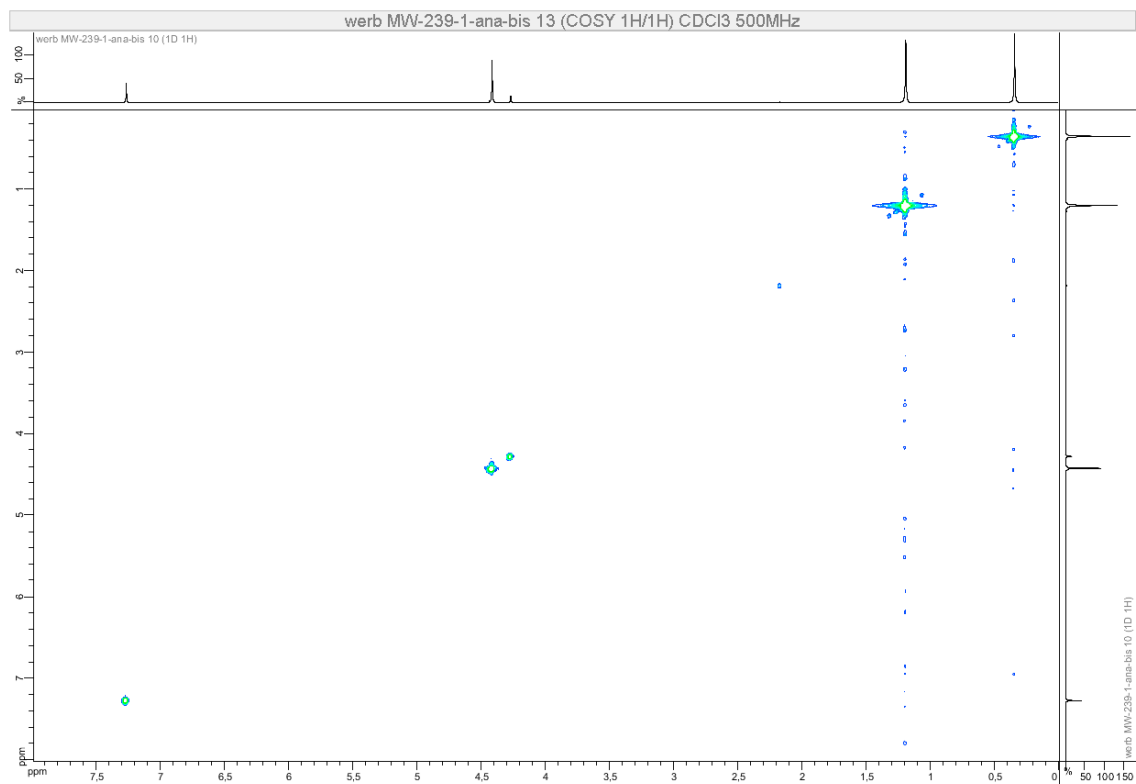
^{13}C NMR (126 MHz, CDCl_3)



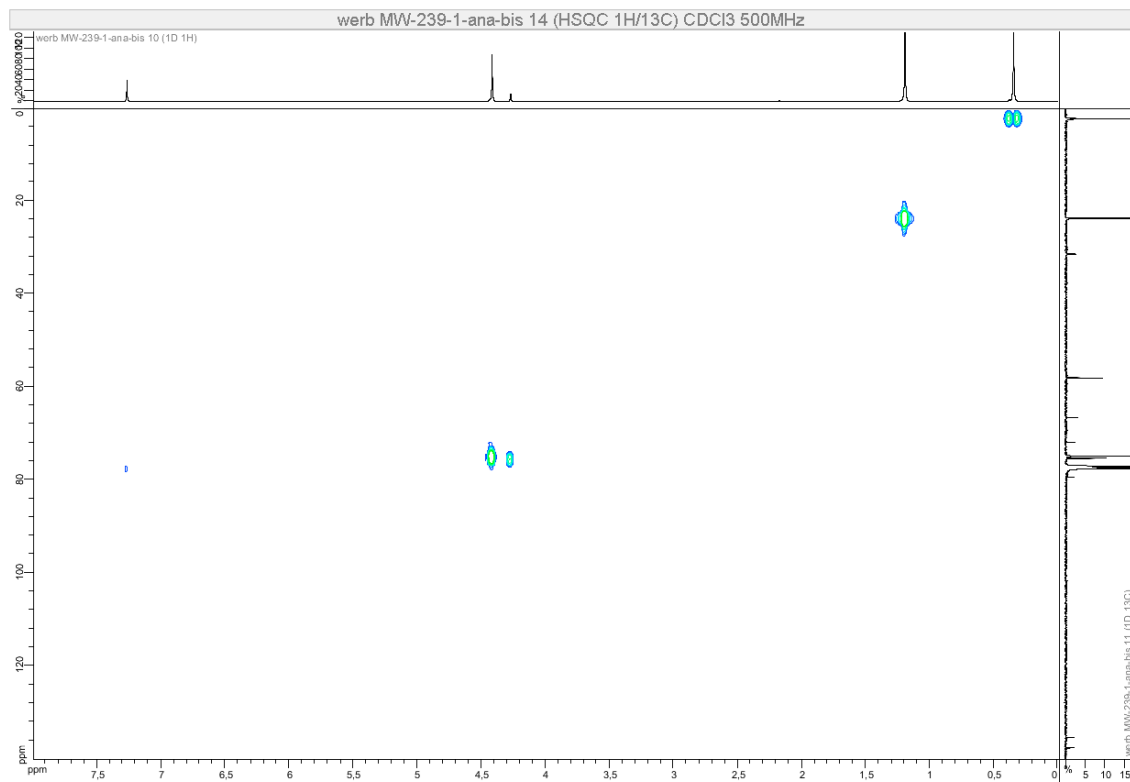
DEPT 135 (126 MHz, CDCl₃)



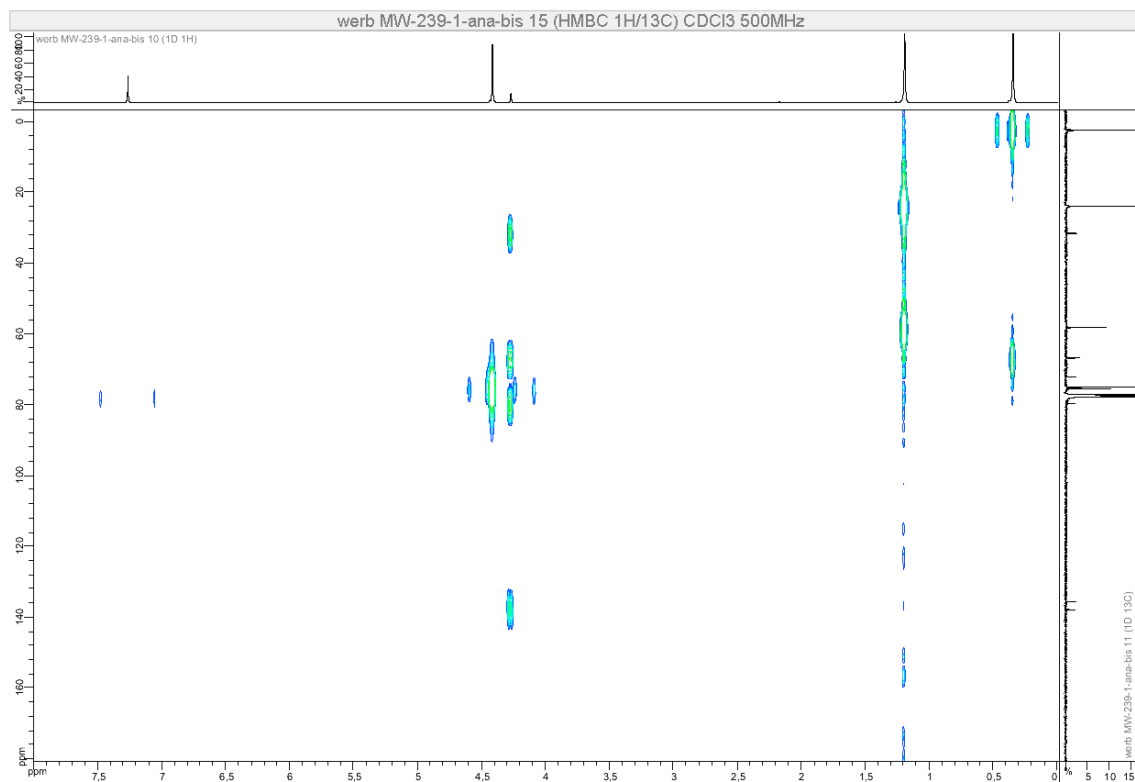
COSY (500 MHz, CDCl₃)



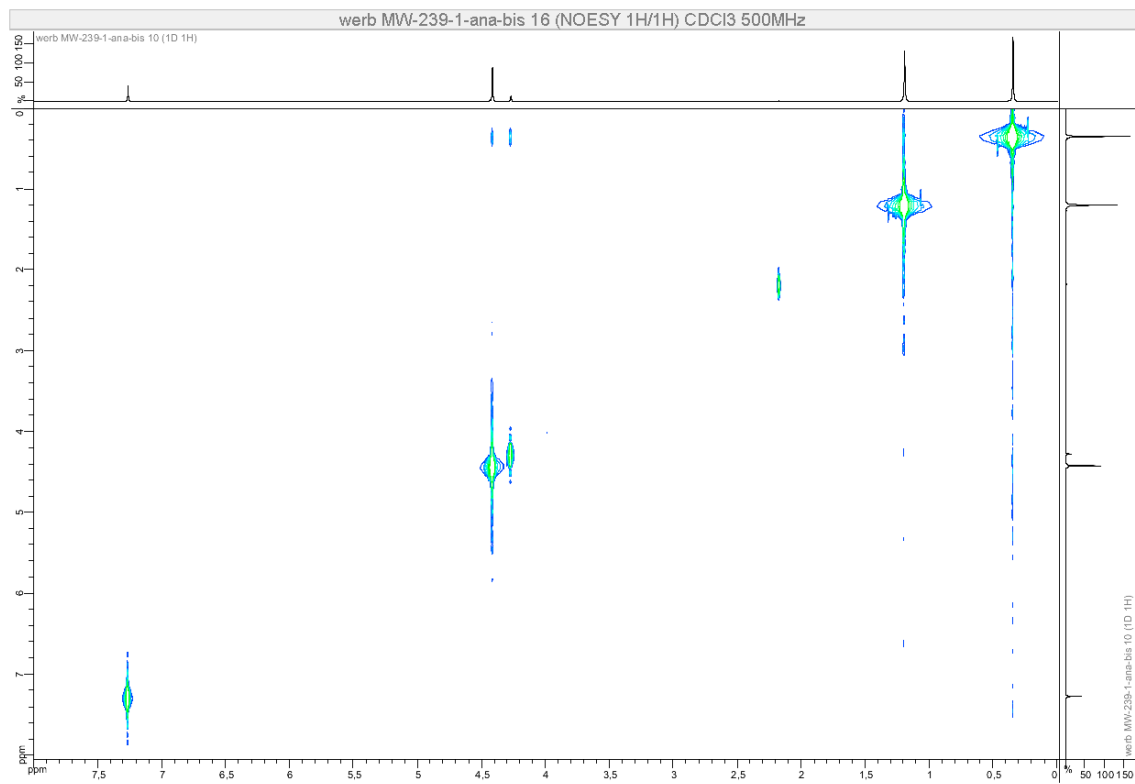
HSQC (500 MHz, CDCl₃)



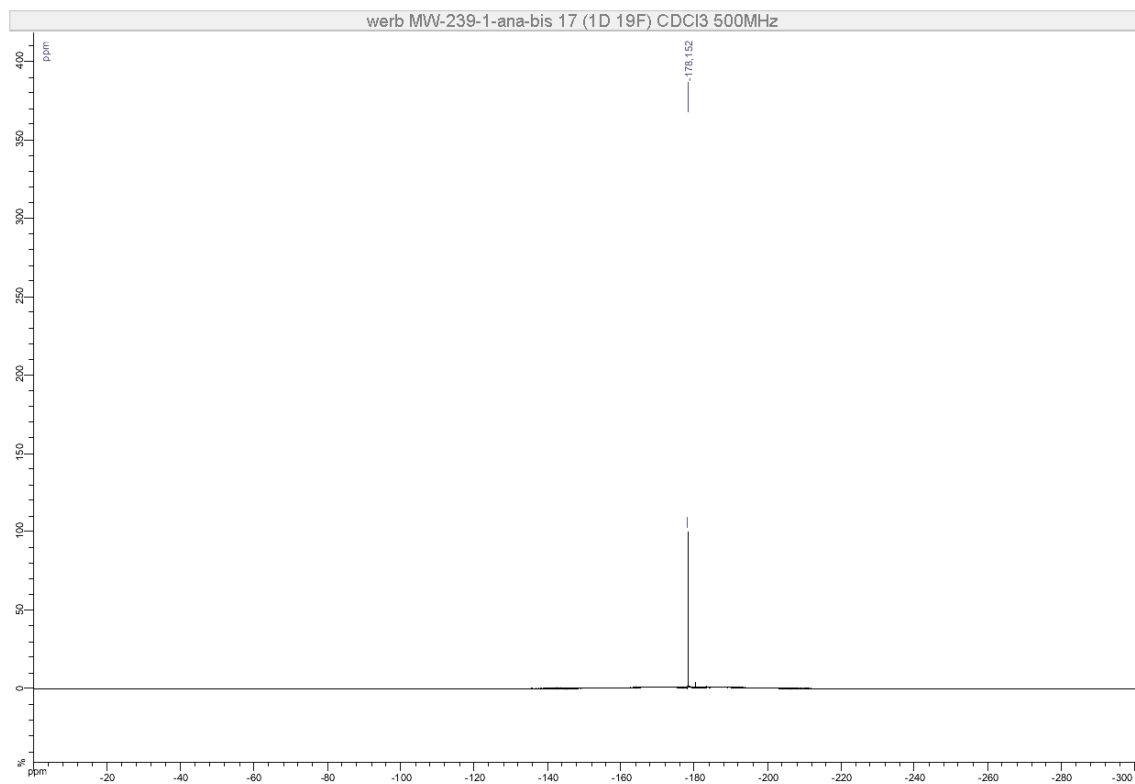
HMBC (500 MHz, CDCl₃)



NOESY (500 MHz, CDCl₃)

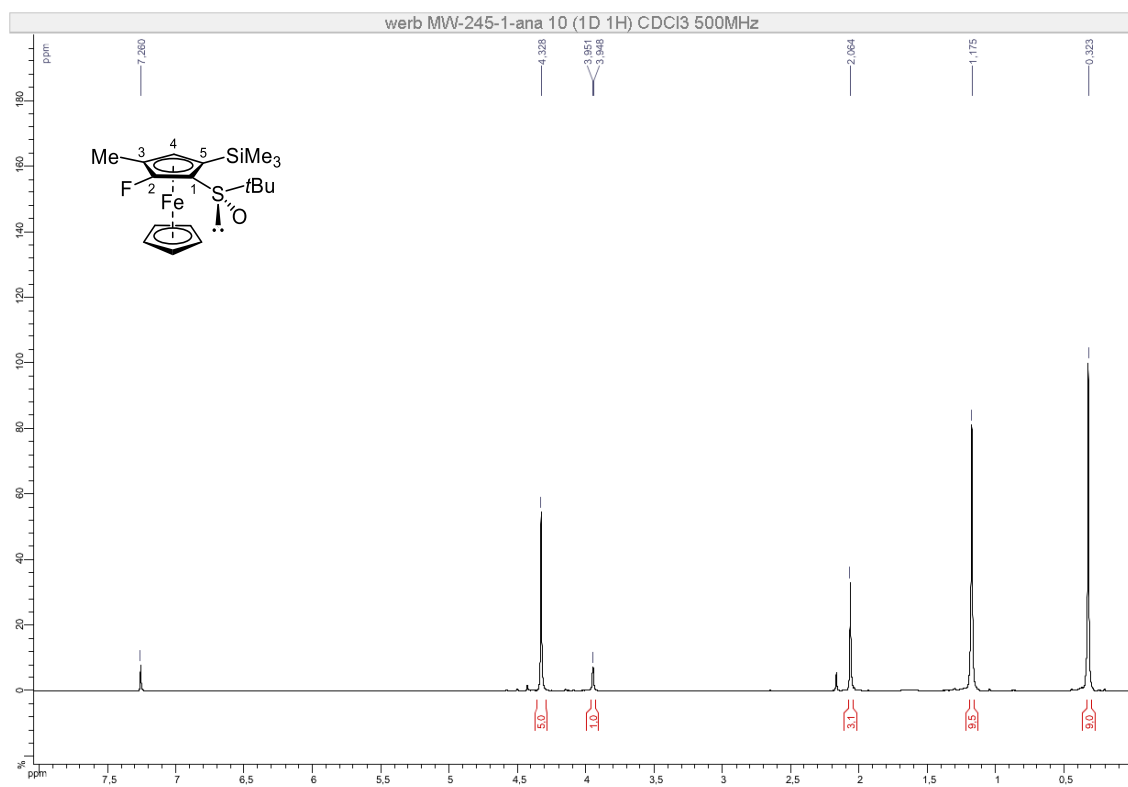


¹⁹F NMR (471 MHz, CDCl₃)

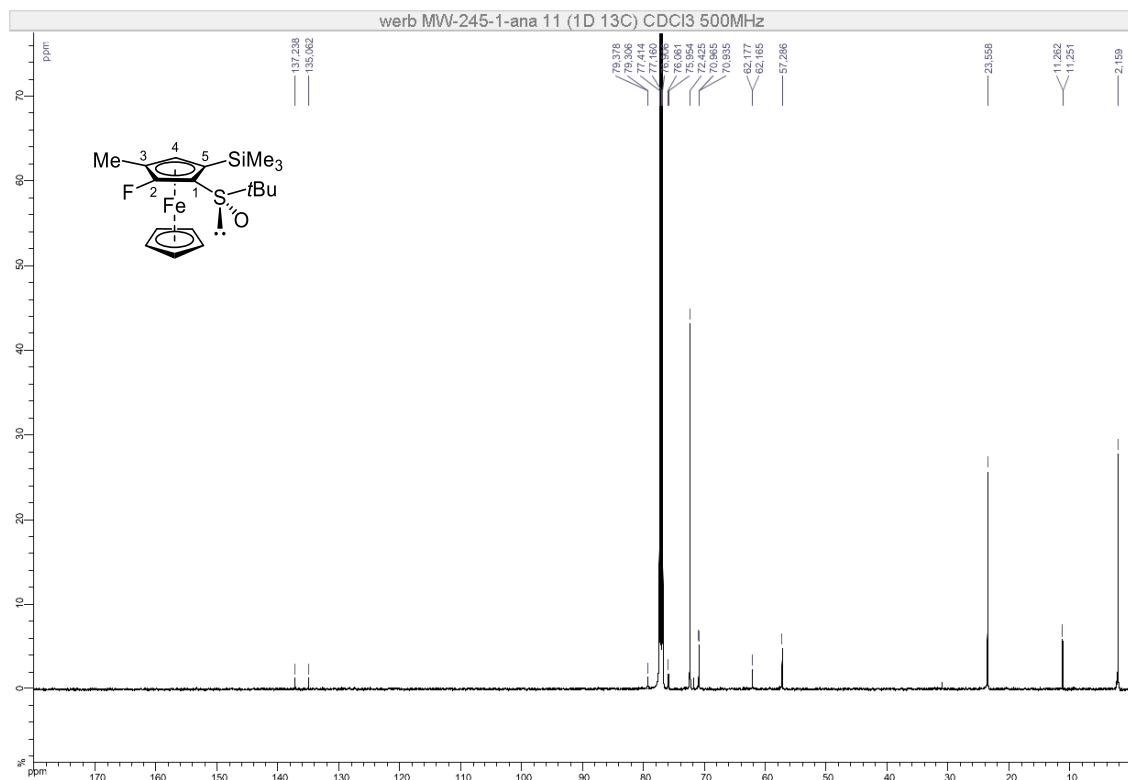


(*S,S*_P)-*S*-tert-Butyl-2-fluoro-3-methyl-5-(trimethylsilyl)ferrocenesulfoxide (*S,S*_P-9d)

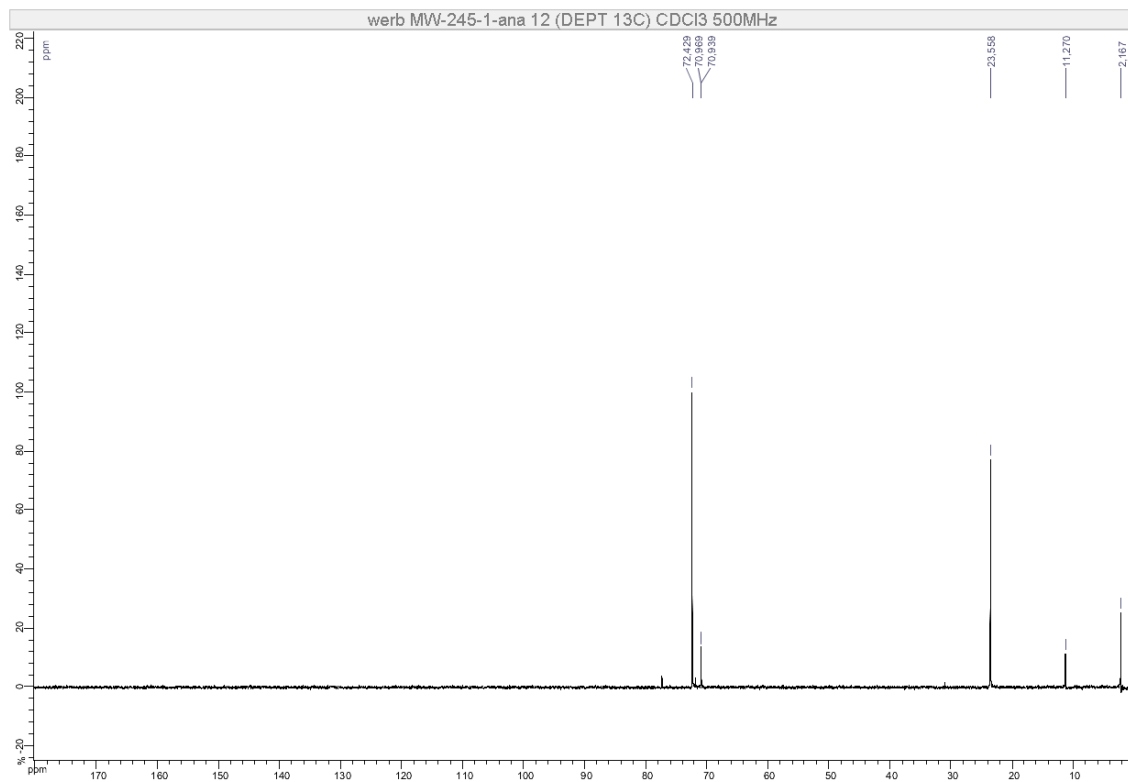
¹H NMR (500 MHz, CDCl₃)



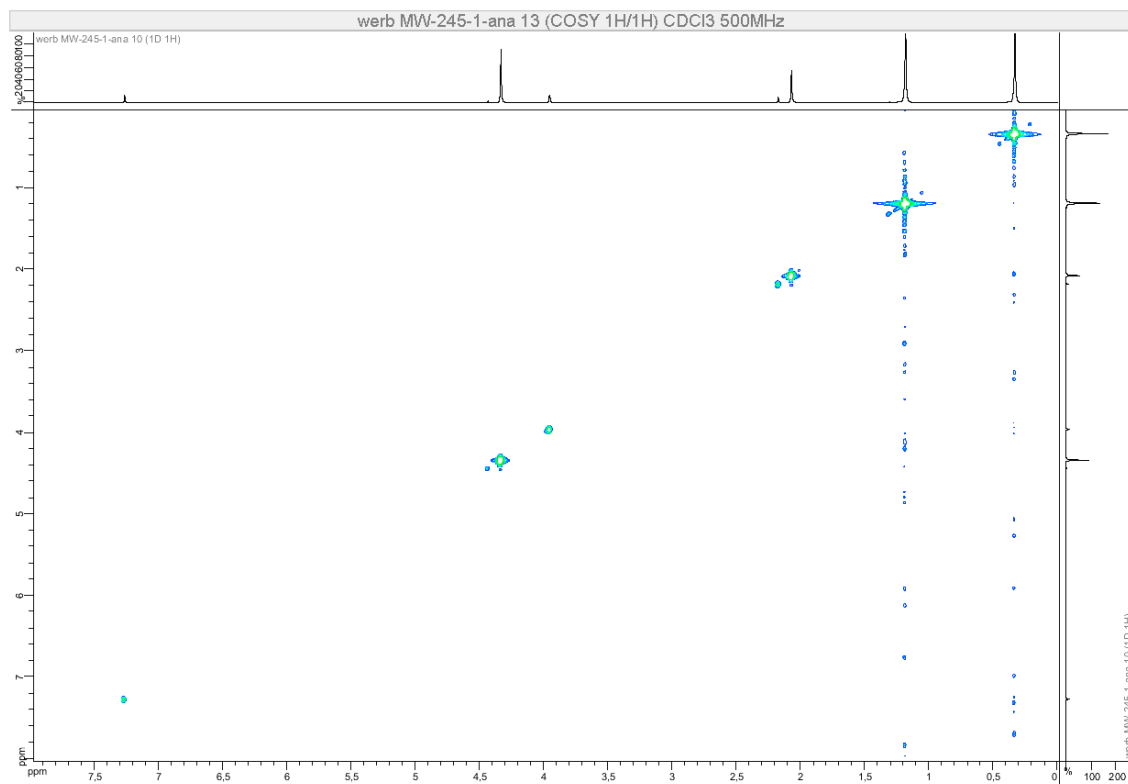
¹³C NMR (126 MHz, CDCl₃)



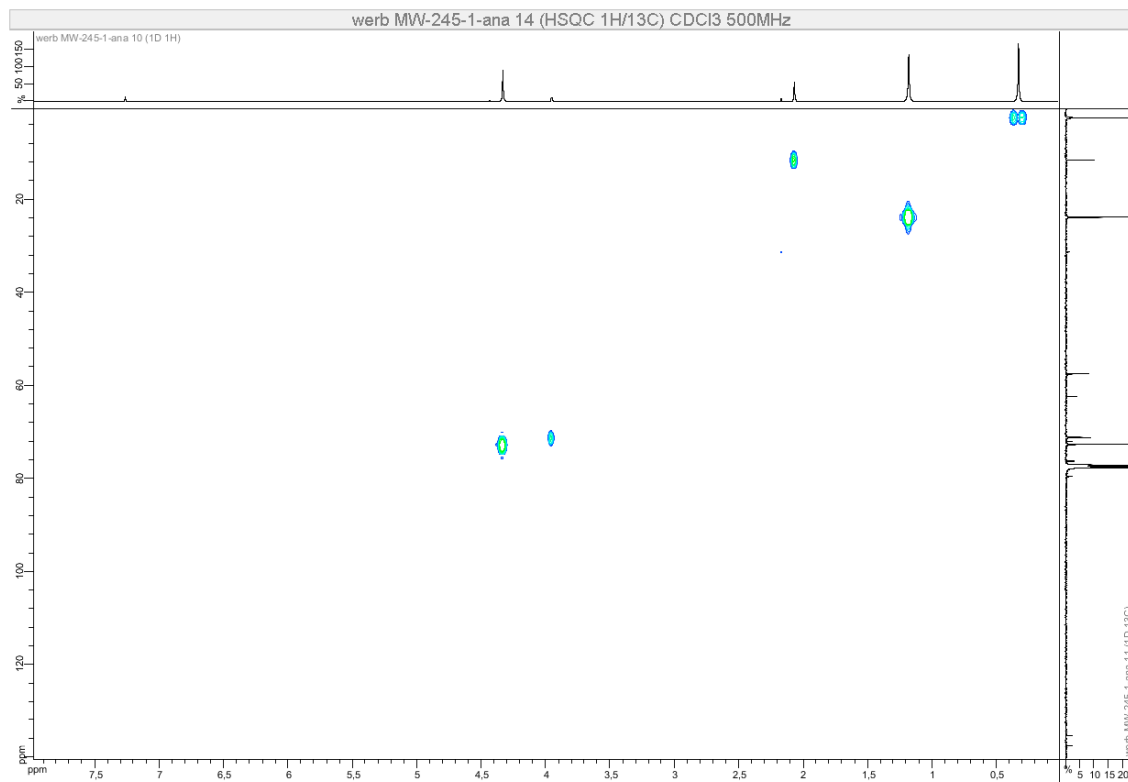
DEPT 135 (126 MHz, CDCl₃)



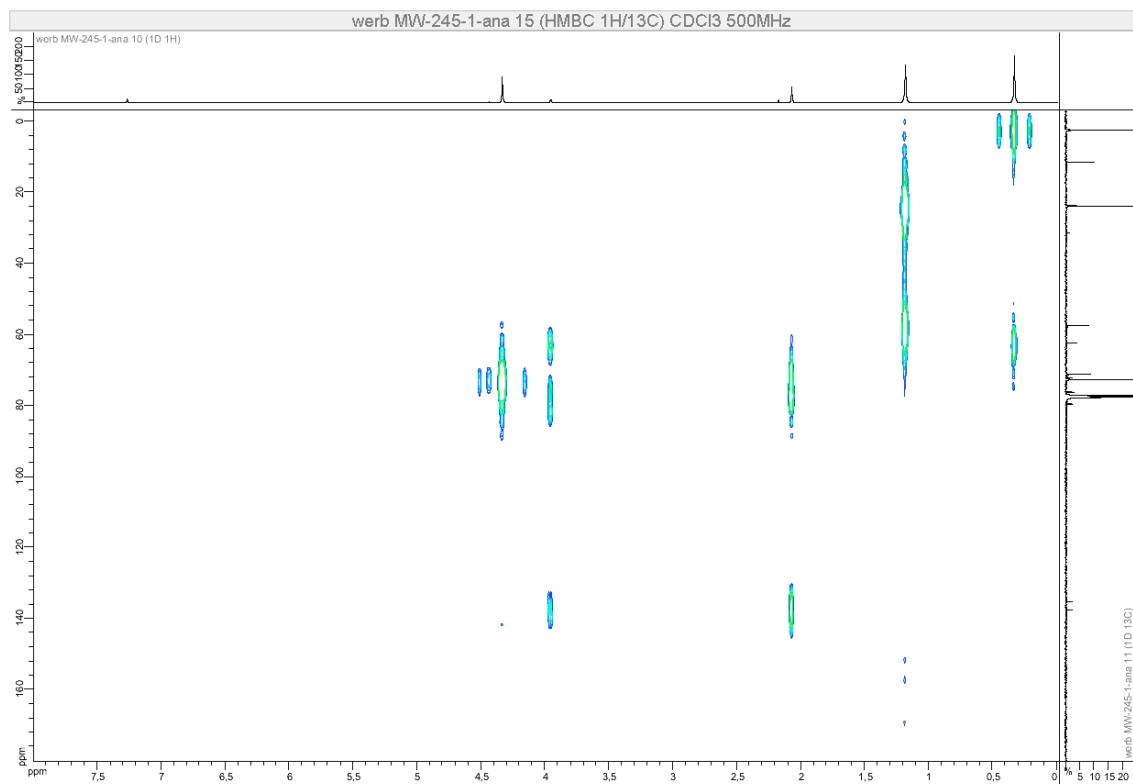
COSY (500 MHz, CDCl₃)



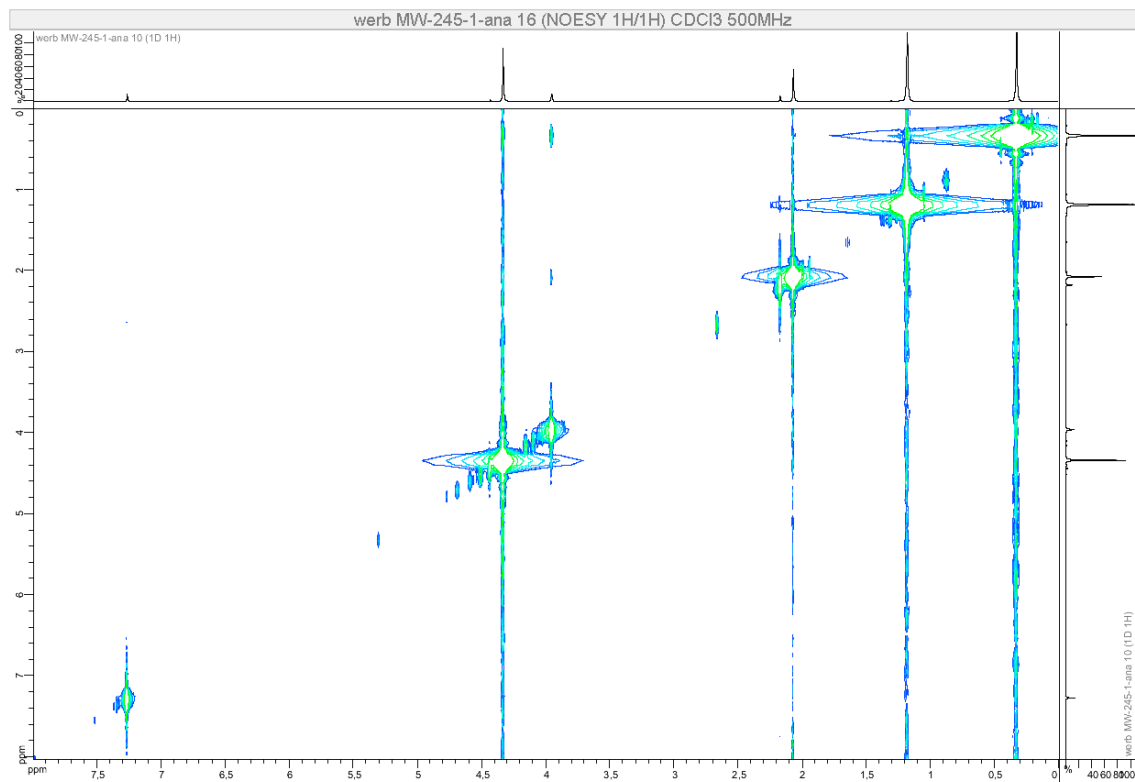
HSQC (500 MHz, CDCl₃)



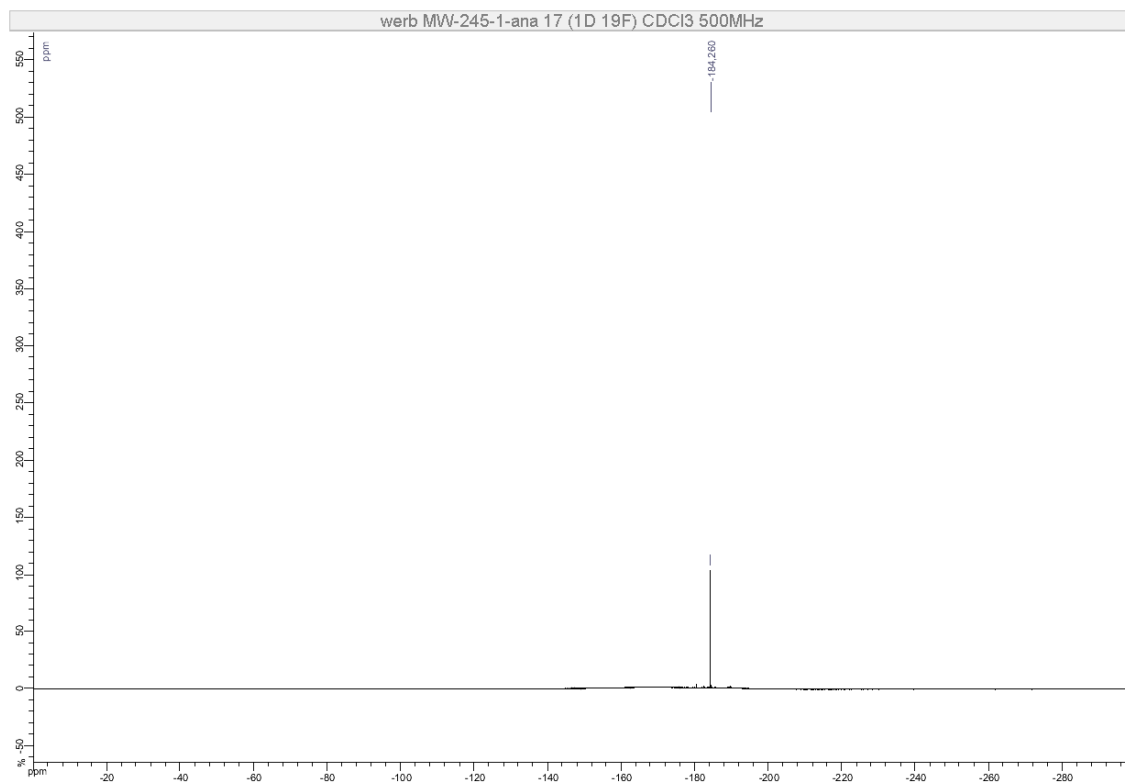
HMBC (500 MHz, CDCl₃)



NOESY (500 MHz, CDCl₃)

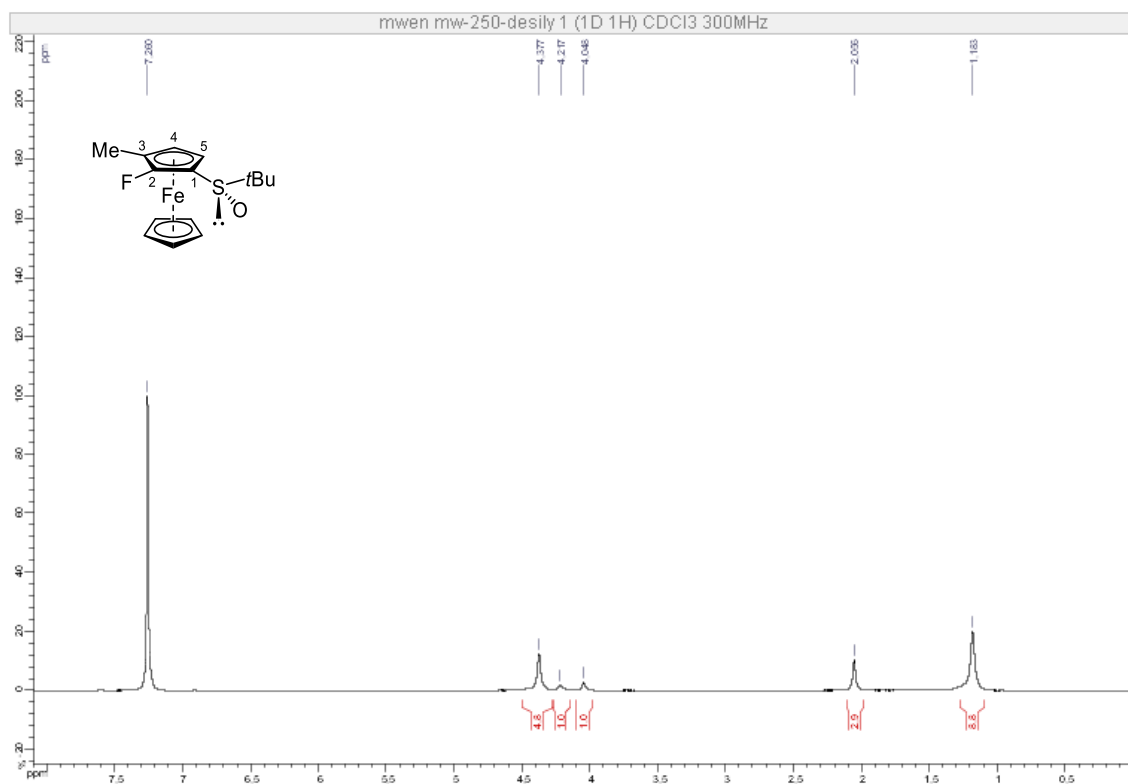


¹⁹F NMR (471 MHz, CDCl₃)



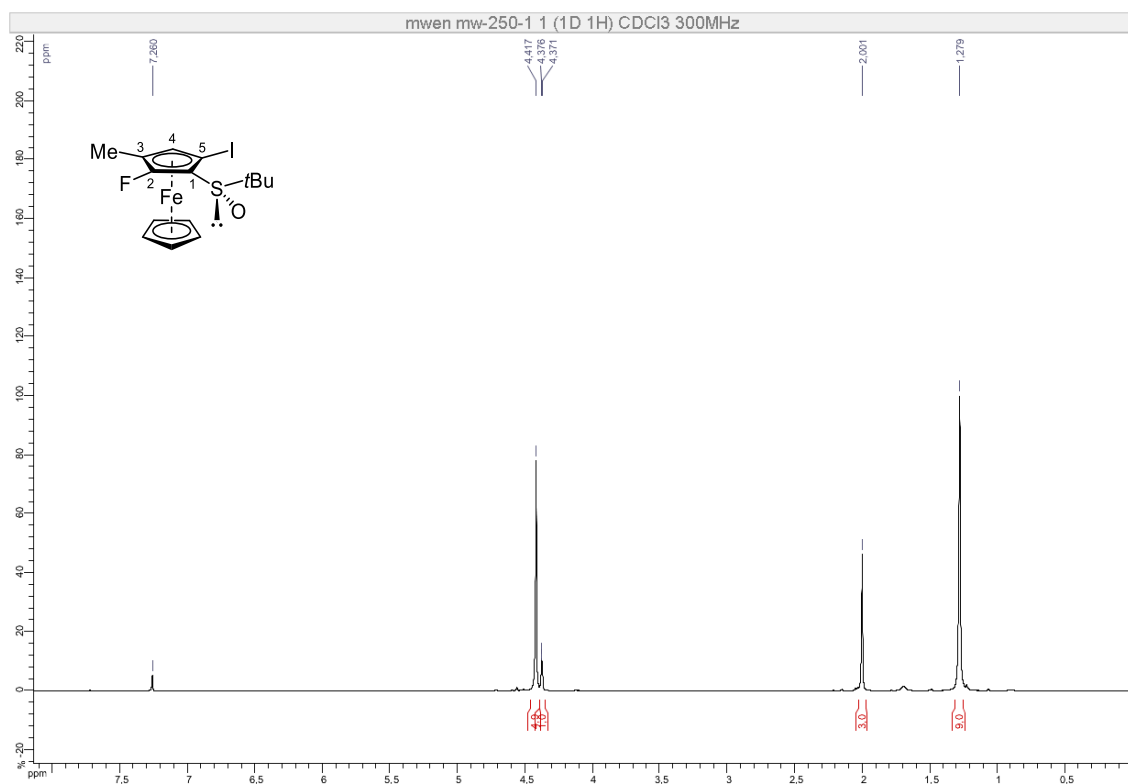
(*S,R*_P)-*S*-tert-Butyl-2-fluoro-3-methylferrocenesulfoxide (*S,R*_P-10)

¹H NMR (300 MHz, CDCl₃)



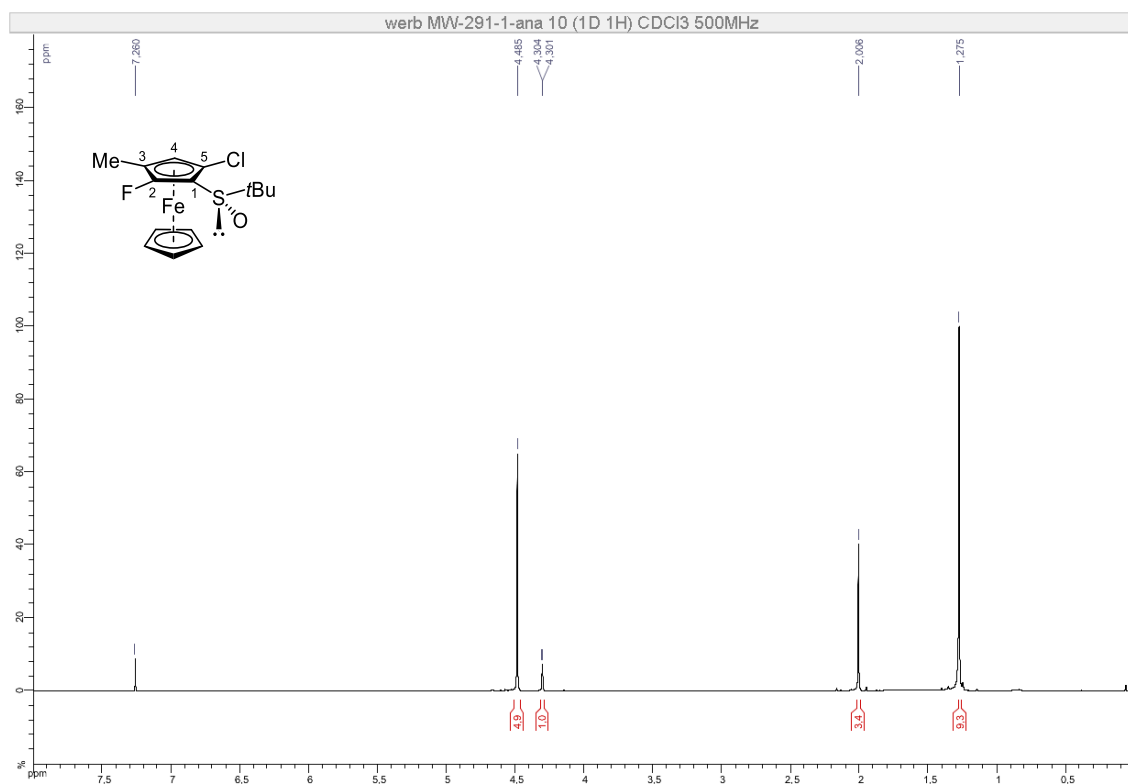
(*S,R_P*)-*S*-tert-Butyl-2-fluoro-5-iodo-3-methylferrocenesulfoxide (*S,R_P*-11b)

^1H NMR (300 MHz, CDCl_3)

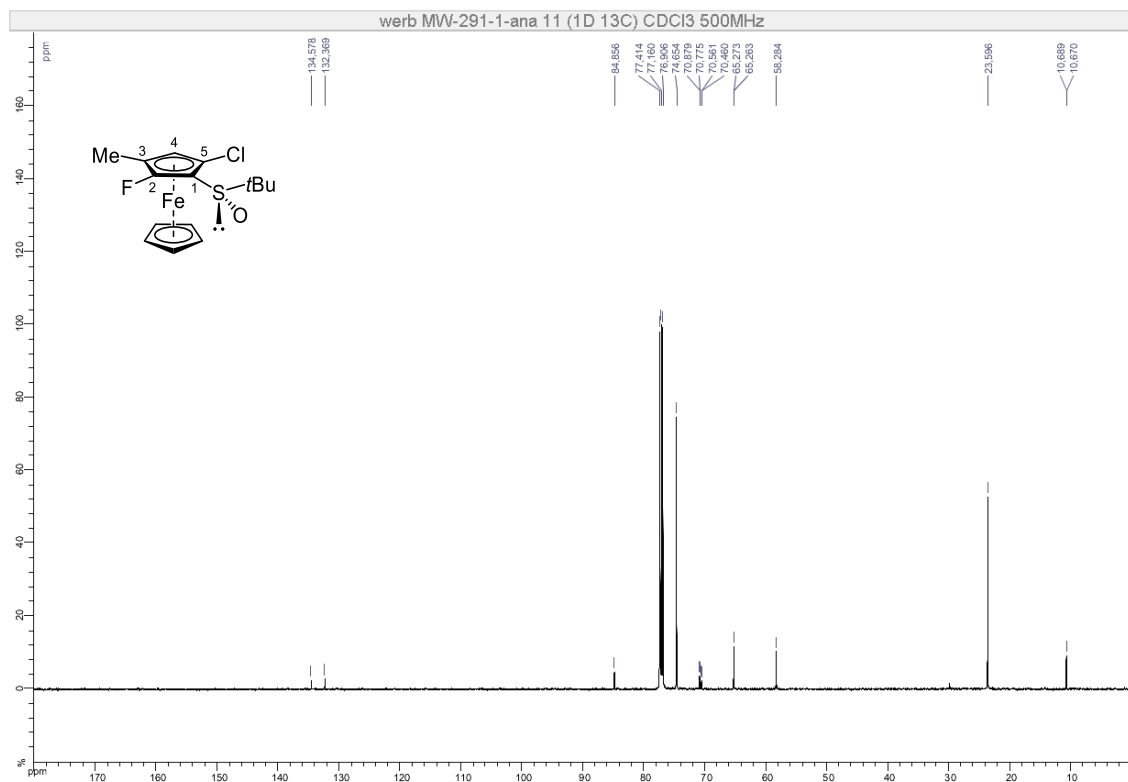


(*S,R*_P)-*S*-tert-Butyl-5-chloro-2-fluoro-3-methylferrocenesulfoxide (*S,R*_P-11k)

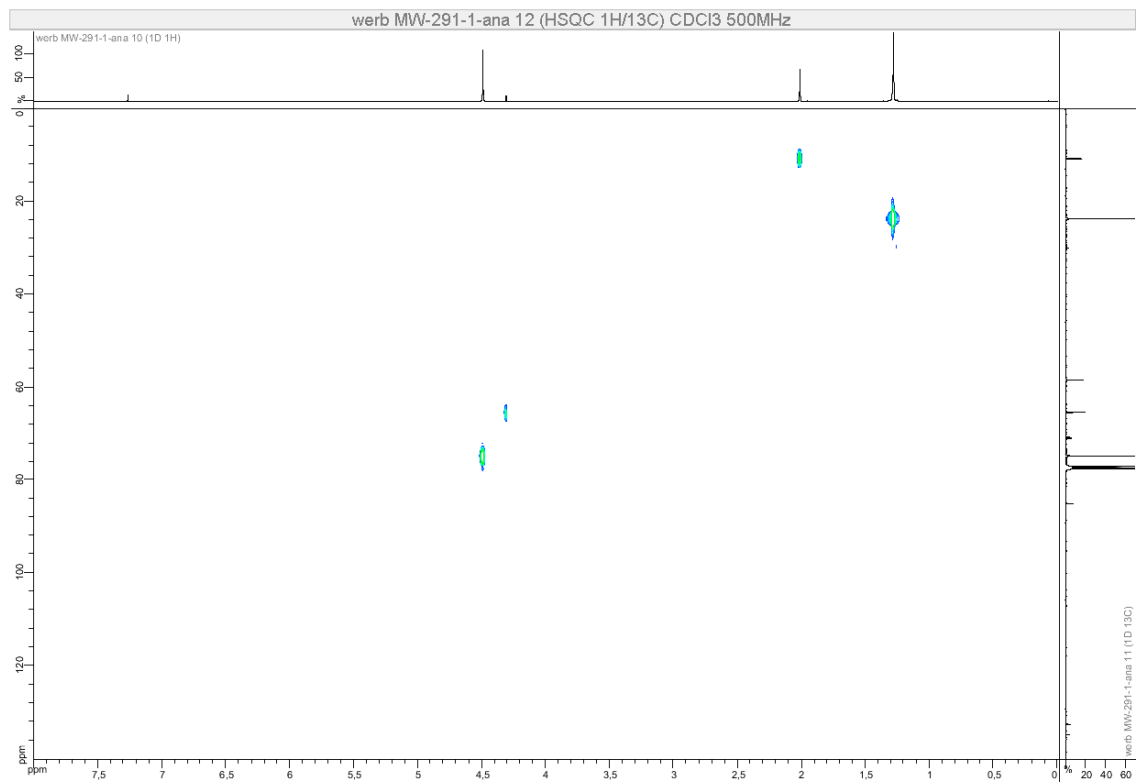
¹H NMR (500 MHz, CDCl₃)



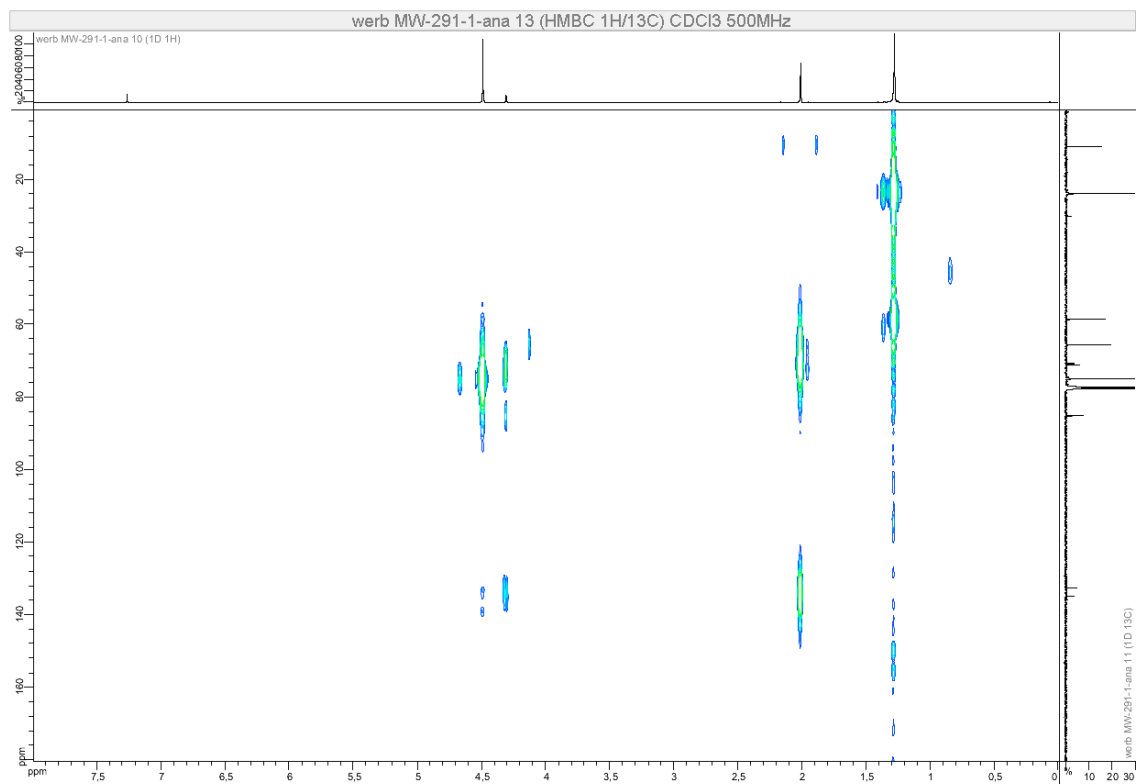
¹³C NMR (126 MHz, CDCl₃)



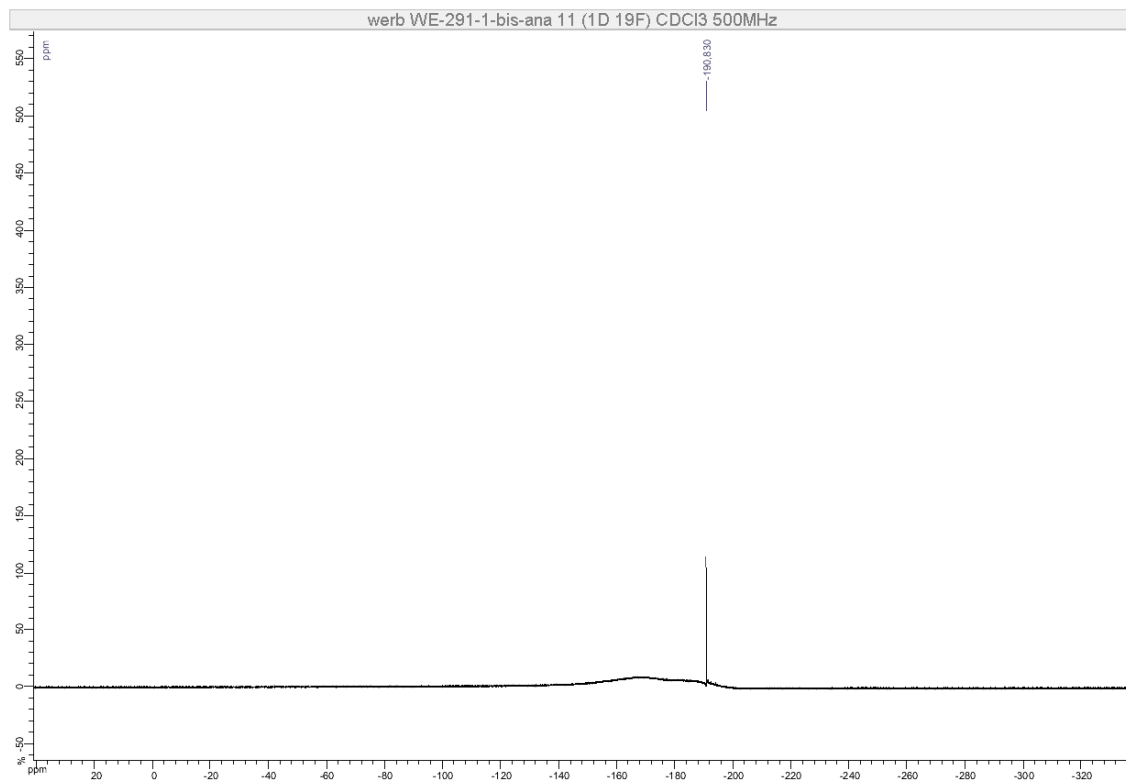
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

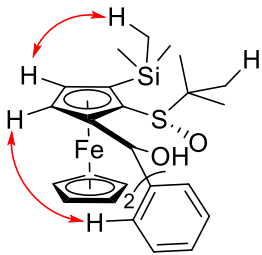
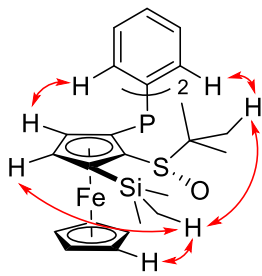
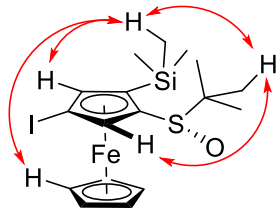
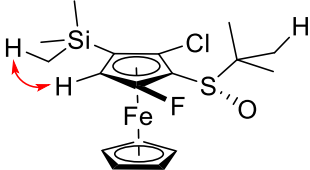
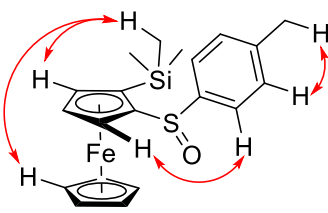
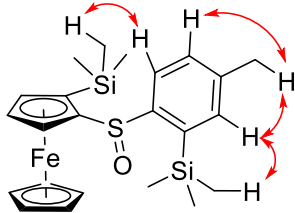
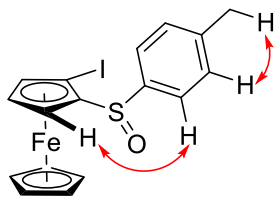
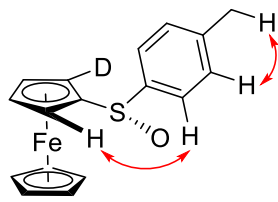
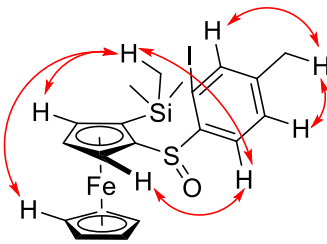
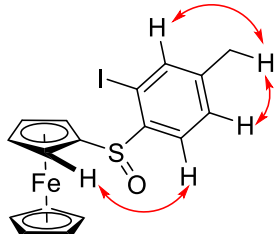
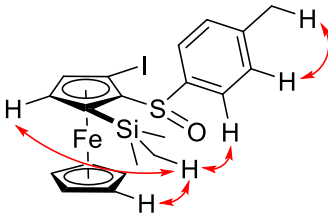
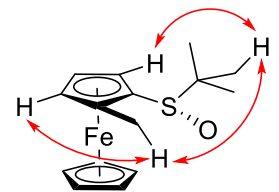
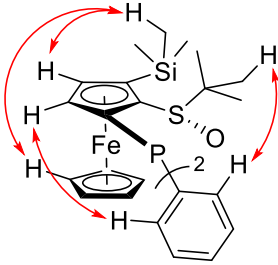
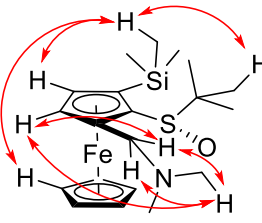
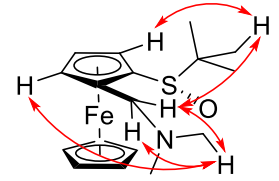


^{19}F NMR (471 MHz, CDCl_3)

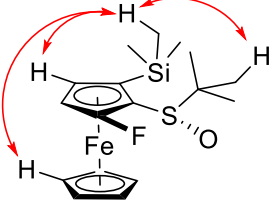
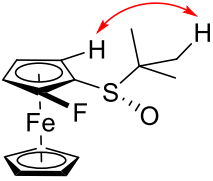
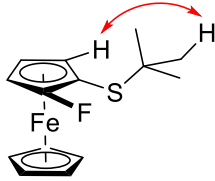
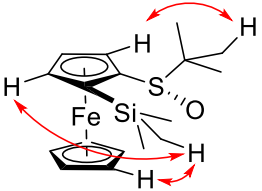
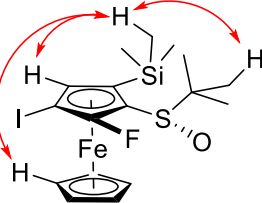
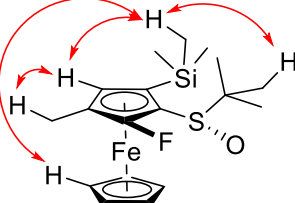


Selected NOESY correlations

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

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

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

