

Supporting Information

Ruthenium Olefin Metathesis Catalysts Bearing Carbohydrate-Based N-Heterocyclic Carbenes

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Contents

General Information.....	S2
Synthesis of 7b , 8a/b	S3-S5
Representative procedures for ROMP, RCM, CM, and AROCM.....	S5-S6
NMR Data for 8a	S6-S20
NMR Data for 8b	S21-S28
Magnetization Transfer Experiment.....	S29
Line Shape Analysis.....	S30-S39
References.....	S39

General Information.

All reactions were carried out in dry glassware under an argon atmosphere using standard Schlenk techniques or in a Vacuum Atmospheres Glovebox under a nitrogen atmosphere unless otherwise specified. All solvents were purified by passage through solvent purification columns and further degassed with argon.¹ NMR solvents were dried over CaH₂ and vacuum transferred to a dry Schlenk flask and subsequently degassed with argon. Commercially available reagents were used as received unless otherwise noted. Silica gel used for the purification of organometallic compounds was obtained from TSI Scientific, Cambridge, MA (60 Å, pH 6.5-7.0).

2D-NMR experiments were conducted on a Varian 600 MHz spectrometer equipped with a Triax (¹H, ¹³C, ¹⁵N) probe while VT and kinetic experiments were conducted on a Varian 500 MHz spectrometer equipped with an AutoX probe. Accurate temperature measurements of the NMR probe were obtained using a thermocouple connected to a multimeter with the probe immersed in an NMR tube containing toluene. Experiments and pulse sequences from Varian's Chempack 4 software were used without modification except for changes in the number of FIDs and scans per FID. Reaction conversions were obtained by comparing the integral values of starting material and product, no internal standard was used. Chemical shifts are reported in ppm downfield from Me₄Si by using the residual solvent peak as an internal standard. Spectra were analyzed and processed using MestReNova Ver. 5.2.5 – 4119.²

Gas chromatography data were obtained using an Agilent 6850 FID gas chromatograph equipped with a DB-Wax Polyethylene Glycol capillary column (J&W Scientific). Response factors were calculated for all relevant compounds before analysis. Enantiomeric excess was determined using an Agilent 1100 series HPLC equipped with Chiracel AD, OD-H, and AS

columns. The retention time of all compounds analyzed has been previously reported³ but was also compared to authentic racemic samples. High-resolution mass spectrometry (HRMS) data was obtained on a JEOL MSRoute mass spectrometer using FAB+ ionization.

Compounds **6a**⁴, **6b**⁴, and **7a**⁵ were prepared according to literature procedures from commercially available precursors.

Synthesis of **7b**.

Mesityl imidazole⁶ (1.06 g, 5.67 mmol), **6b** (2.57 g, 6.24 mmol), and AgOTf (1.60 g, 6.24 mmol) were placed in a dry 100 ml RB flask under argon and dissolved in 30 ml of dry MeCN. The RB was shielded from light and heated to 50 °C for 16 h. The reaction was cooled to 25 °C and the solution filtered through a pad of celite washing with MeCN then concentrated *in vacuo*. The resulting residue was dissolved in CH₂Cl₂ and MTBE was added until the solution became slightly cloudy. After cooling to -5 °C, an oily residue crashed out. The supernatant was removed and the oil was triturated with cold hexanes and concentrated to a light brown powder (1.8 g, 47%). **5b** was recovered as a 1.3:1 mixture of β:α anomers ¹H NMR (CDCl₃, 300 MHz): δ 9.39 (s, 1H), 8.69 (s, 1H), 7.91 (s, 1H), 7.77 (s, 1H), 7.31 (s, 1H), 7.18 (s, 1H), 7.02 (s, 4H), 6.37 (m, 1H), 5.57 (m, 1H), 5.36 (m, 3H), 4.48 (t, J = 6.18 Hz, 1H), 4.19-4.03 (m, 4H), 2.18-1.97 (m, 42H).

Synthesis of **8a**.

In a glovebox, a 100 ml RB was charged with **1** (0.497 g, 0.604 mmol), **7a** (0.604 g, 0.906 mmol), and NaO^tBu (0.087 g, 0.906 mmol). 50 ml of dry THF was added and the reaction was stirred for 1 h at 25 °C after which it was removed from the glovebox and conc. *in vacuo*. The residue was dissolved in a minimal amount of CH₂Cl₂, loaded onto a column of TSI silica gel,

and eluted with 10% diethyl ether/pentane to first collect excess **1** as a dark purple band, followed by 30% ether/pentane, and finally 60% ether/pentane until a dark pink/red band was collected. After concentration of the relevant fractions, a dark pink residue was obtained which could be lyophilized from benzene to yield **8a** (208 mg, 33%) as a dark pink powder. ¹H NMR (C₆D₆, 600 MHz, major isomer): δ 19.74 (s, 1H), 8.4-7.8 (br s, 2H), 7.10 (d, J = 1.8 Hz, 1H), 6.95 (m, 3H), 6.31 (br s, 1H), 6.03 (d, J = 1.8 Hz, 1H), 5.98 (br s, 1H), 5.94 (t, J = 9 Hz, 1H), 5.88 (t, J = 9.6 Hz, 1H), 5.57 (t, J = 9.6 Hz, 1H), 4.39 (m, 2H), 4.26 (ad, J = 10.8 Hz, 1H), 2.53 (m, 3H), 2.23 (s, 6H), 1.98 (br s, 3H), 1.88 (br s, 6H), 1.80 (br s, 12H), 1.73 (m, 9H), 1.59 (m, 6H), 1.23 (m, 9H). ¹³C NMR (151 MHz, C₆D₆) δ 298.0, 192.6, 170.39, 170.22, 169.94, 152.44, 138.70, 137.03, 136.86, 136.51, 129.46, 129.14, 128.90, 124.55, 124.54, 120.36, 120.34, 87.17, 75.50, 74.74, 71.13, 69.30, 62.00, 33.17, 33.06, 30.49, 28.52, 28.49, 28.46, 28.43, 27.24, 21.42, 21.31, 20.94, 20.55, 20.53, 18.97, 18.69. ³¹P NMR (202 MHz, C₆D₆) δ 30.86 (major), 28.17 (minor). HRMS (FAB+) Calculated: 1058.332, Experimental: 1058.329.

Synthesis of **8b**.

An analogous procedure to that of **8a** was followed yielding **8b** (17%) as a 1.2:1 mixture of anomers. ¹H NMR (C₆D₆, 600 MHz, major isomer): δ 19.78 (s, 1H), 8.4-7.9 (br s, 4H), 7.46 (d, J = 1.56 Hz, 1H), 7.06 (d, J = 5.1 Hz, 1H), 6.95 (br t, J = 7.38 Hz, 2H), 6.76 (d, J = 3.54 Hz, 1H), 6.32 (br s, 1H), 6.27 (t, J = 9.48 Hz, 1H), 6.03 (d, J = 2.04 Hz, 1H), 6.00 (br s, 1H), 5.91 (d, J = 2.88 Hz, 1H), 5.82 (m, 1H), 5.71 (m, 1H), 5.67 (m, 1H), 5.63 (m, 1H), 4.64 (br t, J = 6.78 Hz, 1H), 4.38 (m, 1H), 4.22 (m, 1H), 4.17 (m, 1H), 4.10 (m, 2H), 2.54 (m, 6H), 2.26 (s, 6H), 1.98-1.55 (m, 77H), 1.24 (m, 15H). ¹³C NMR (151 MHz, C₆D₆) δ 193.04, 170.52, 170.37, 170.35, 170.20, 170.13, 169.94, 169.92, 169.81, 168.82, 152.49, 138.71, 137.09, 136.88, 136.52, 129.46, 129.17, 128.66, 128.61, 128.53, 128.45, 128.37, 128.29, 128.21, 128.10, 124.60, 124.59, 120.54,

120.52, 92.94, 90.54, 87.65, 74.31, 72.66, 72.22, 71.67, 69.65, 68.86, 68.55, 68.25, 68.17, 68.03, 67.57, 67.51, 61.69, 61.47, 61.21, 33.08, 33.04, 32.97, 30.51, 30.49, 30.37, 30.15, 28.54, 28.51, 28.49, 28.44, 28.43, 27.60, 27.28, 27.16, 27.01, 21.58, 21.32, 20.73, 20.63, 20.53, 20.52, 20.49, 20.47, 20.43, 20.41, 20.39, 20.24, 20.18, 19.01, 18.67. ³¹P NMR (121 MHz, C₆D₆) δ 31.19 (major), 28.53 (minor). HRMS (FAB+) Calculated: 1057.324, Experimental 1057.321.

Representative procedure for ROMP/RCM kinetics.

In a glovebox, catalyst **8a** (2.5 mg, 0.0024 mmol) was dissolved in CD₂Cl₂ (0.8 ml) and placed in a NMR tube equipped with a rubber septum. The NMR tube was removed from the glovebox and COD (distilled prior to use) (30 μL, 0.24 mmol) was injected after which the tube was immediately placed in the spectrometer and a spectral array started by arraying the “pad” variable for Varian spectrometers.

Representative procedure for CM Kinetics.

Allyl benzene and *cis*-diacetoxybutene were distilled prior to use. In a glovebox, a scintillation vial was charged with allyl benzene (20 μL, 0.153 mmol), *cis*-diacetoxybutene (49 μL, 0.305 mmol), and tridecane standard (50 μL, 0.205 mmol). CH₂Cl₂ (0.75 ml) was added followed by **8a** (4 mg, 0.004 mmol) as a solution in CH₂Cl₂. The vial was equipped with a septa top, removed from the glovebox and stirred under argon. Aliquots were removed via syringe at the specified time points and added to a GC vial containing a solution of ethyl vinyl ether in CH₂Cl₂ in order to quench the catalyst. GC retention times were as follows (min): allyl benzene (10.87), tridecane (11.55), *cis*-diacetoxybutene (18.13), *trans*-diacetoxybutene (18.70), *cis*-**12** (21.27), *trans*-**12** (21.48), *trans*-homocoupled allyl benzene (24.09), *cis*-homocoupled allyl benzene (24.34).

Representative procedure for AROCM.

A 10 ml RB was dried and charged with the norbornene substrate (0.109 mmol), styrene (0.125 mL, 1.09 mmol) which had been passed through a small plug of silica gel, and dry toluene (2 mL). Catalyst **8a** (6 mg, 0.005 mmol) was injected as a solution in toluene and the reaction stirred at 40°C for 14 h. The solvent was evaporated and the remaining residue was purified by flash chromatography to yield the desired product. Chromatography and HPLC conditions for all compounds studied have been previously reported.³

Spectroscopic characterization.

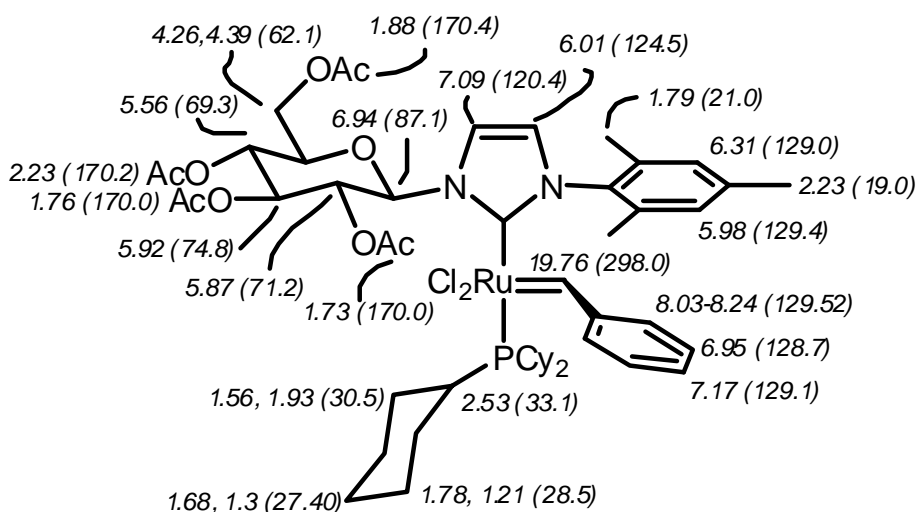


Figure S1. ^1H (^{13}C) assignments for major isomer of catalyst **8a** based on spectroscopic data.

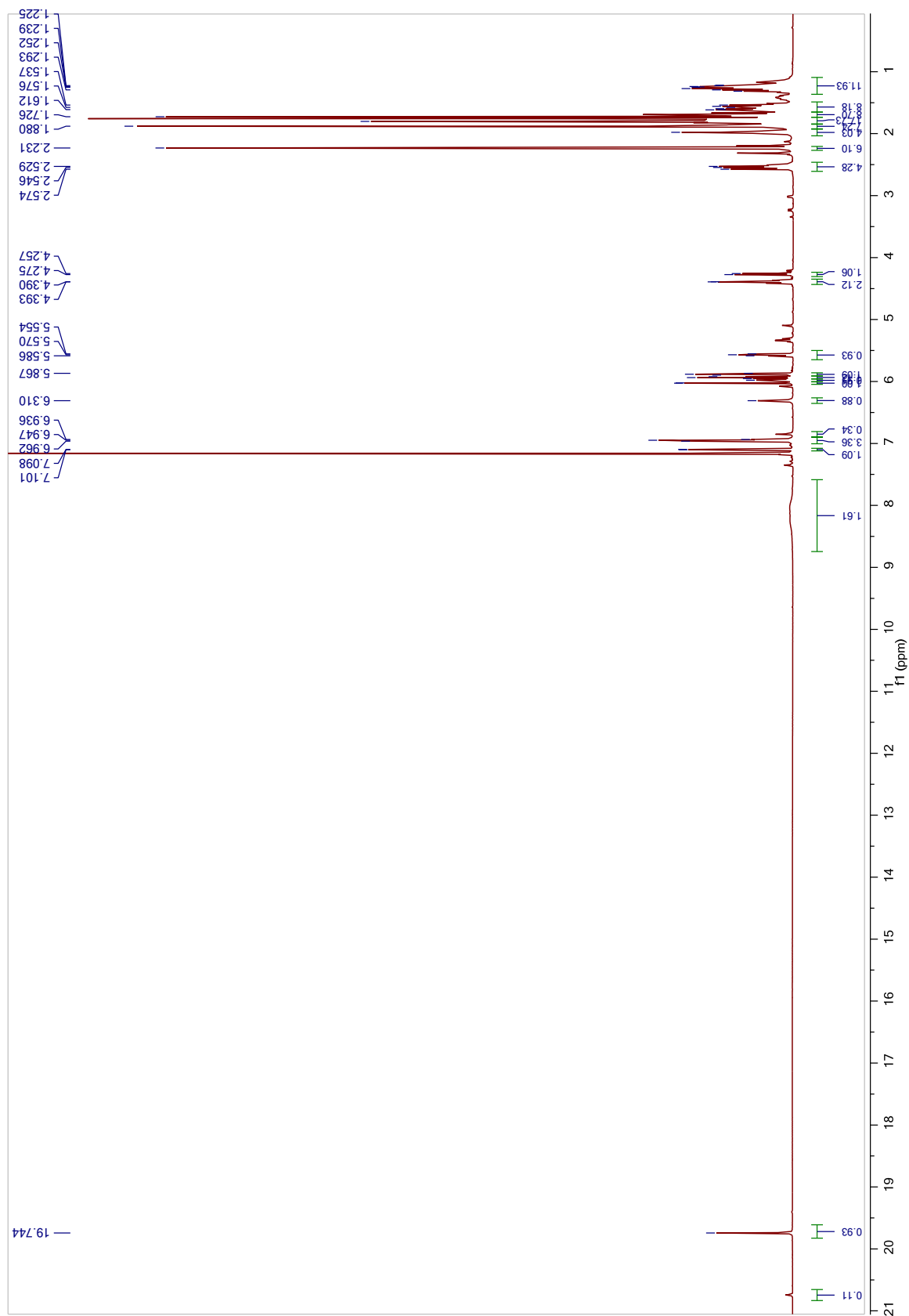


Figure S2. ^1H NMR (600 MHz) spectrum of catalyst **8a** in C_6D_6

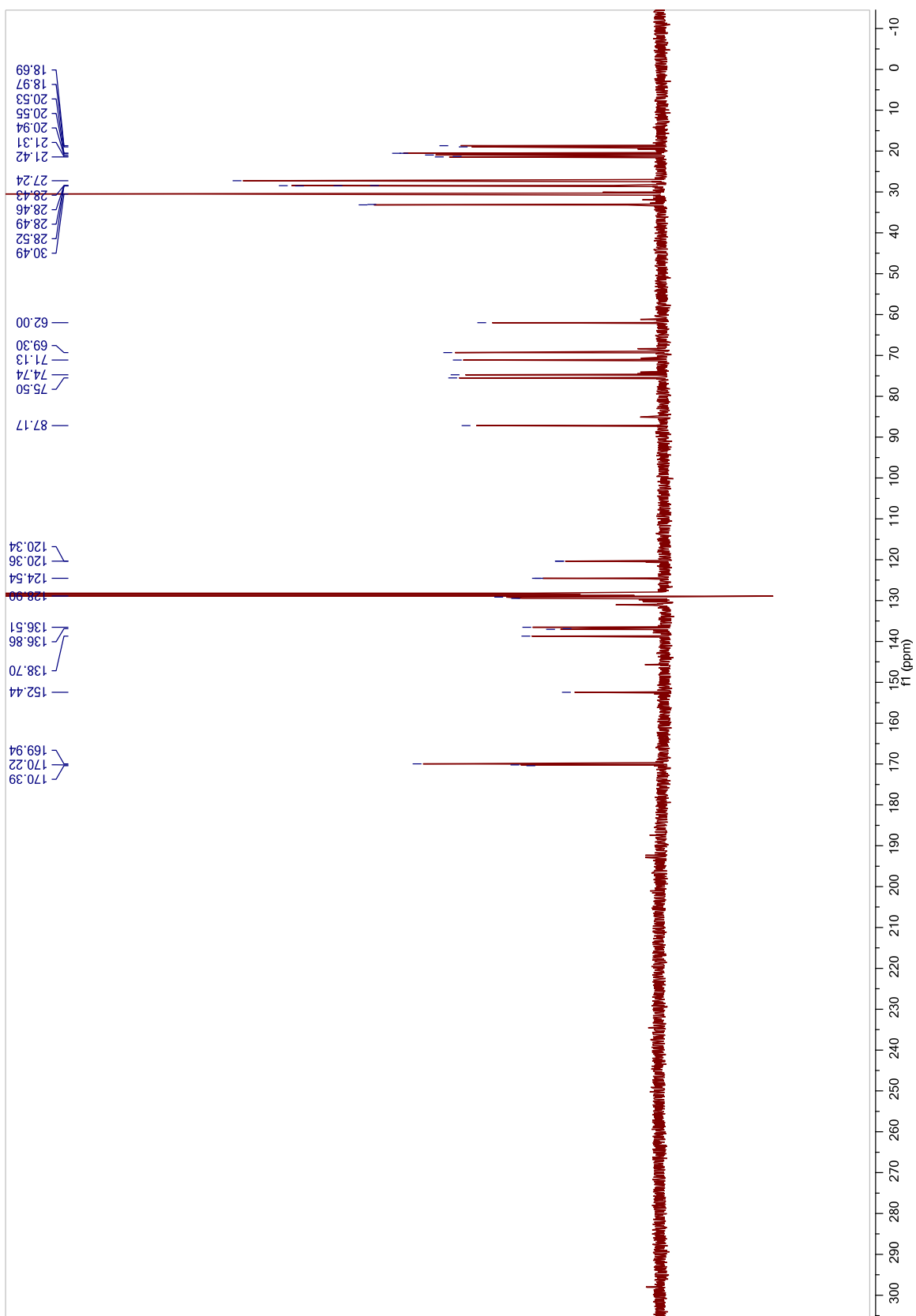


Figure S3. ^{13}C NMR spectrum of catalyst **8a** in C_6D_6 .

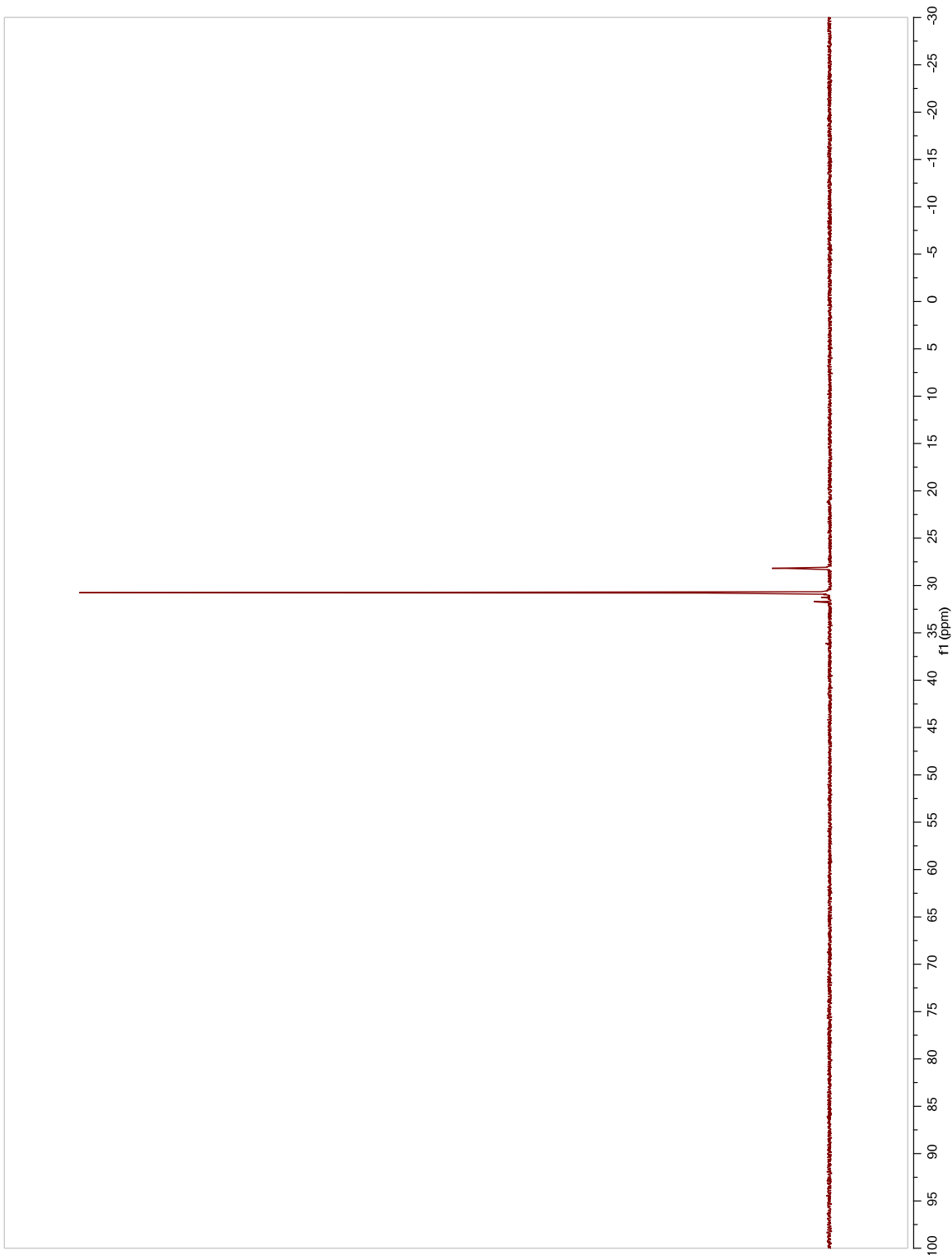


Figure S4. ^{31}P NMR Spectrum of catalyst **8a** in C_6D_6 .

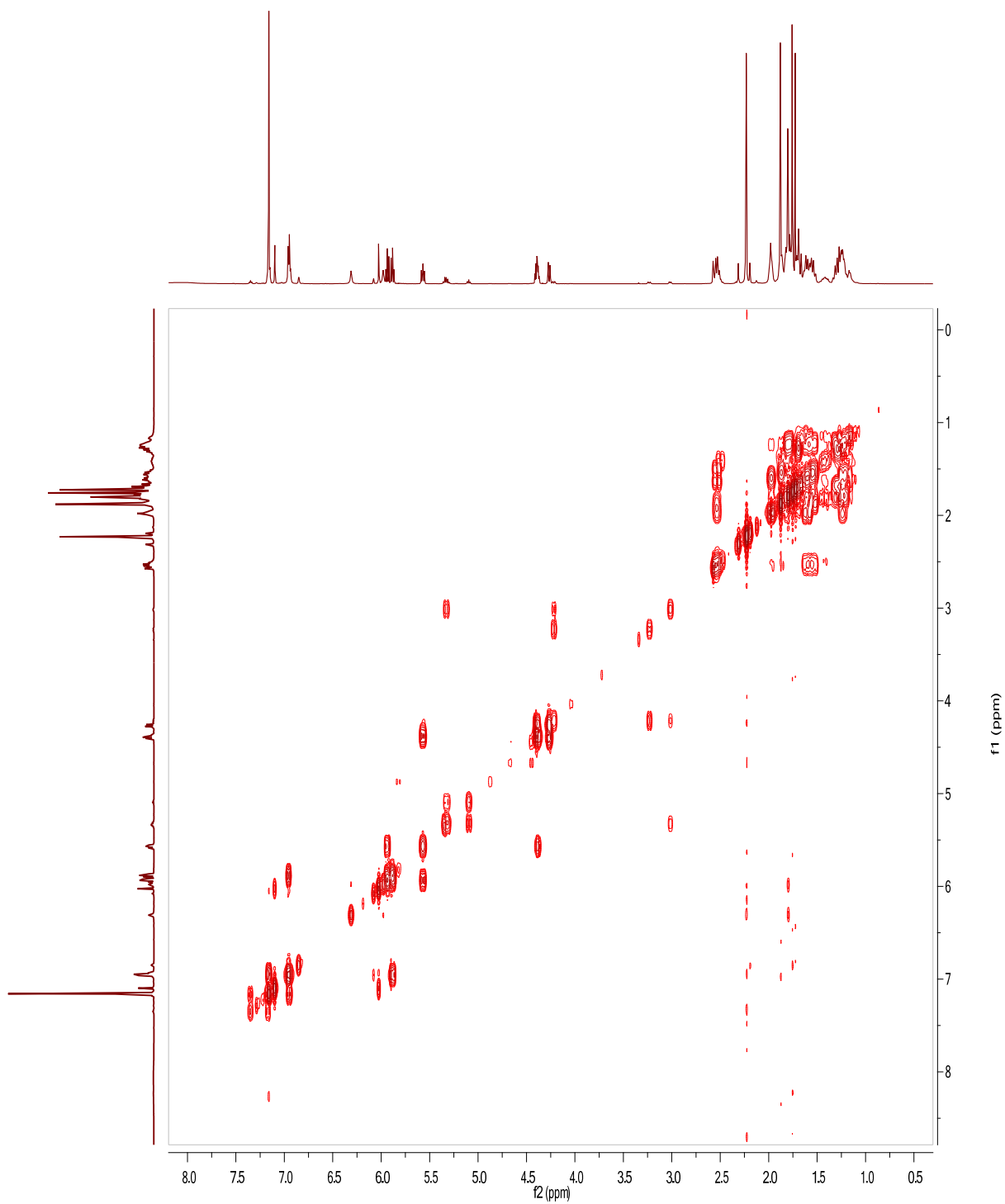


Figure S5. 600 MHz ¹H-¹H gCOSY spectrum of **8a** in C₆D₆ at 25 °C.

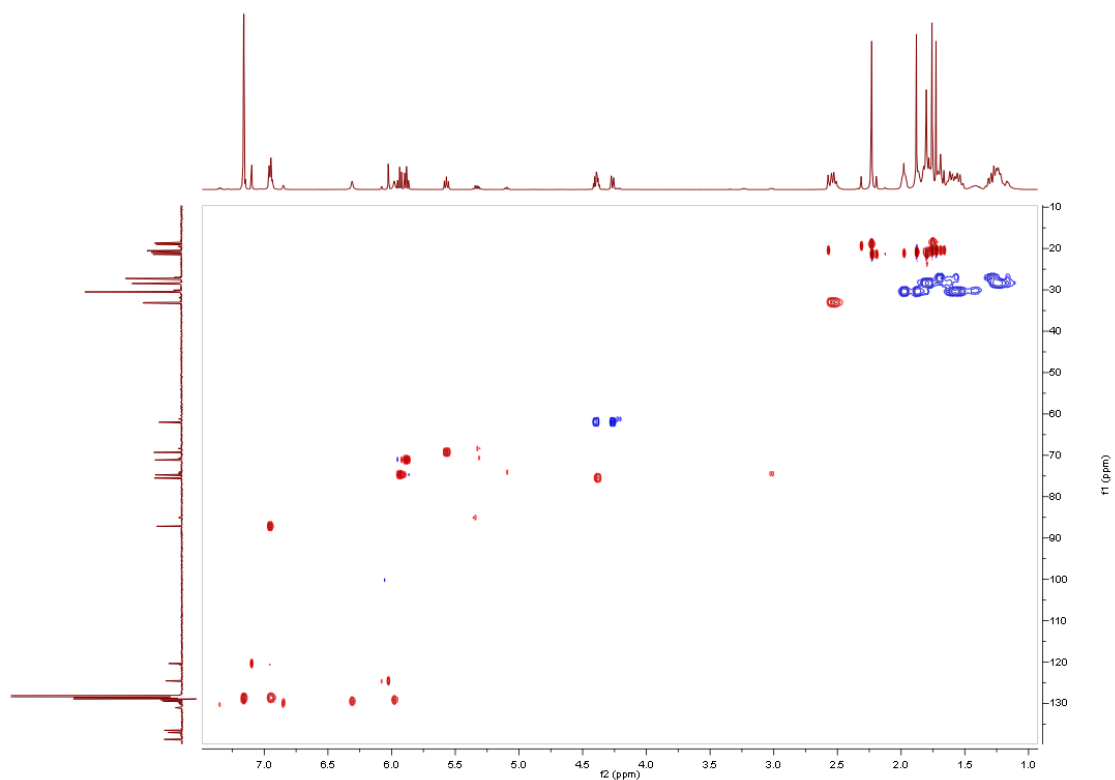


Figure S6. Upfield 600 MHz ^1H - ^{13}C gHSQCad spectrum of **8a** in C_6D_6 at 25 °C.

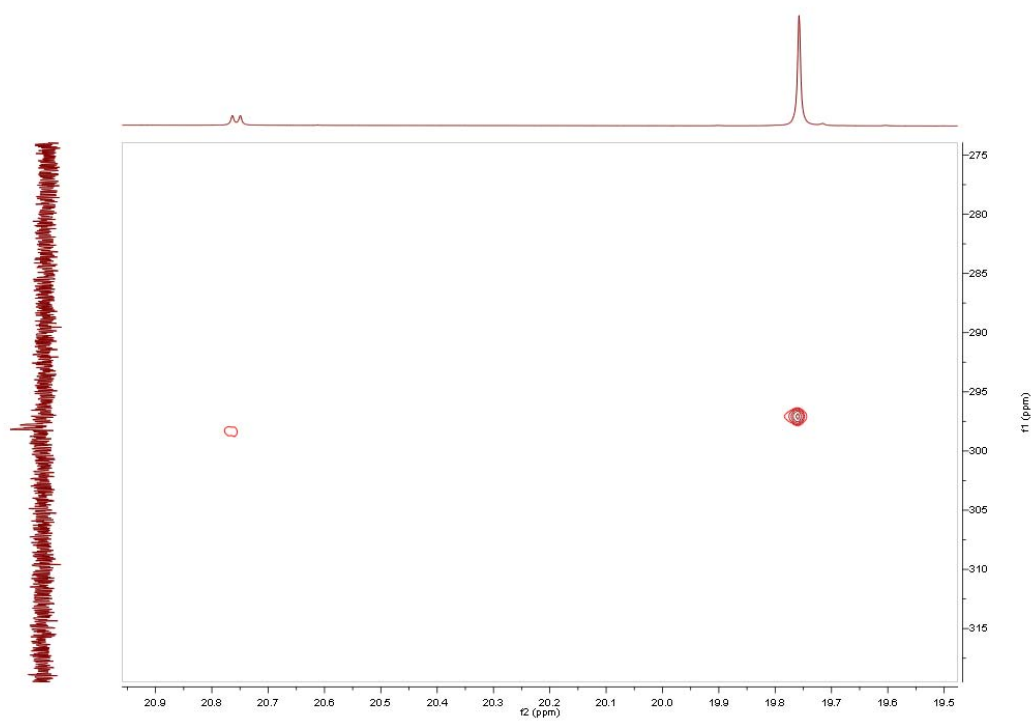


Figure S7. Downfield 600 MHz ^1H - ^{13}C gHSQCad spectrum of **8a** in C_6D_6 at 25 °C.

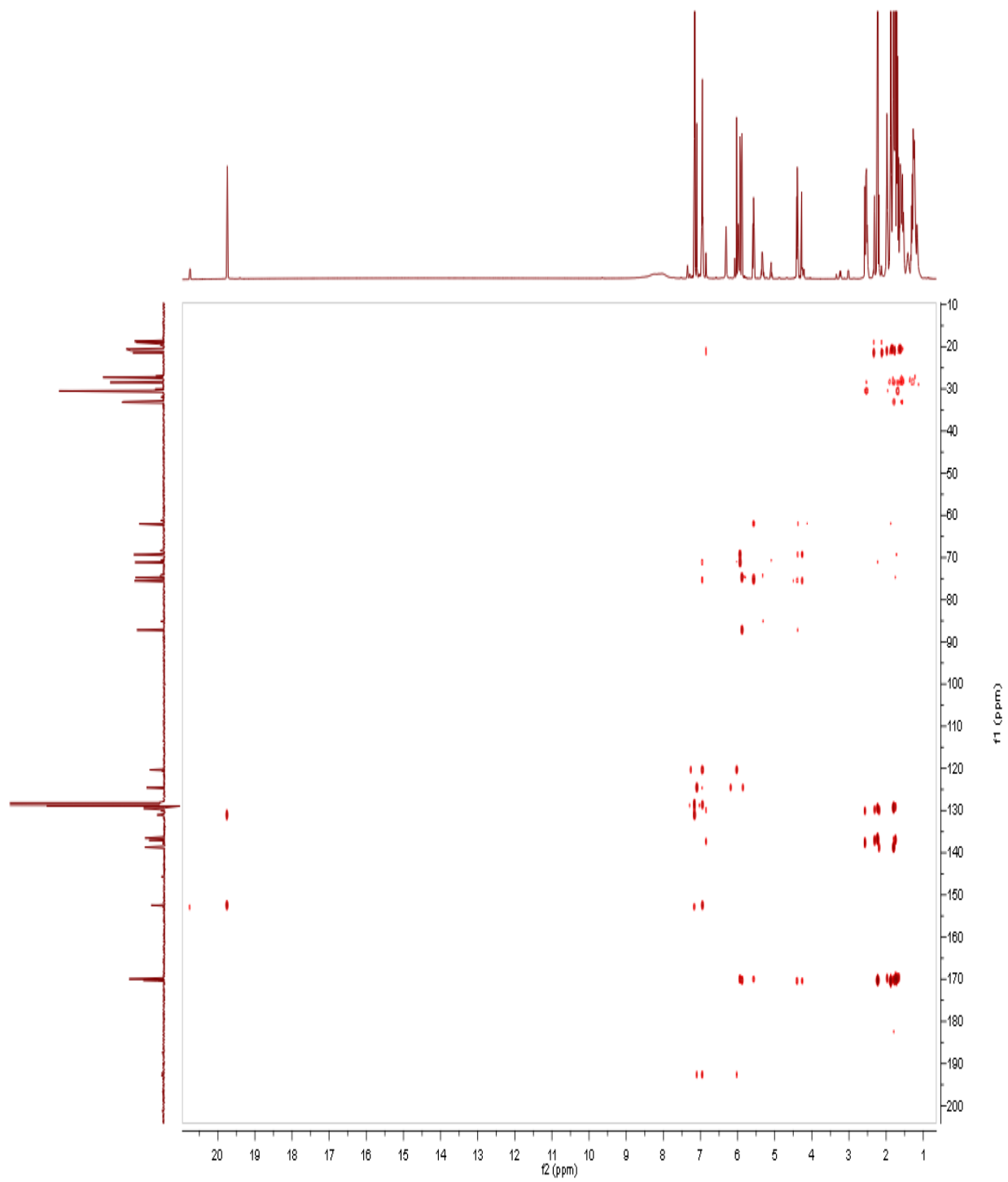


Figure S8. 600 MHz ^1H - ^{13}C gHMBCad spectrum of **8a** in C_6D_6 at 25 °C.

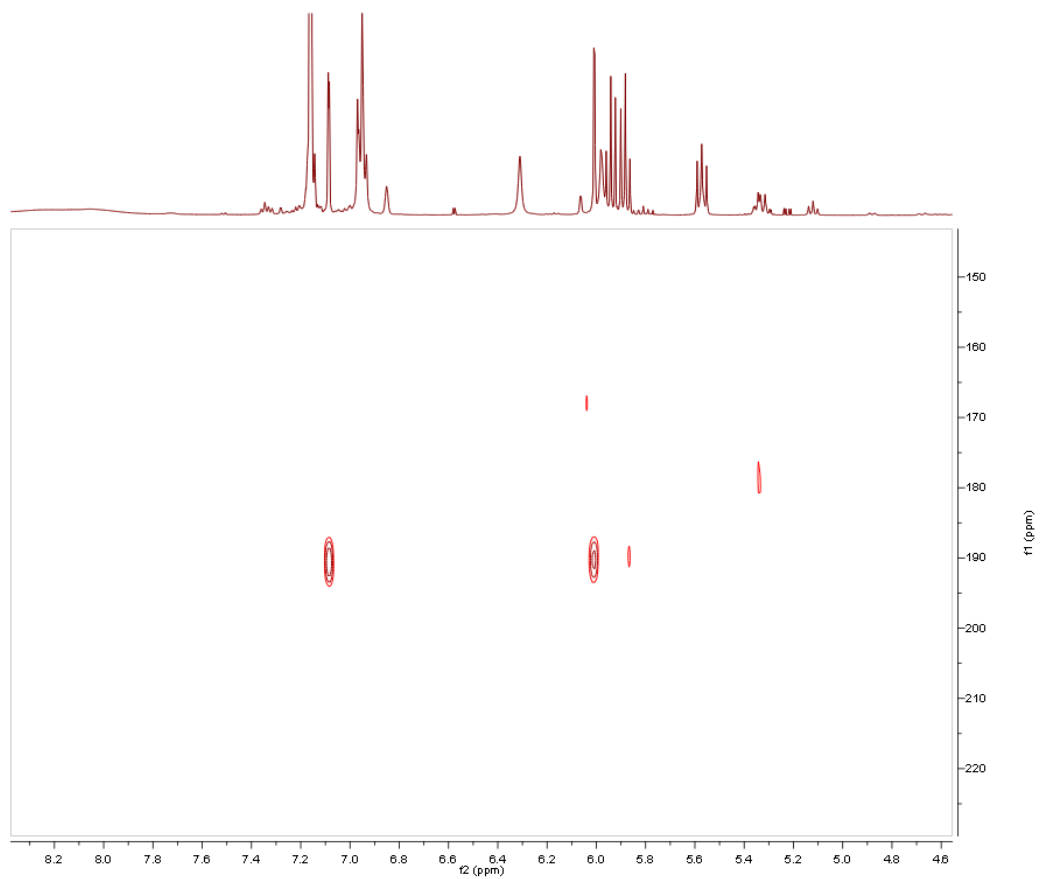


Figure S9. 600 MHz ^1H - ^{15}N gHMBCad of **8a** in C_6D_6 at 25 $^\circ\text{C}$.

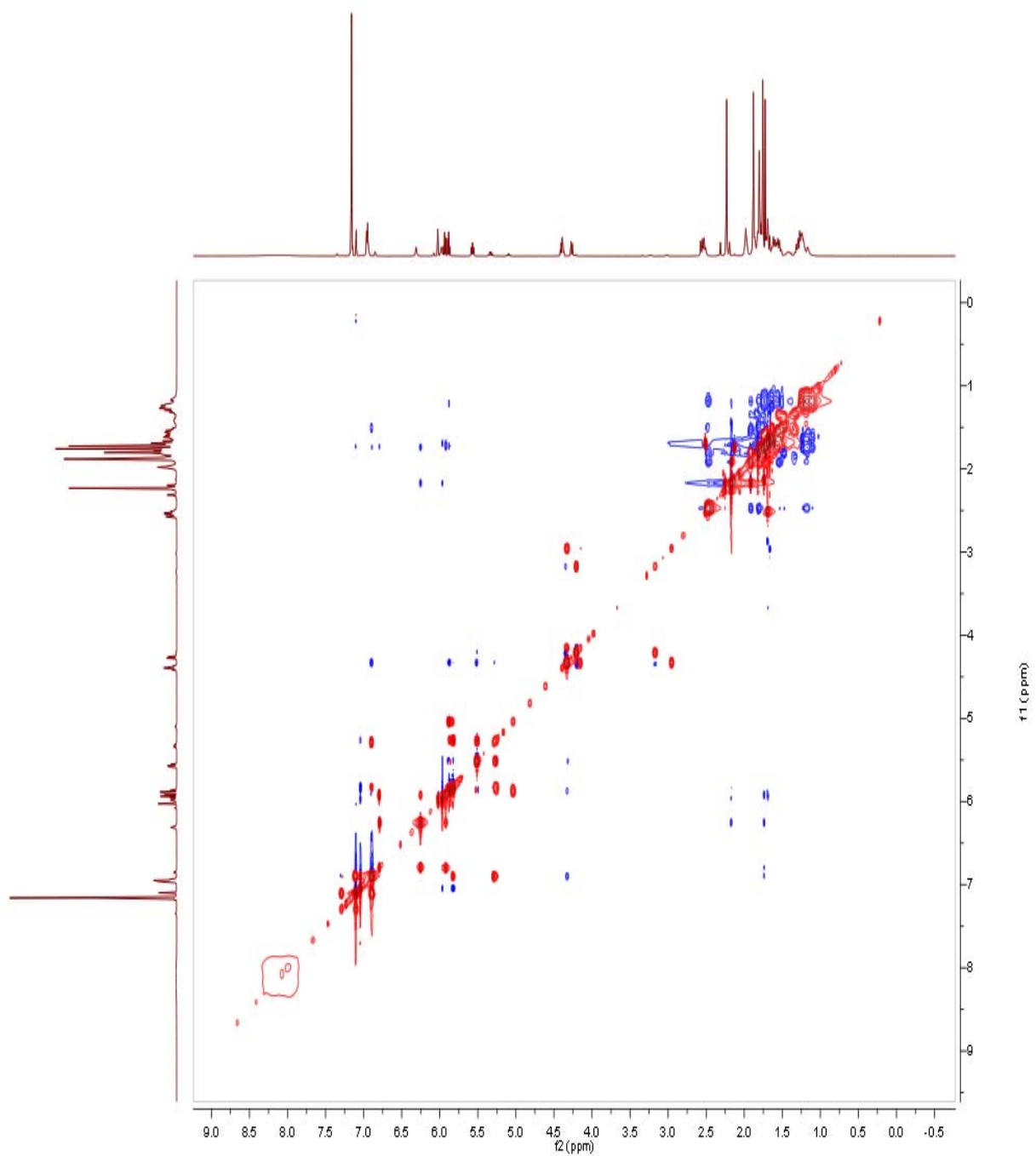


Figure S10. 600 MHz ^1H - ^1H NOESY of **8a** in C_6D_6 at 25 °C. Mixing time = 200 ms. Red peaks show chemical exchange, blue peaks show NOE.

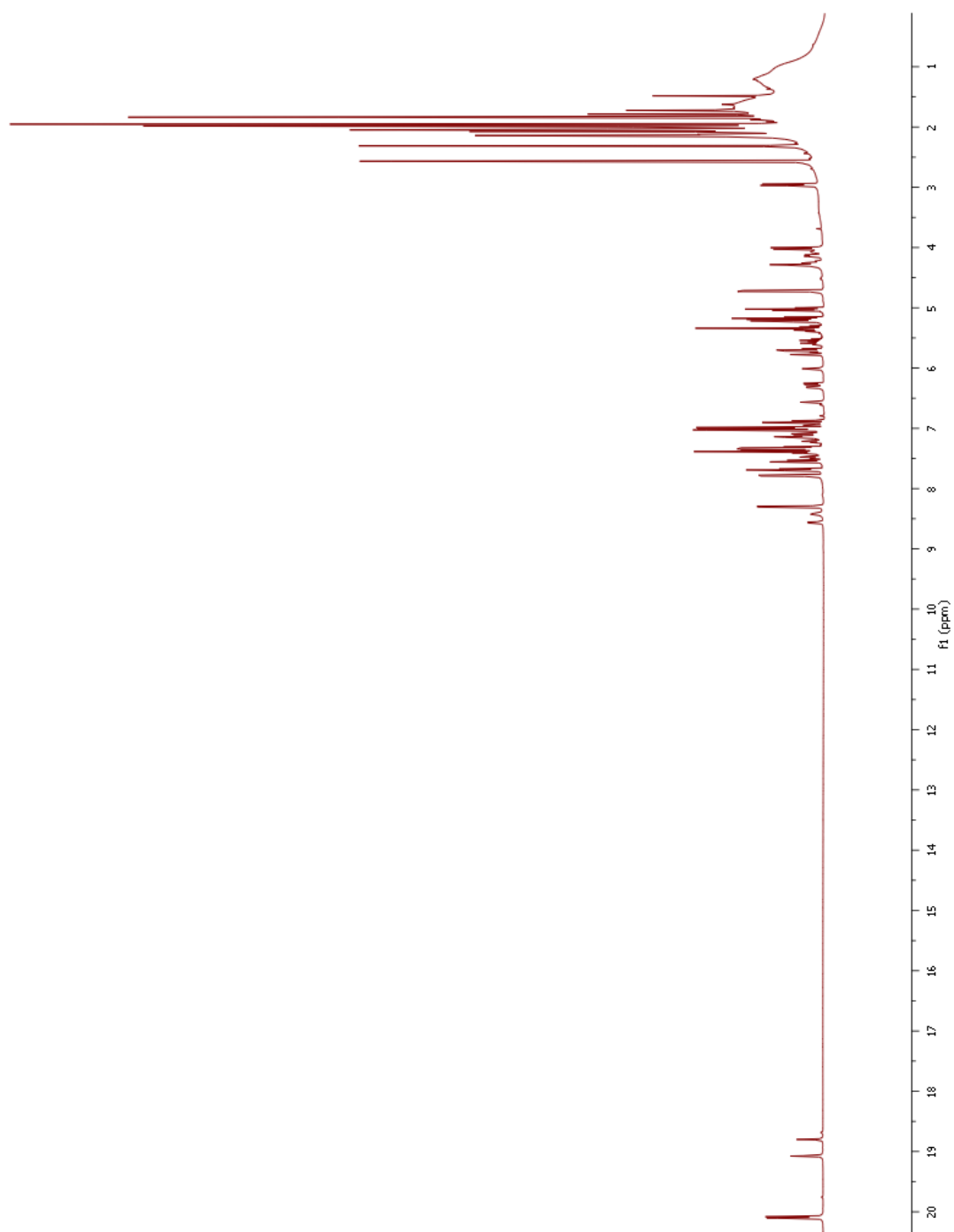


Figure S11. 500 MHz ^1H NMR spectrum of **8a** in CD_2Cl_2 at -75°C .

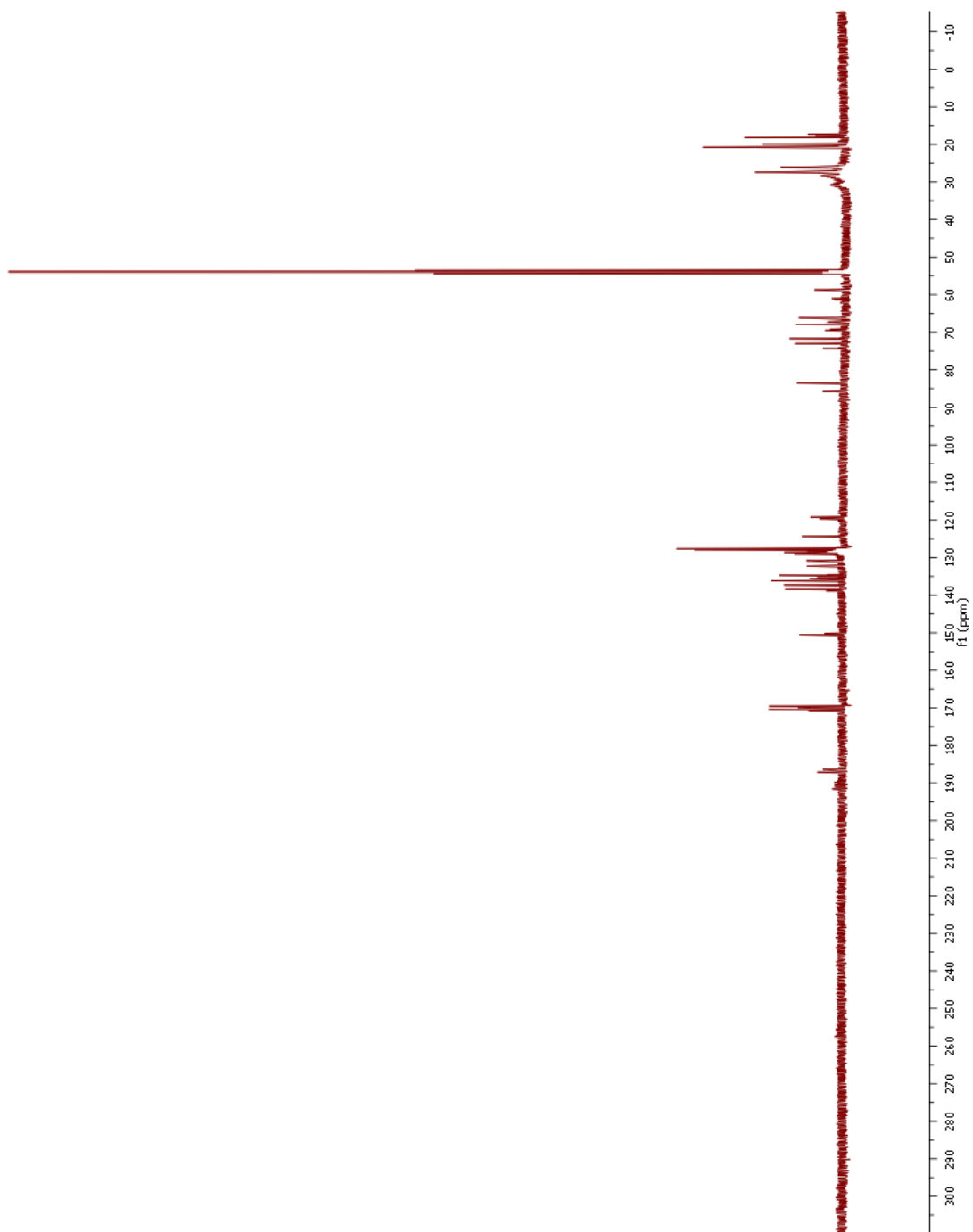


Figure S12. 500 MHz ^{13}C NMR spectrum of **8a** in CD_2Cl_2 at -75°C .

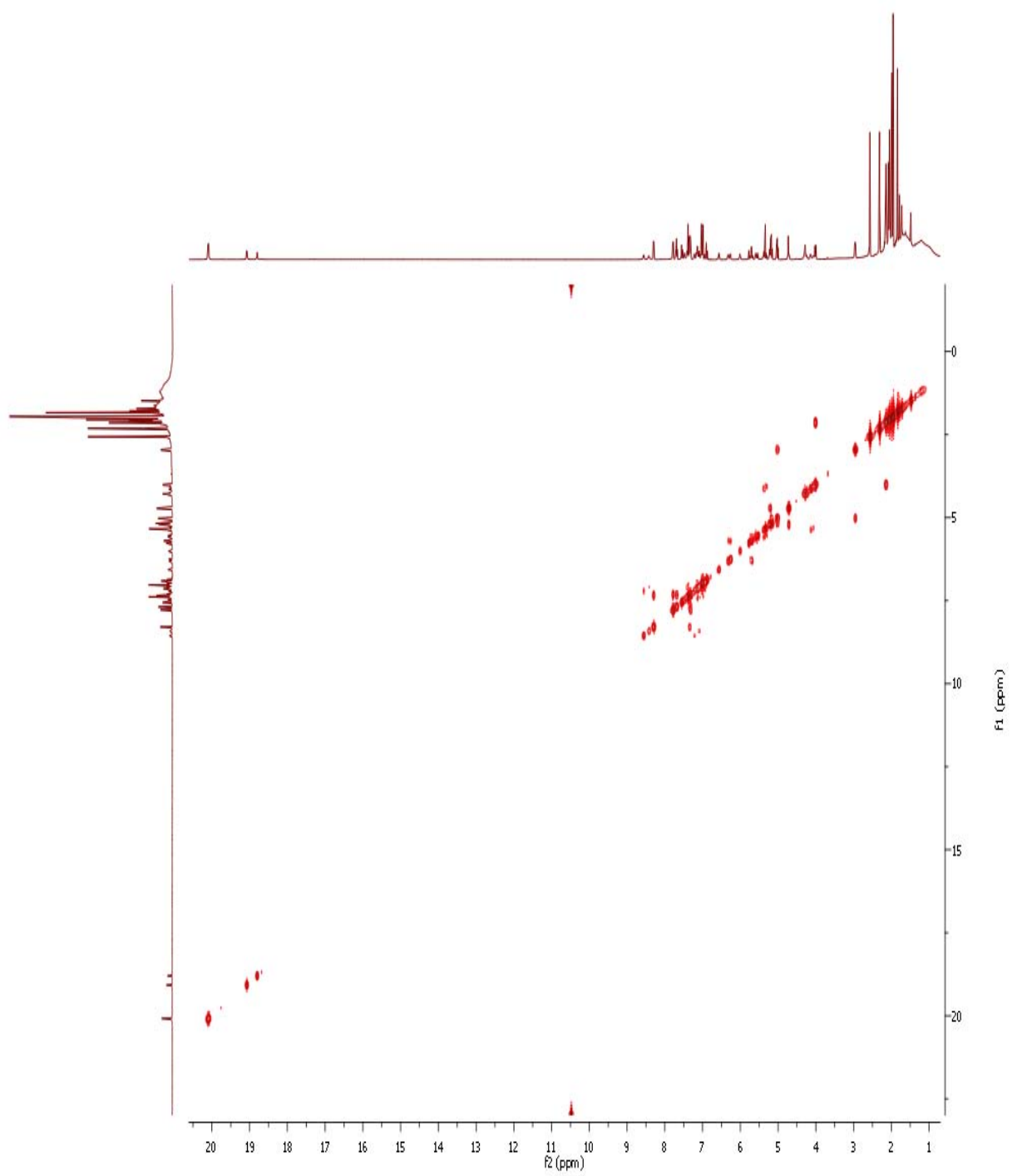


Figure S13. 500 MHz ¹H-¹H gCOSY of **8a** in CH₂Cl₂ at -75°C.

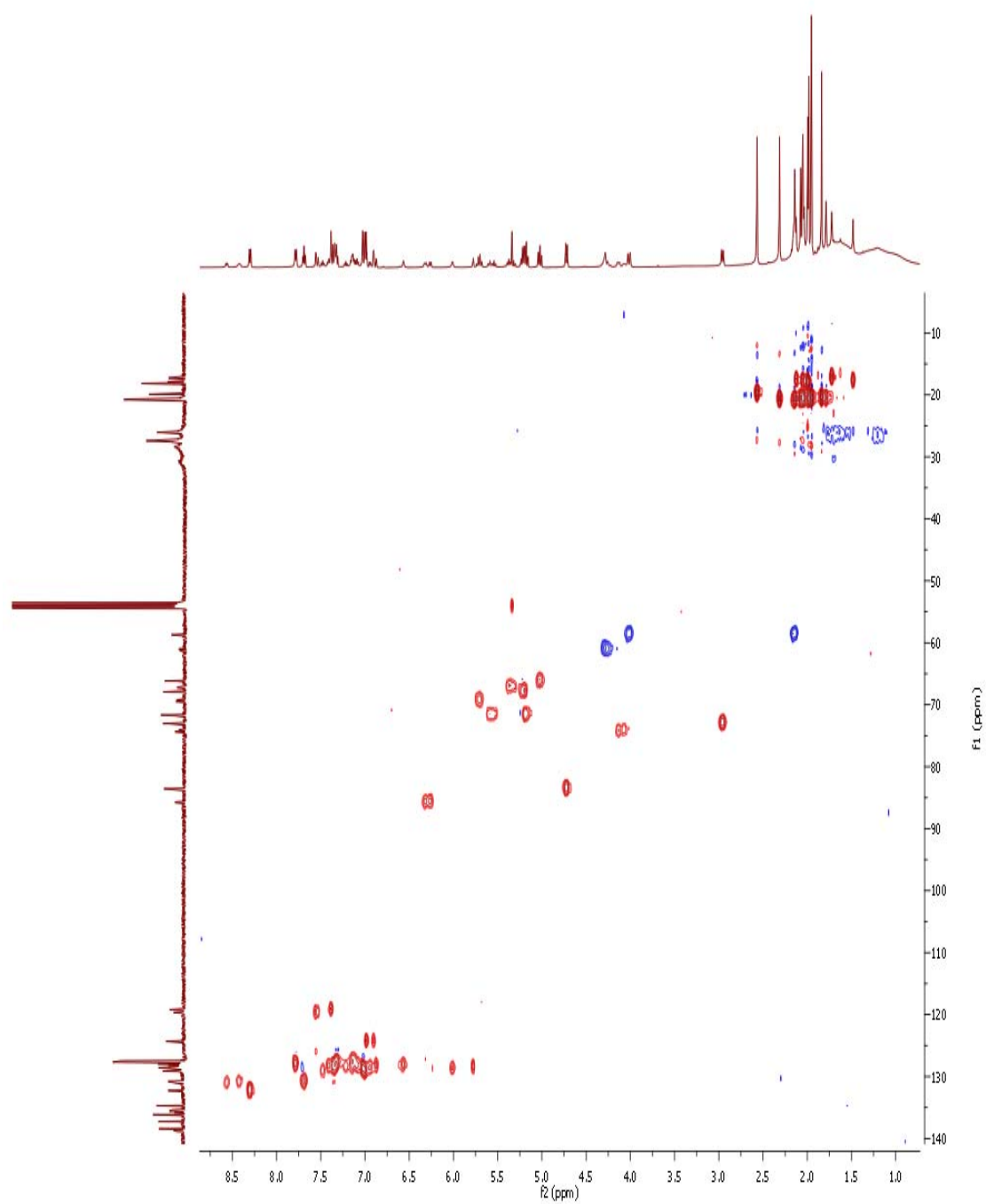


Figure S14. 500 MHz ^1H - ^{13}C gHSQCad spectrum of **8a** in C_6D_6 at -75°C .

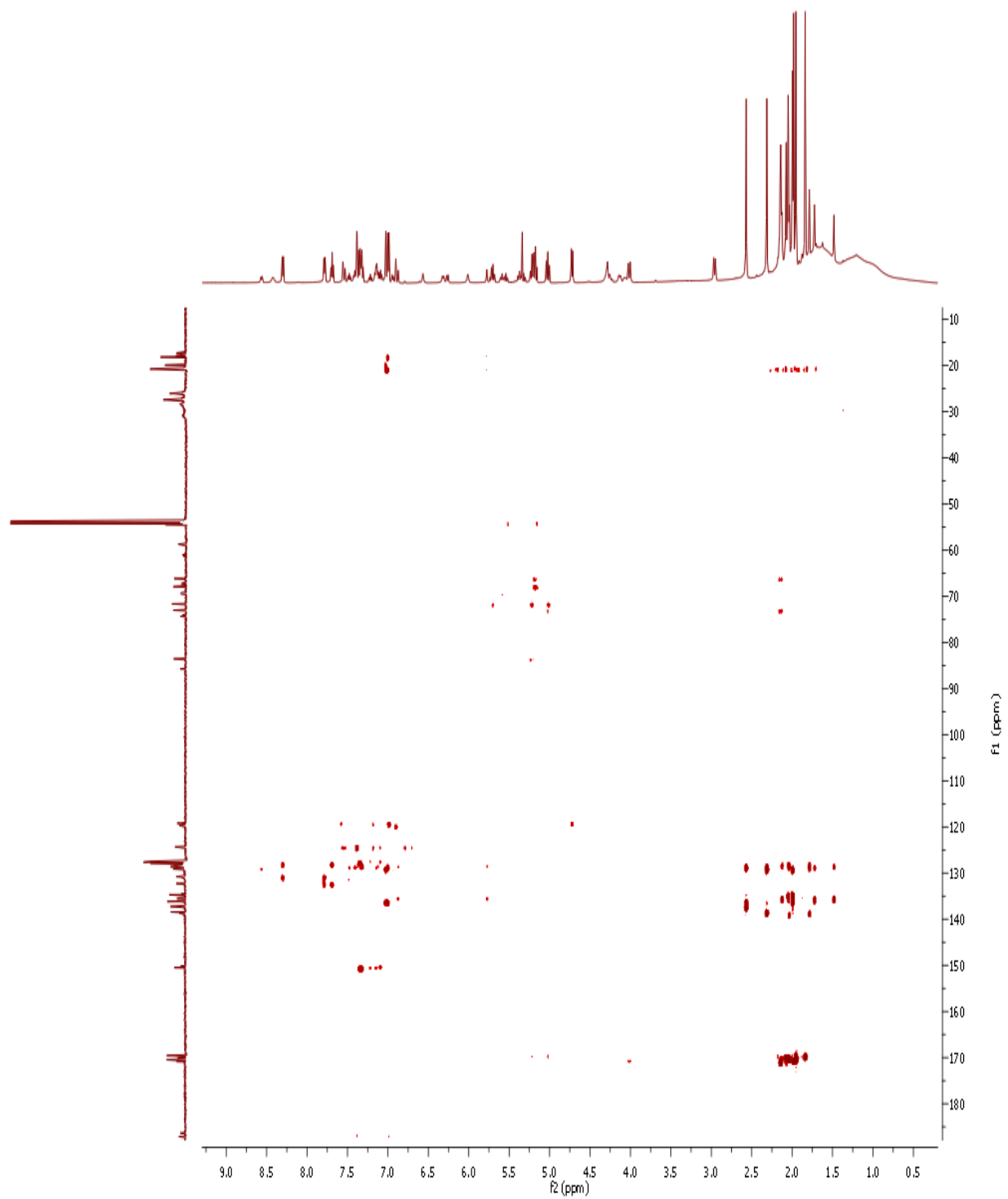


Figure S15. 500 MHz ^1H - ^{13}C gHMBCad spectrum of **8a** in C_6D_6 at -75°C .

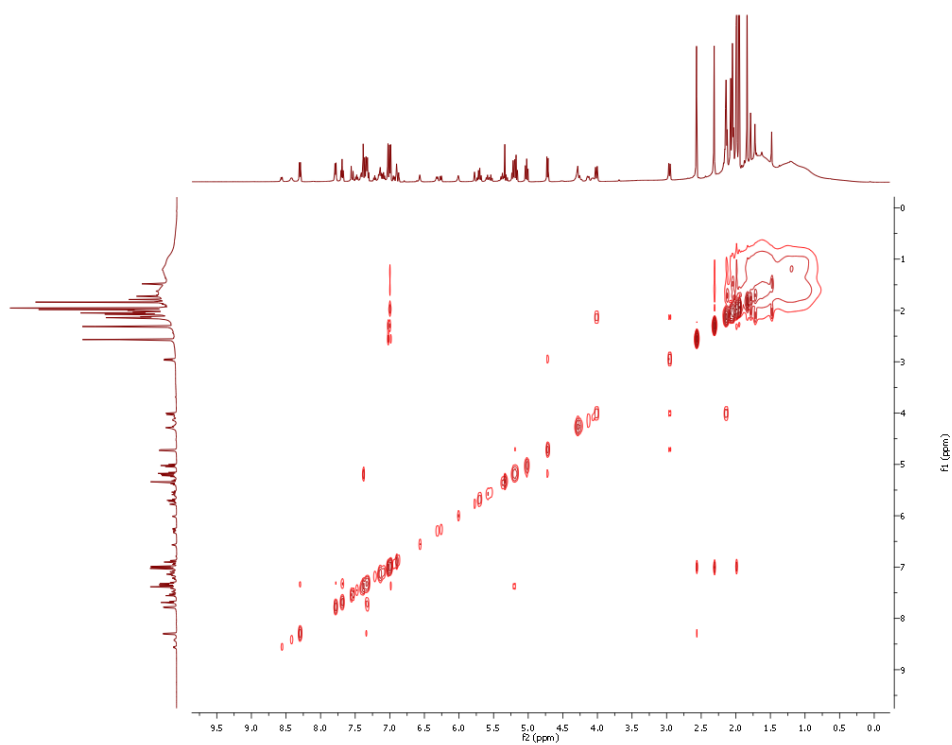


Figure S16. 500 MHz ^1H - ^1H NOESY of **8a** in C_6D_6 at -75°C . Mixing time = 500 ms.

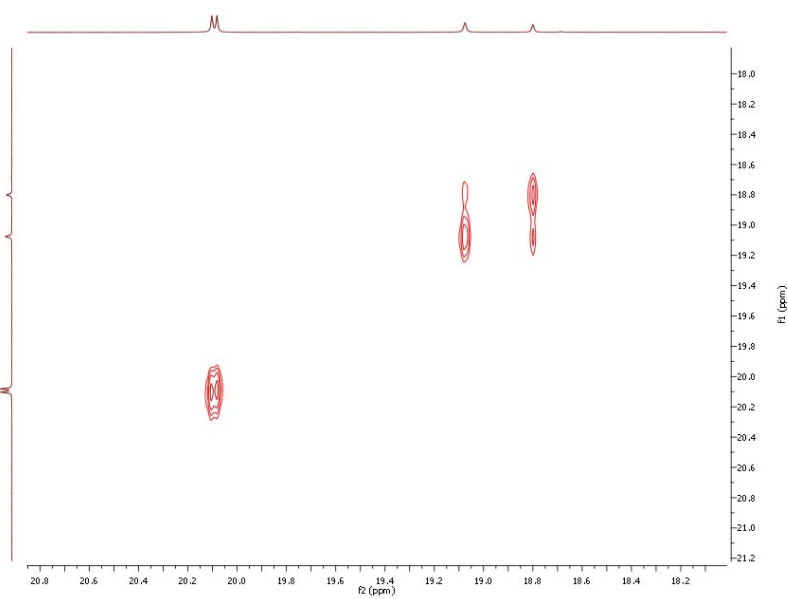


Figure S17. 500 MHz ^1H - ^1H NOESY of **8a** in C_6D_6 at -75°C . Mixing time = 500 ms.

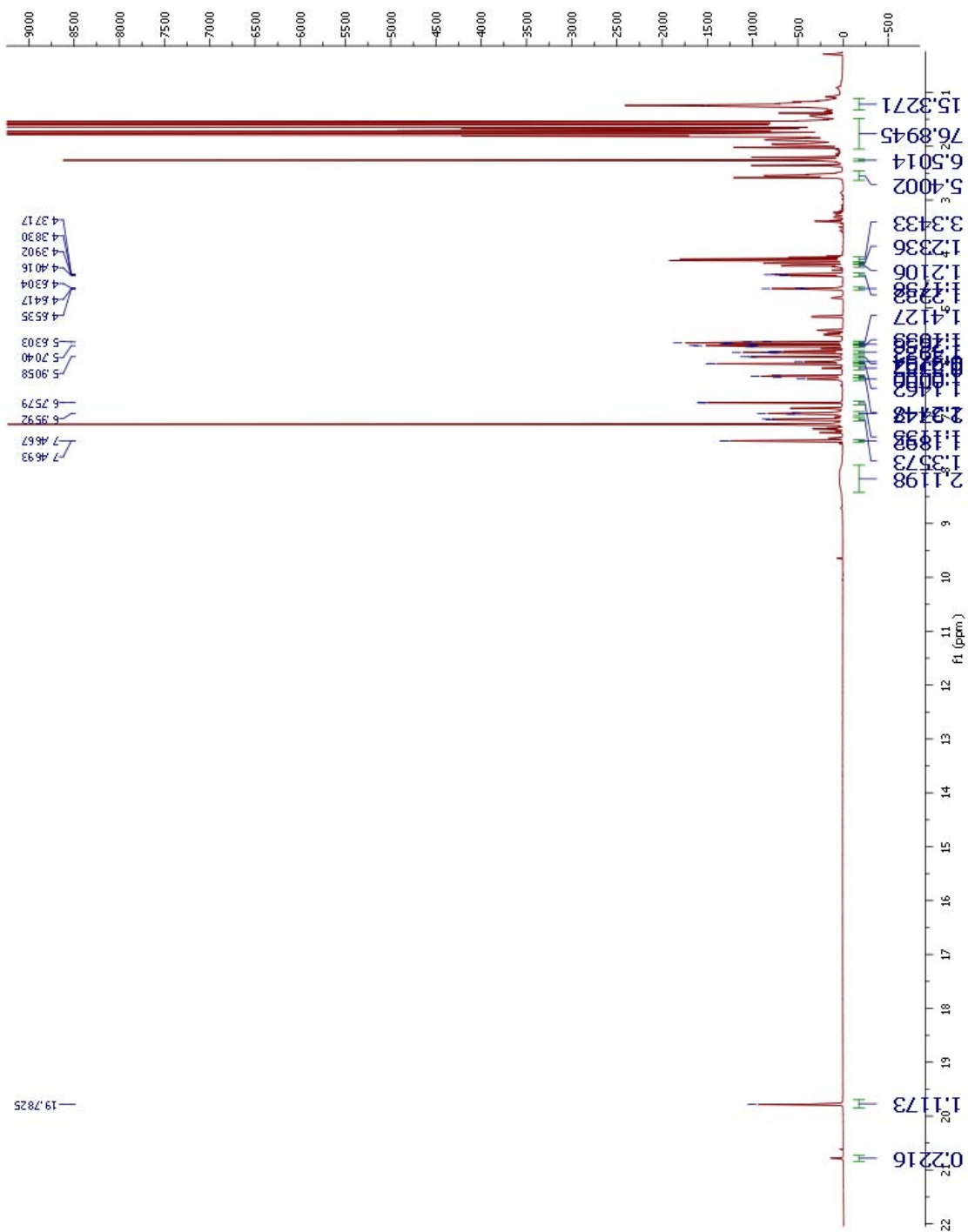
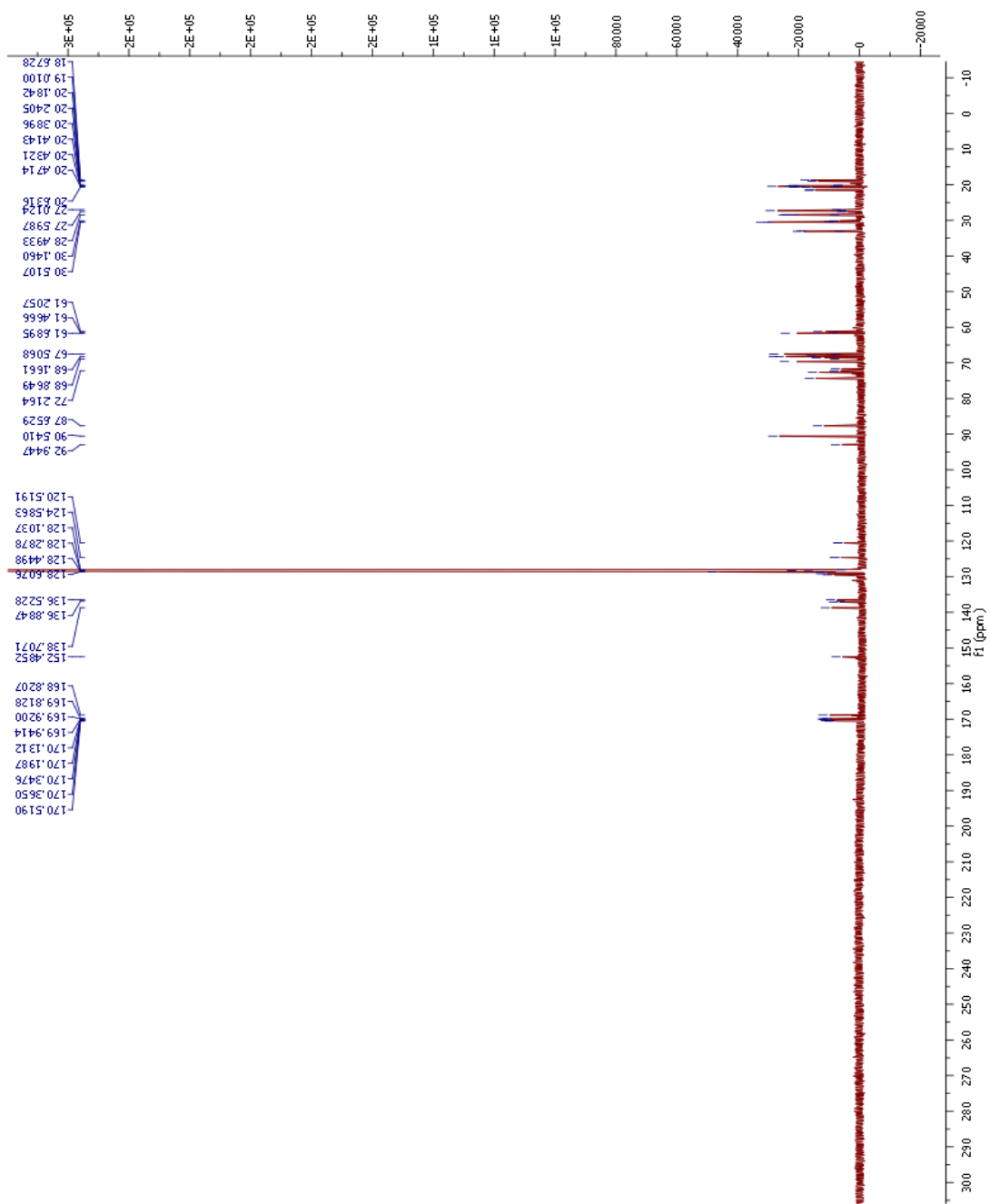


Figure S19. 600 MHz ^1H NMR spectrum of **8b** in C_6D_6 at 25 °C.

Figure S20. ^{13}C NMR spectrum of **8b** in C_6D_6 at 25 $^\circ\text{C}$.



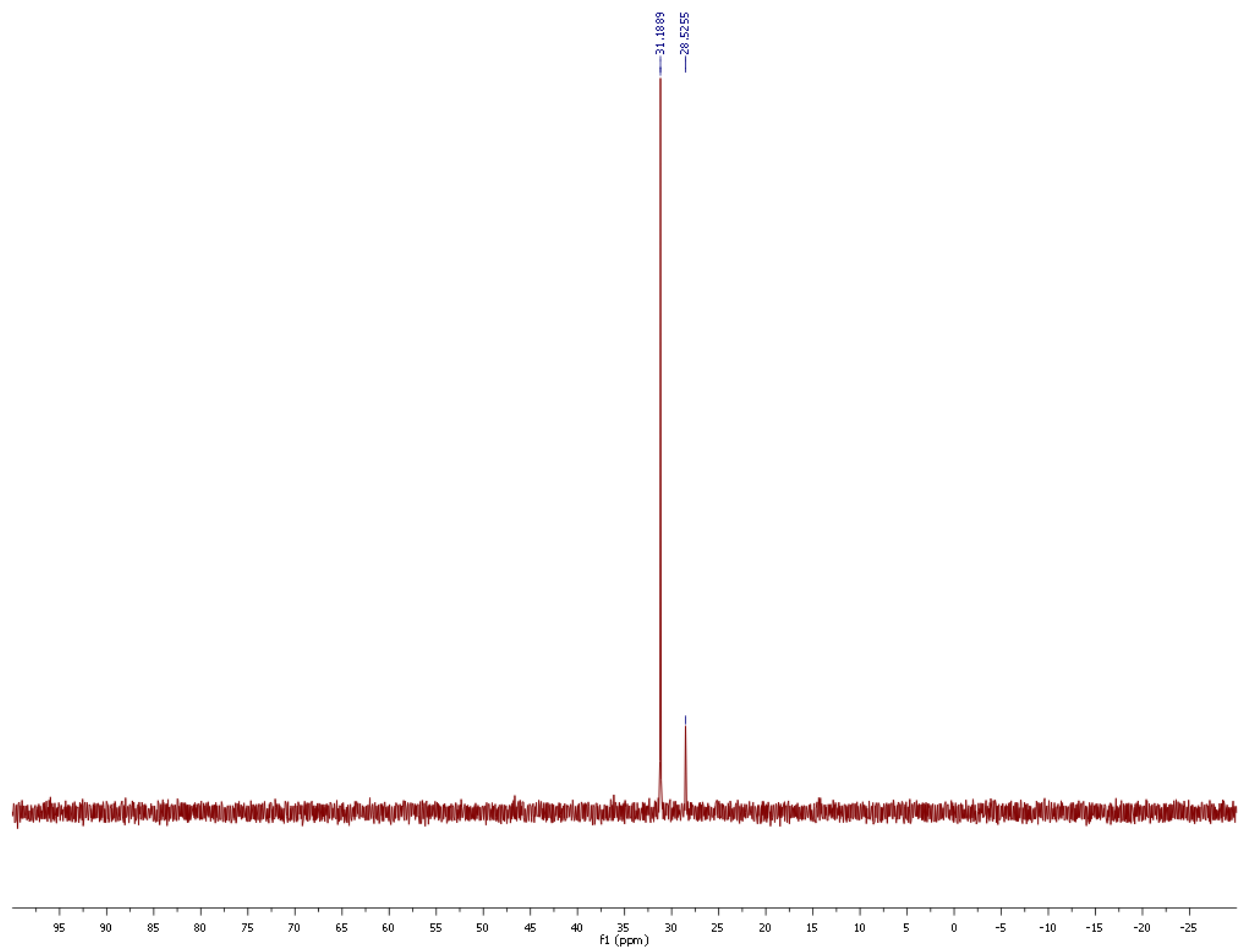


Figure S21. ^{31}P NMR spectrum of **8b** in C_6D_6 at 25 °C.

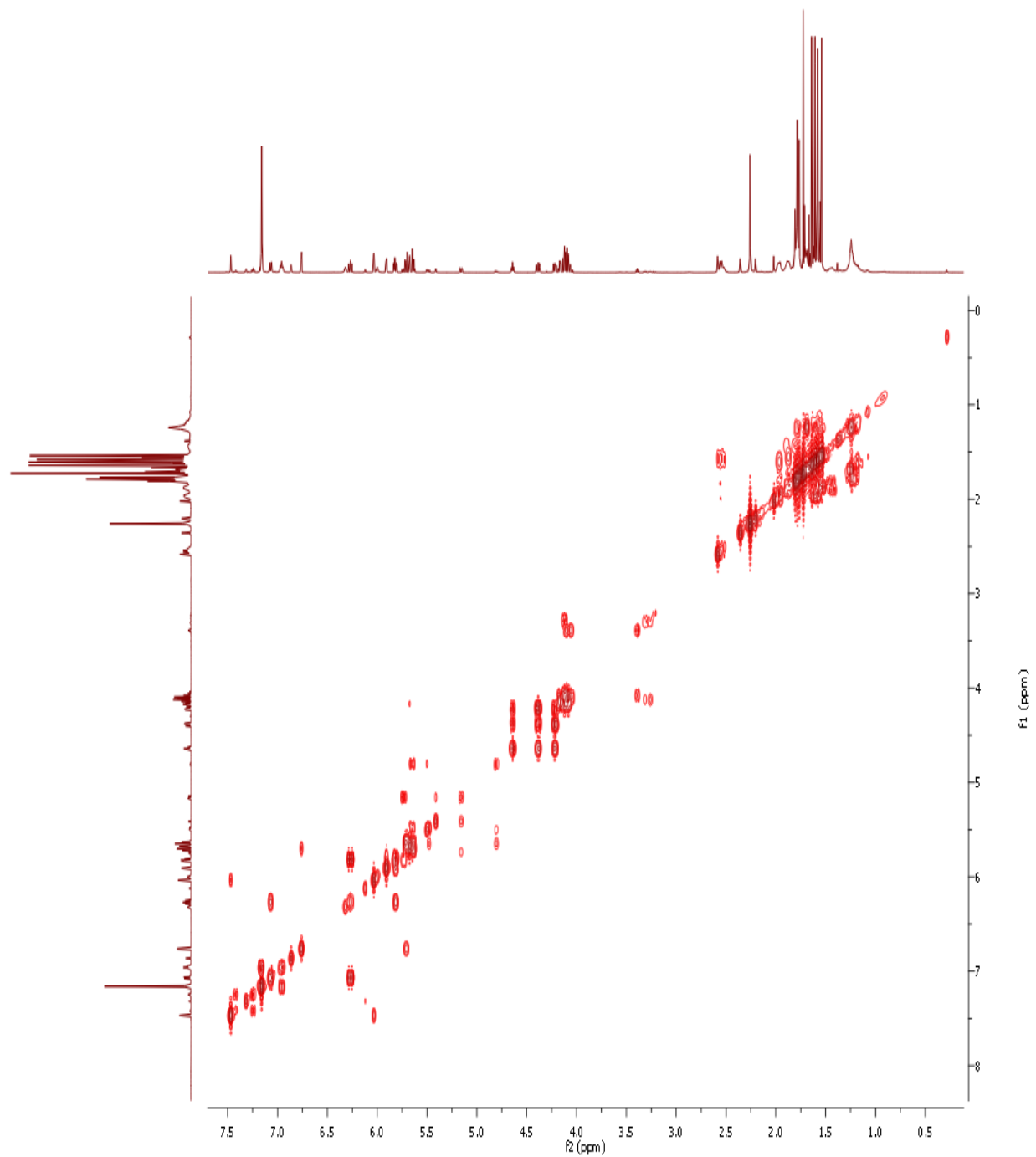


Figure S22. 600 MHz ¹H-¹H gCOSY spectrum of **8b** in C₆D₆ at 25 °C.

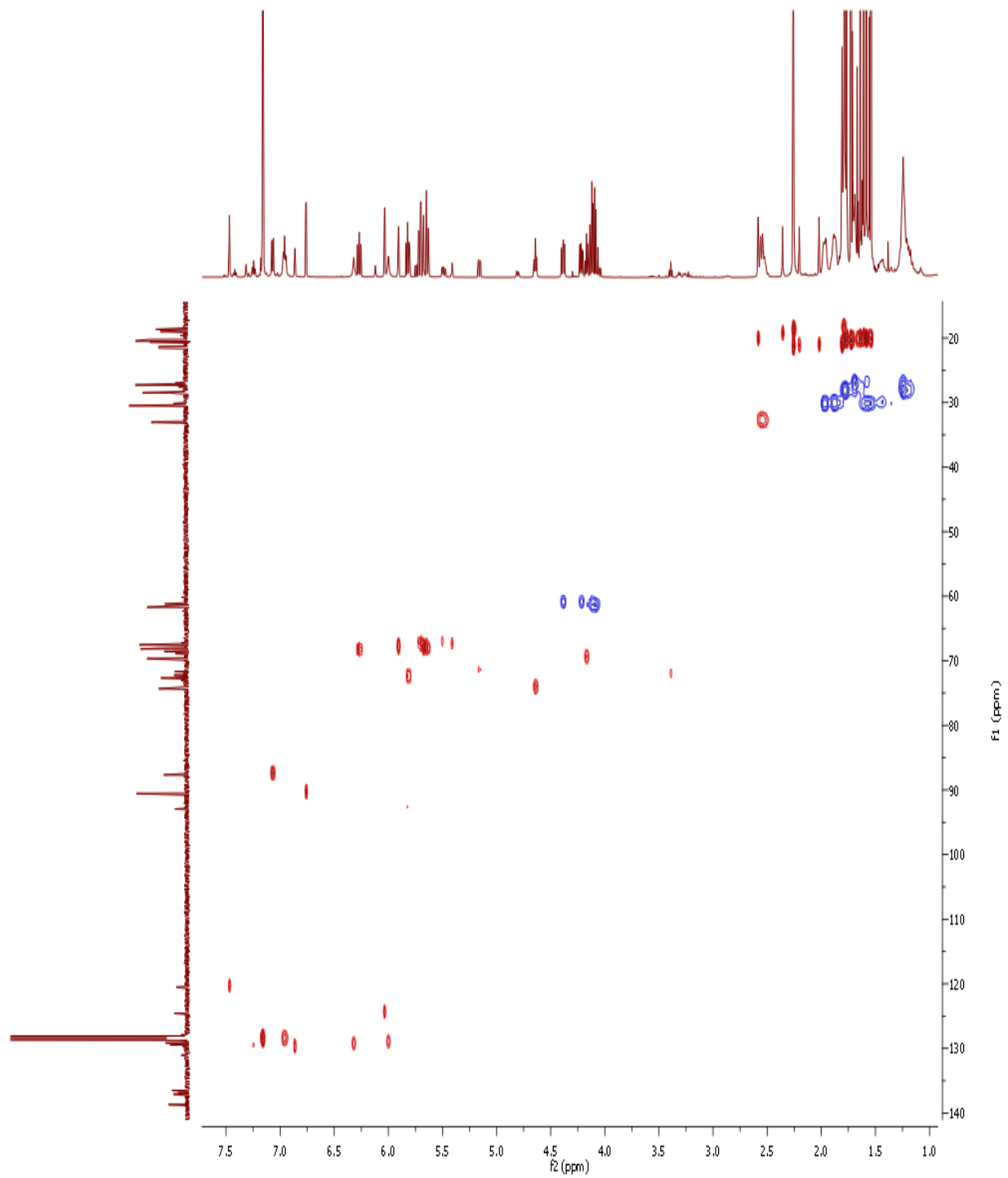


Figure S23. 600 MHz ^1H - ^{13}C gHSQCad spectrum of **8b** in C_6D_6 at 25 °C.

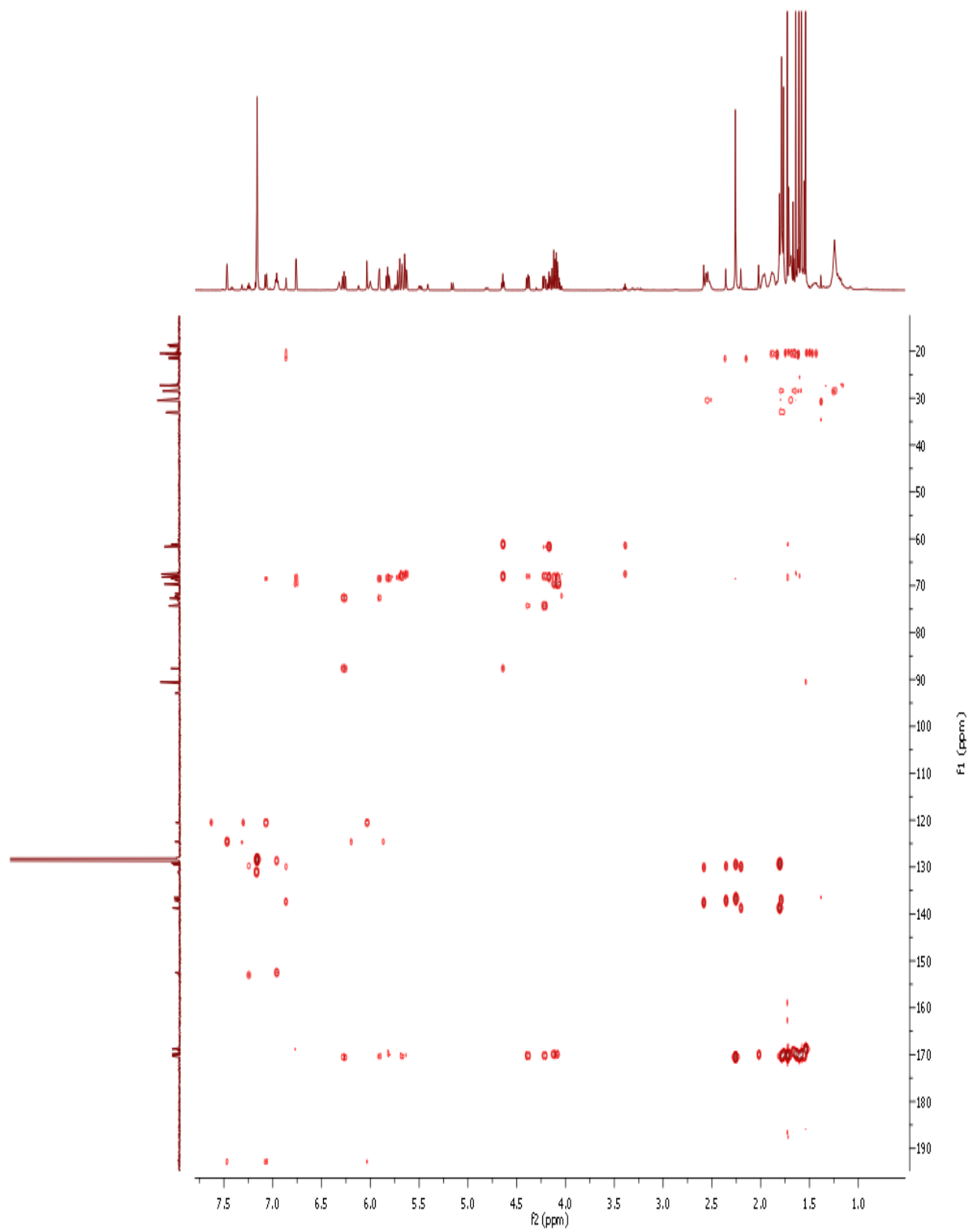


Figure S24. 600 MHz ^1H - ^{13}C gHMBCad spectrum of **8b** in C_6D_6 at 25 °C.

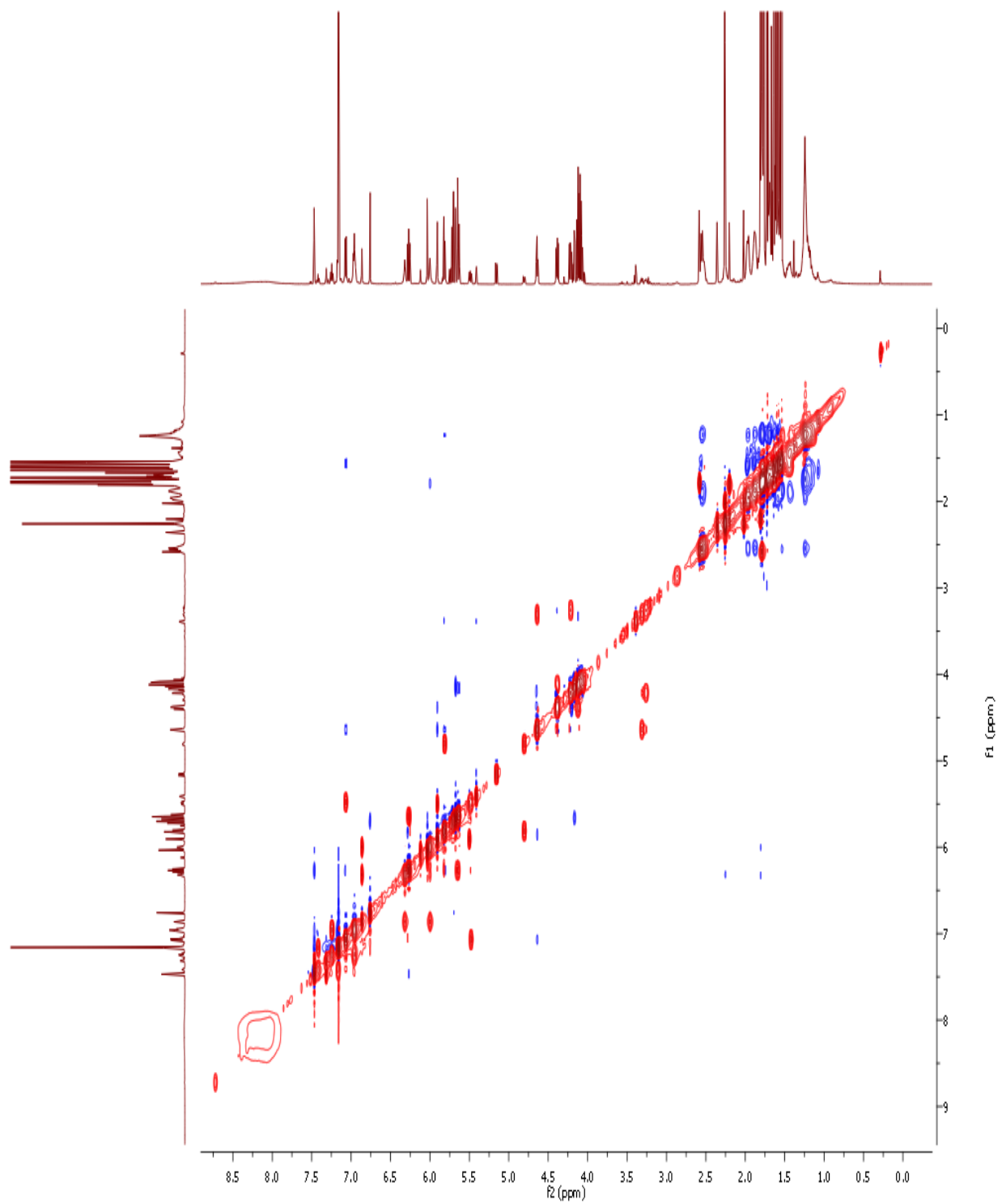


Figure S25. 600 MHz ^1H - ^1H NOESY spectrum of **8b** in C_6D_6 at 25 °C.

Measurement of benzylidene rotation rate based on T₁.

The first method used to measure the rotation rate about the benzylidene C – Ru bond was the spin saturation transfer method. This method entails the observation of one of the sites of an exchanging system while the other site is saturated with a selective inversion pulse. As a result of the chemical exchange, the intensity of the observed peak decreases until a new steady state is reached. The ratio of the intensity of this new steady state resonance to the original peak intensity is related to the T₁ of the observed resonance and the rate of chemical exchange by Eq. 1.⁷

$$M_{zA}(\infty) = M_{0A} \frac{T_A}{\tau_A + T_{1A}} \quad (1)$$

Rearranging Eq. 1 with $k_A = 1/\tau_A$ and $R_A = 1/T_{1A}$ yields Eq. 2.

$$\frac{M_{zA}(\infty)}{M_{0A}} = \frac{R_A}{R_A + k_A} \quad (2)$$

The T₁'s were measured using the inversion recovery method and are shown in Table S1.

Table S1. Measured T₁'s using inversion recovery of **8a** in C₆D₆ at 25°C.

Peak	Shift (ppm)	T ₁ (s)	Error (s)
1	19.74	0.615	0.002
2	20.78	0.569	0.007

The VNMRj PRESAT pulse sequence was used to selectively invert the desired peak and an array of delay times (d1) was set up in order to determine the steady state intensity. A sample calculation is given below.

$$\frac{M_{zA}(\infty)}{M_{0A}} = 0.249 = \frac{1.75}{1.75 + k_A}$$

$$k_A = 5.28 \text{ s}^{-1} \text{ (reported value)}$$

Measurement of benzylidene rotation rate using line shape analysis.

A lineshape analysis of the benzylidene rotation in **8a** was performed in order to obtain a more accurate estimate of ΔG^\ddagger . The coalescence temperature could not be reached due to catalyst decomposition, however, a suitable temperature range from 12.5-73.1 °C was found in which there was no observable catalyst decomposition. To measure the rate of benzylidene rotation, **8a** was dissolved in ca. 0.6 mL of dry C₆D₆ and placed into a J. Young tube inside of a glove box. The tube was sealed and removed from the box and placed inside the spectrometer where it was allowed to equilibrate at the appropriate temperature for ca. 10 min before acquisition. The probe was calibrated at each temperature according to the method described in the **General Information**. Each experiment was run with ³¹P decoupling in order to simplify the line shape analysis of the resulting spectrum. These spectra, along with the overlaid fits, are shown in Figure S25. Experimental spectra were simulated using the MEXICO set of programs developed by Professor Alex Bain.⁸ The non-iterative version of MEXICO was used through the SpinWorks (Ver. 3) NMR program which overlays the MEXICO simulation with the experimental spectrum and calculates an RMS value immediately.⁹ Table S2 summarizes the fit parameters and results from each simulation.

Table S2. Simulation parameters and results from manual MEXICO fitting.

Number	$\delta 1$ (ppm)	$\delta 2$ (ppm)	Temp (K)	Pop. 1	Pop. 2	T1 (s)	k (s ⁻¹)	R ²
1	19.7429	20.7398	285.5	1	0.221	0.075	0.4	0.016869
2	19.7573	20.7604	295.3	1	0.2227	0.1	0.91	0.014485
3	19.7714	20.7793	305.3	1	0.2491	0.125	1.6	0.016267
4	19.786	20.7987	315.4	1	0.2347	0.15	4.3	0.021245
5	19.8006	20.8163	325.1	1	0.2575	0.175	11	0.03155
6	19.815	20.8333	335.9	1	0.3759	0.2	24.5	0.035247
7	19.8301	20.8387	346.1	1	0.2575	0.225	75	0.132513

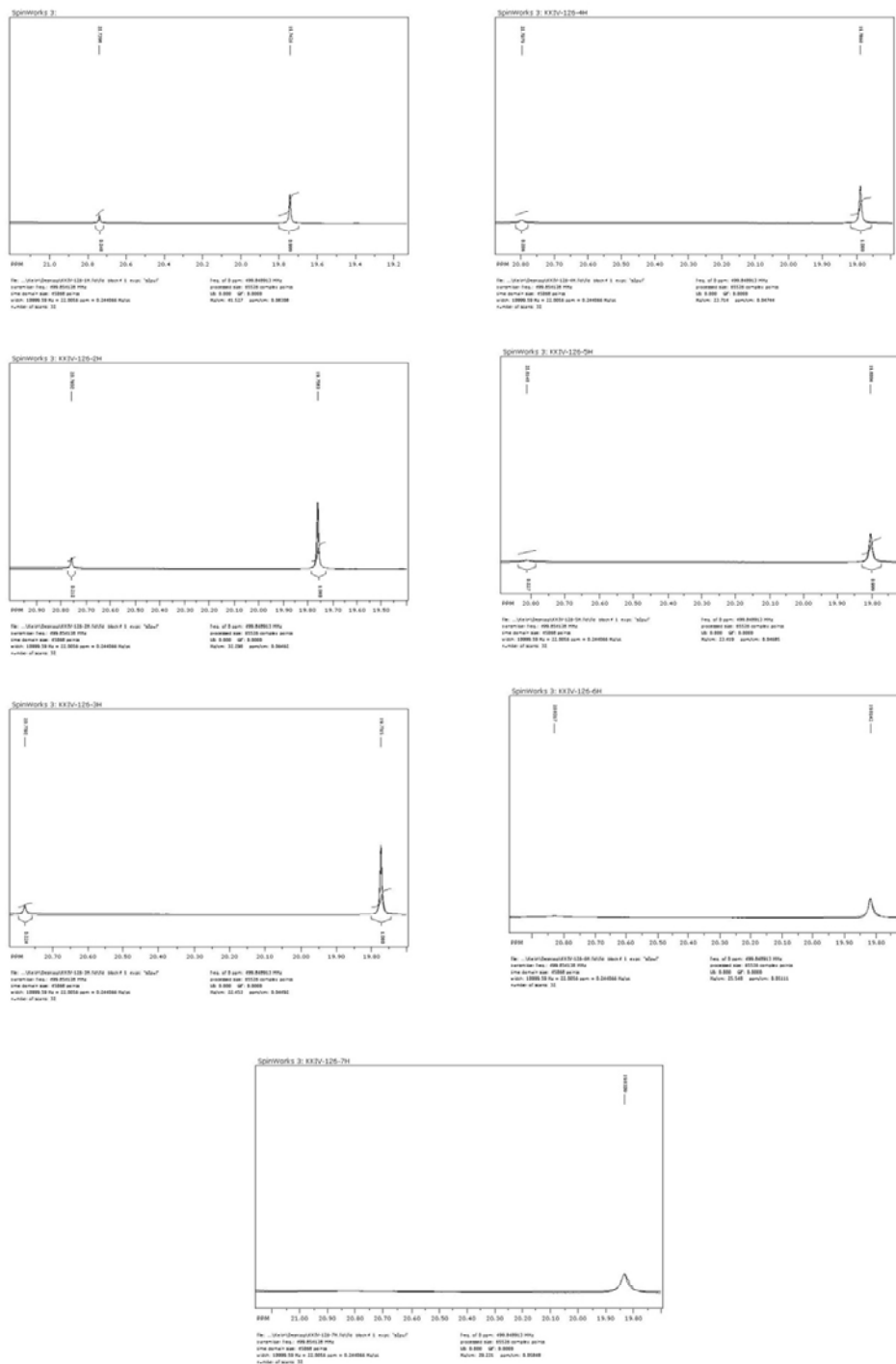


Figure S26. Experimental spectra and MEXICO fits of the benzylidene region of **8a** in C₆D₆ at temperatures ranging from 285.5 K to 346.1 K.

Eyring Plots and Error Analysis

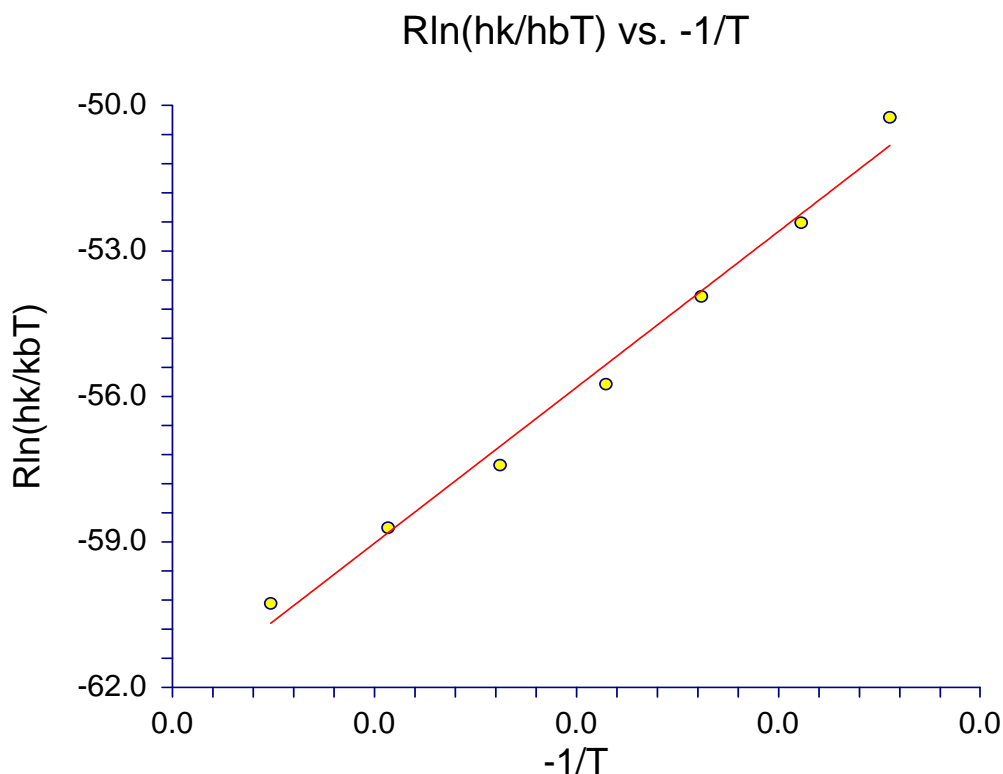
According to the Activated Complex Theory of Henry Eyring,

$$k = \left(\frac{k_B T}{h} e^{\Delta S^\ddagger / R} \right) e^{-\Delta H^\ddagger / RT} \quad (3)$$

where k is the rate in s^{-1} , k_B is Boltzmann's constant, h is Planck's constant, R is the gas constant, and T is the temperature in Kelvin. Eq. 3 can be re-worked to yield a linear equation which gives ΔH^\ddagger as the slope and ΔS^\ddagger as the intercept (Eq. 4).

$$R \ln \frac{hk}{k_B T} = \Delta S^\ddagger + \left(\frac{1}{T} \right) \Delta H^\ddagger \quad (4)$$

The uncertainty in the slope and intercept was determined directly from the output provided by the linear regression function of the NCSS statistical software package (shown below).¹⁰



Run Summary Section

Parameter	Value	Parameter	Value
Dependent Variable	C2	Rows Processed	7
Independent Variable	C1	Rows Used in Estimation	7

Frequency Variable	None	Rows with X Missing	0
Weight Variable	None	Rows with Freq Missing	0
Intercept	-4.4239	Rows Prediction Only	0
Slope	16060.7710	Sum of Frequencies	7
R-Squared	0.9885	Sum of Weights	7.0000
Correlation	0.9943	Coefficient of Variation	-0.0075
Mean Square Error	0.1747487	Square Root of MSE	0.4180296

Descriptive Statistics Section

Parameter	Dependent	Independent
Variable	C2	C1
Count	7	7
Mean	-55.5371	-0.0032
Standard Deviation	3.5655	0.0002
Minimum	-60.2700	-0.0035
Maximum	-50.2500	-0.0029

Regression Estimation Section

Parameter	Intercept B(0)	Slope B(1)
Regression Coefficients	-4.4239	16060.7710
Lower 95% Confidence Limit	-10.7621	14073.2819
Upper 95% Confidence Limit	1.9143	18048.2602
Standard Error	2.4657	773.1670
Standardized Coefficient	0.0000	0.9943
T Value	-1.7942	20.7727
Prob Level (T Test)	0.1327	0.0000
Reject H0 (Alpha = 0.0500)	No	Yes
Power (Alpha = 0.0500)	0.3086	1.0000
Regression of Y on X	-4.4239	16060.7710
Inverse Regression from X on Y	-3.8316	16246.8727
Orthogonal Regression of Y and X	-3.8316	16246.8727

Estimated Model

$(-4.42385374824523) + (16060.7710380801) * (C1)$

Correlation and R-Squared Section

Parameter	Pearson Correlation Coefficient	R-Squared	Spearman Rank Correlation Coefficient
Estimated Value	0.9943	0.9885	1.0000
Lower 95% Conf. Limit (r dist'n)	0.9532		
Upper 95% Conf. Limit (r dist'n)	0.9989		
Lower 95% Conf. Limit (Fisher's z)	0.9599		1.0000
Upper 95% Conf. Limit (Fisher's z)	0.9992		1.0000
Adjusted (Rbar)		0.9863	
T-Value for H0: Rho = 0	20.7727	20.7727	
Prob Level for H0: Rho = 0	0.0000	0.0000	0.0000

Analysis of Variance Section

Source	DF	Sum of Squares	Mean Square	F-Ratio	Prob Level	Power (5%)
Intercept	1	21590.62	21590.62			

Slope	1	75.405	75.405	431.5053	0.0000	1.0000
Error	5	0.8737436	0.1747487			
Adj. Total	6	76.27874	12.71312			
Total	7	21666.9				

$s = \text{Square Root}(0.1747487) = 0.4180296$

Summary Matrices

	X'X	X'X	X'Y	X'X Inverse	X'X Inverse
Index	0	1	2	0	1
0	7	-2.227745E-02	-388.76	34.79001	10886.8
1	-2.227745E-02	7.119015E-05	1.241921	10886.8	3420839
2 (Y'Y)			21666.9		
Determinant		2.046282E-06			488691.3

Variance - Covariance Matrix of Regression Coefficients

	VC(b)	VC(b)
Index	0	1
0	6.079509	1902.454
1	1902.454	597787.3

Tests of Assumptions Section

Assumption/Test	Test Value	Prob Level	Is the Assumption Reasonable at the 0.2000 Level of Significance?
Residuals follow Normal Distribution?			
Shapiro Wilk	0.9158	0.437789	Yes
Anderson Darling	0.3309	0.513157	Yes
D'Agostino Skewness	0.0000		
D'Agostino Kurtosis		1.000000	Yes
D'Agostino Omnibus			
Constant Residual Variance?			
Modified Levene Test	0.1252	0.737872	Yes
Relationship is a Straight Line?			
Lack of Linear Fit F(0, 0) Test	0.0000	0.000000	No

The uncertainty in ΔG^\ddagger was calculated using the error in the slope, intercept, and the off-diagonal component of the variance-covariance matrix (because ΔH^\ddagger and ΔS^\ddagger are correlated) created by NCSS.¹¹

Measurement of NHC rotation rate using line shape analysis.

The general procedure for the line shape analysis of the benzylidene rotation was followed with the exception of substituting CD_2Cl_2 for C_6D_6 .

Table S3. Simulation parameters and results from manual MEXICO fitting.

Number	δ_1 (ppm)	δ_2 (ppm)	Temp (K)	Pop. 1	Pop. 2	T1 (s)	k (s^{-1})	R2
1	19.0408	18.7754	199.3	1	0.82	0.04	0.004	0.028476
2	19.0854	18.8064	206.8	1	0.73	0.05	0.01	0.017213
3	19.172	18.8741	223.5	1	0.6	0.04	1.35	0.018617
4	19.2137	18.9127	234.6	1	0.65	0.04	29	0.044761
5	19.2401	18.954	241.8	1	0.7	0.03	75	0.09729
6	19.0408	18.7754	272	1	0.65	0.04	1454	0.016645

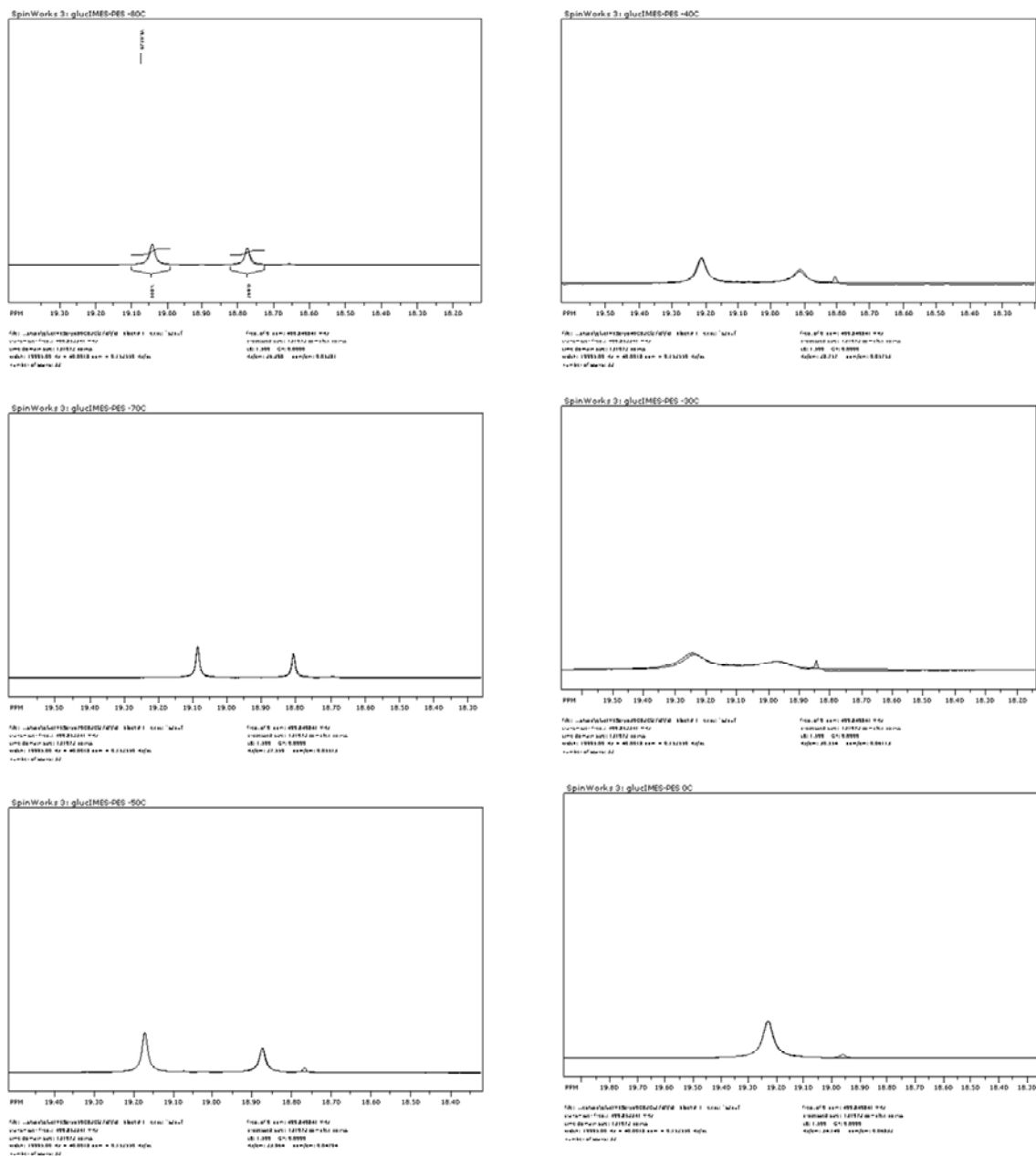
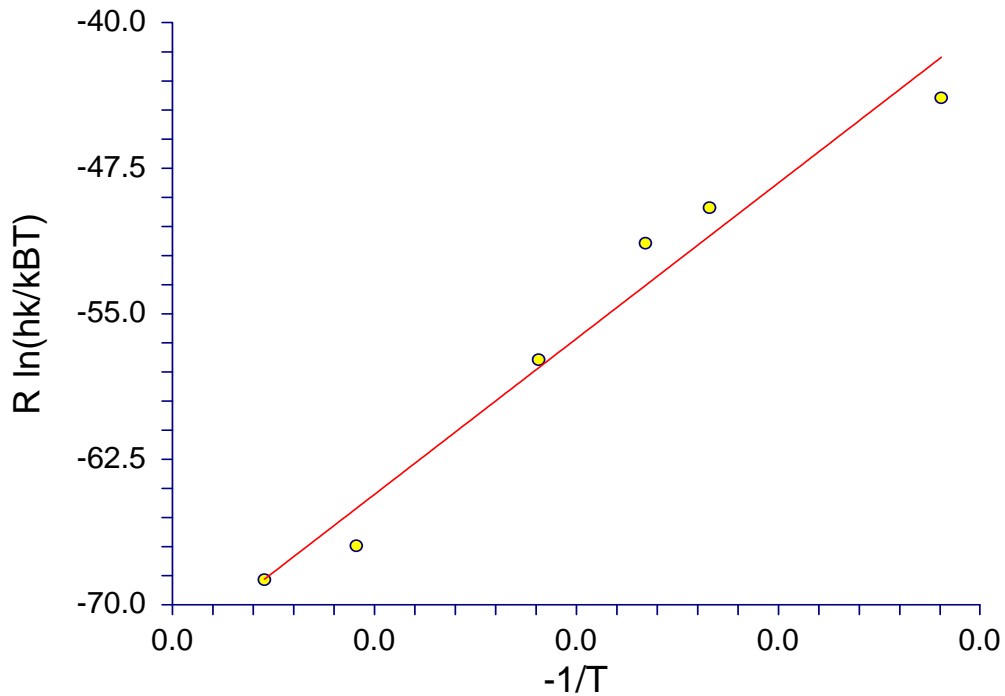


Figure S27. Experimental spectra and MEXICO fits of the benzylidene region of **8a** in CD_2Cl_2 at temperatures ranging from 199.3 K to 272 K.

Rln(hk/kBT) vs. -1/T



Run Summary Section

Parameter	Value	Parameter	Value
Dependent Variable	C2	Rows Processed	6
Independent Variable	C1	Rows Used in Estimation	6
Frequency Variable	None	Rows with X Missing	0
Weight Variable	None	Rows with Freq Missing	0
Intercept	31.9226	Rows Prediction Only	0
Slope	20050.1186	Sum of Frequencies	6
R-Squared	0.9694	Sum of Weights	6.0000
Correlation	0.9846	Coefficient of Variation	-0.0345
Mean Square Error	3.775506	Square Root of MSE	1.943066

Descriptive Statistics Section

Parameter	Dependent	Independent
Variable	C2	C1
Count	6	6
Mean	-56.3050	-0.0044
Standard Deviation	9.9302	0.0005
Minimum	-68.7100	-0.0050
Maximum	-43.8800	-0.0037

Regression Estimation Section

Intercept	Slope
31.9226	20050.1186

Parameter	B(0)	B(1)
Regression Coefficients	31.9226	20050.1186
Lower 95% Confidence Limit	10.0398	15102.4055
Upper 95% Confidence Limit	53.8054	24997.8317
Standard Error	7.8816	1782.0317
Standardized Coefficient	0.0000	0.9846
T Value	4.0503	11.2513
Prob Level (T Test)	0.0155	0.0004
Reject H0 (Alpha = 0.0500)	Yes	Yes
Power (Alpha = 0.0500)	0.8515	1.0000
Regression of Y on X	31.9226	20050.1186
Inverse Regression from X on Y	34.7104	20683.6584
Orthogonal Regression of Y and X	34.7104	20683.6584

Notes:

The above report shows the least-squares estimates of the intercept and slope followed by the corresponding standard errors, confidence intervals, and hypothesis tests. Note that these results are based on several assumptions that should be validated before they are used.

Estimated Model

$$(31.9226028569538) + (20050.1185962279) * (C1)$$

Analysis of Variance Section

Source	DF	Sum of Squares	Mean Square	F-Ratio	Prob Level	Power (5%)
Intercept	1	19021.52	19021.52			
Slope	1	477.9453	477.9453	126.5911	0.0004	1.0000
Error	4	15.10202	3.775506			
Adj. Total	5	493.0474	98.60947			
Total	6	19514.57				

$$s = \text{Square Root}(3.775506) = 1.943066$$

Notes:

The above report shows the F-Ratio for testing whether the slope is zero, the degrees of freedom, and the mean square error. The mean square error, which estimates the variance of the residuals, is used extensively in the calculation of hypothesis tests and confidence intervals.

Tests of Assumptions Section

Assumption/Test	Test Value	Prob Level	Is the Assumption Reasonable at the 0.2000 Level of Significance?
Residuals follow Normal Distribution?			
Shapiro Wilk	0.9212	0.514354	Yes
Anderson Darling	0.3146	0.544607	Yes
D'Agostino Skewness	0.0000		
D'Agostino Kurtosis		1.000000	Yes
D'Agostino Omnibus			
Constant Residual Variance?			
Modified Levene Test	0.2717	0.629714	Yes

Relationship is a Straight Line?

Lack of Linear Fit F(0, 0) Test 0.0000 0.000000 No

$\Delta H^\ddagger = 20.1 \pm 1.8 \text{ kcal/mol}$ (reported value)

$\Delta S^\ddagger = 31.9 \pm 7.9 \text{ e.u.}$ (reported value)

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