Supporting Information

for

Control over cyclisation sequences of 1,1'-bifunctional octamethylferrocenes to ferrocenophanes

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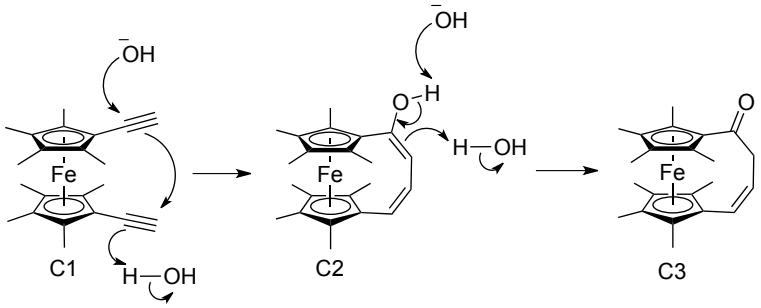


Scheme S1. Alternative mechanism for formation of compound **3** by cyclisation of 1,1'-bis(alkyne)octamethylferrocene.

Table S1. Calculated reaction energies for pathway according Scheme S1 at 333.15 K.

Transformation	**ΔH [kJ/mol]**	**ΔG [kJ/mol]**
Elimination of HCl	+91	+38
C1 → C2	-242	-168
C2 → C2	-54	-54

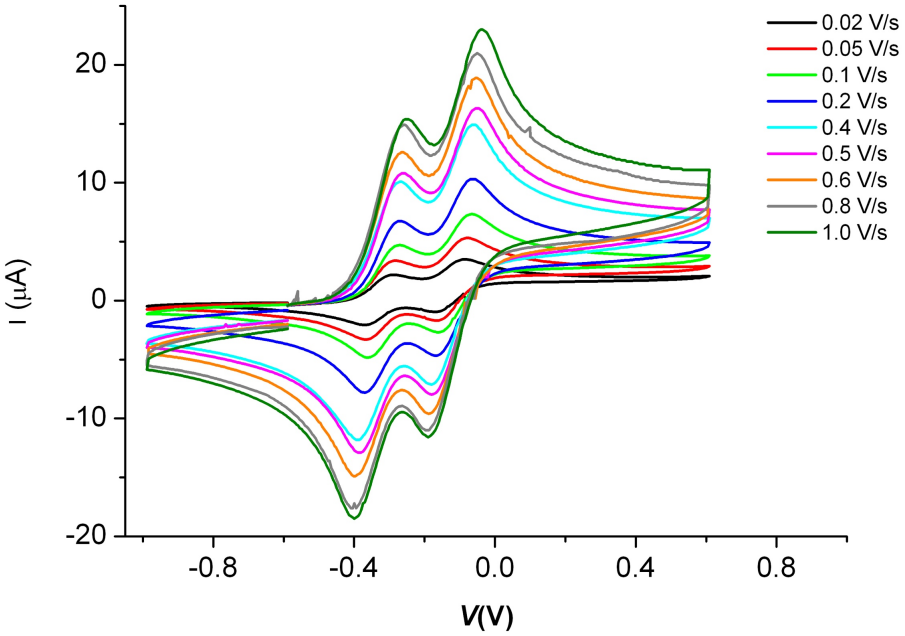


Figure S1. Scan rate dependent cyclic voltammograms of the mixture of *cis*/*trans*-**5** in 0.1 M solutions of Bu_4NPF_6 as supporting electrolyte. Analyte concentration: 1 mM.

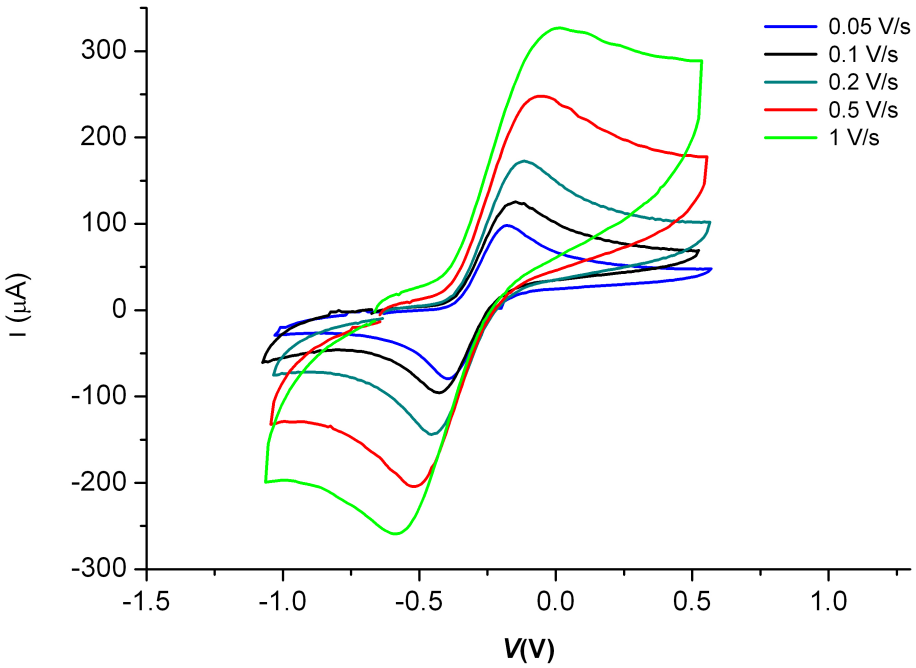


Figure S2. Scan rate dependent cyclic voltammograms of ferrocenophane **3** in 0.1 M solutions of Bu_4NPF_6 as supporting electrolyte. Analyte concentration: 3 mM.

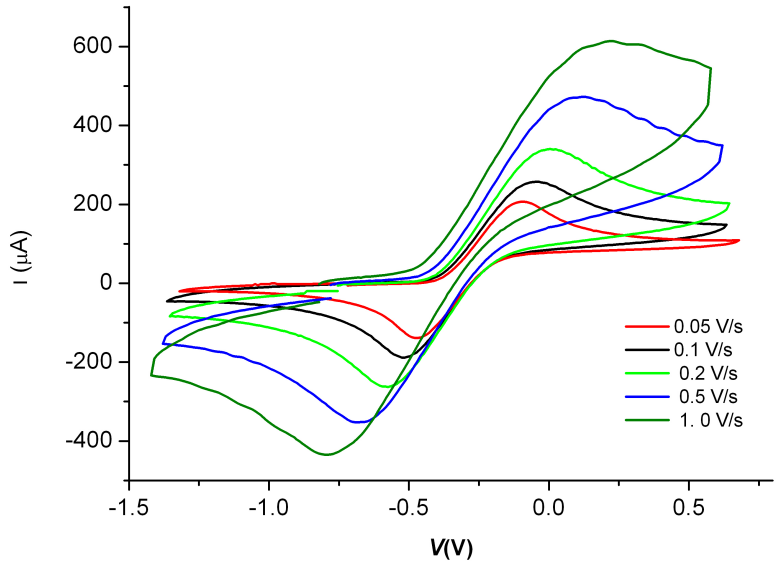


Figure S3. Scan rate dependent cyclic voltammogram of ferrocenophane **3** in 0.1 M solutions of Bu_4NPF_6 as supporting electrolyte. Analyte concentration: 6 mM.

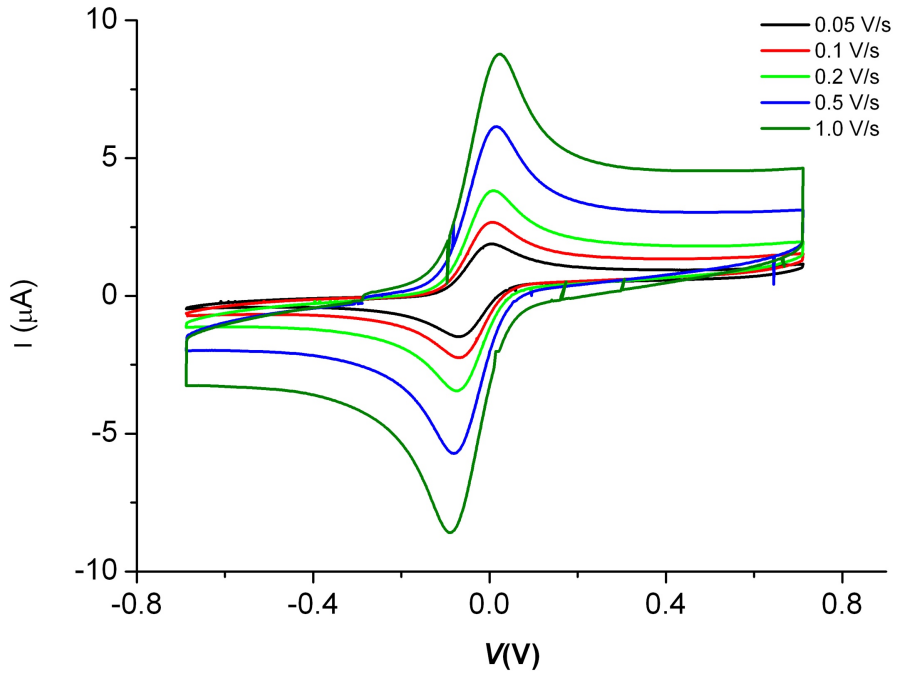


Figure S4. Scanrate dependent cyclic voltammograms of ferrocenophane **6** in 0.1 M solutions of Bu_4NPF_6 as supporting electrolyte. Analyte concentration: 1 mM.

7. ^{1}H and ^{13}C NMR spectra

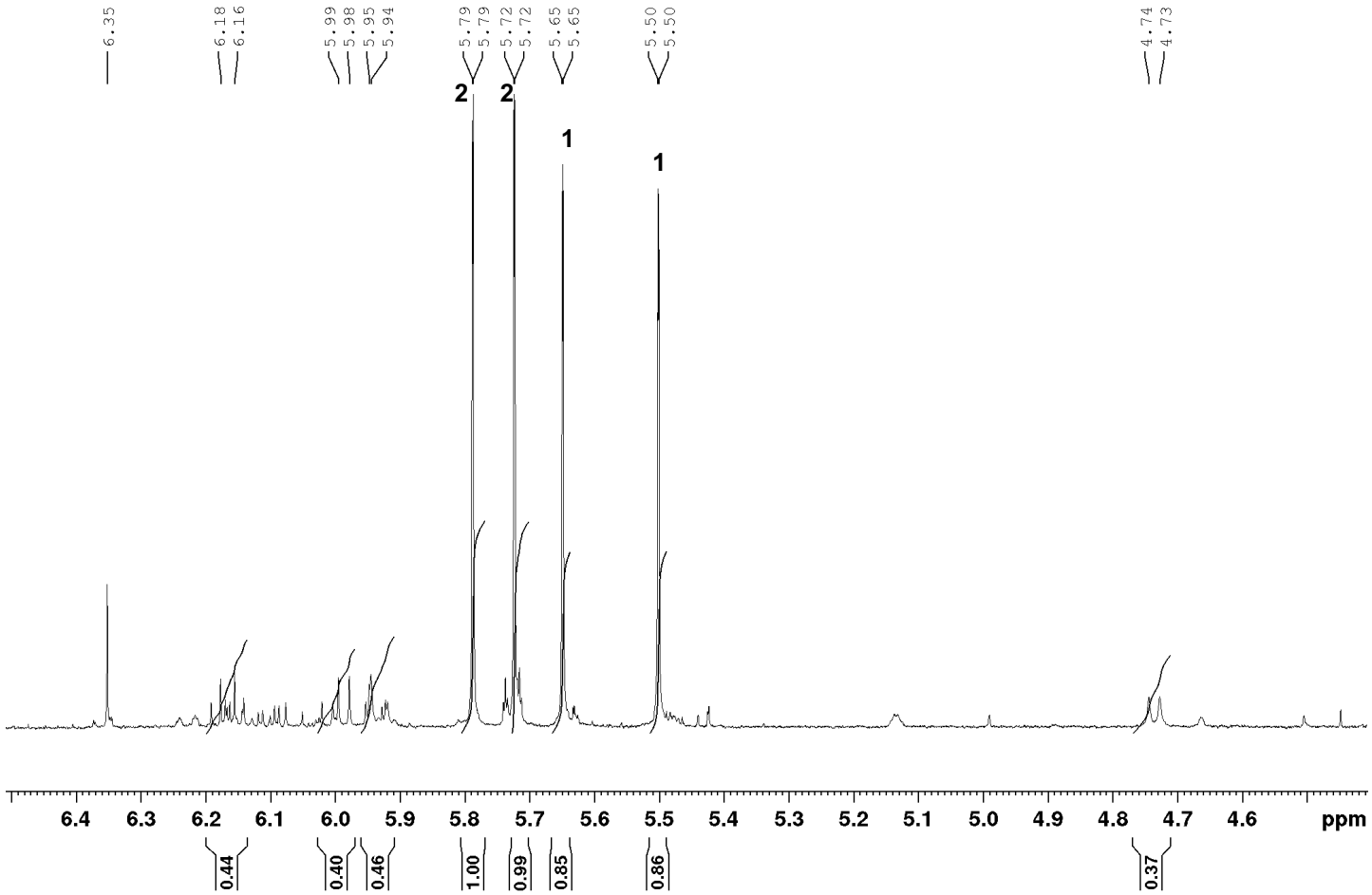


Figure S5. Selected range of the ^{1}H NMR spectrum (500 MHz) in C_6D_6 after aqueous work-up of experiment A.

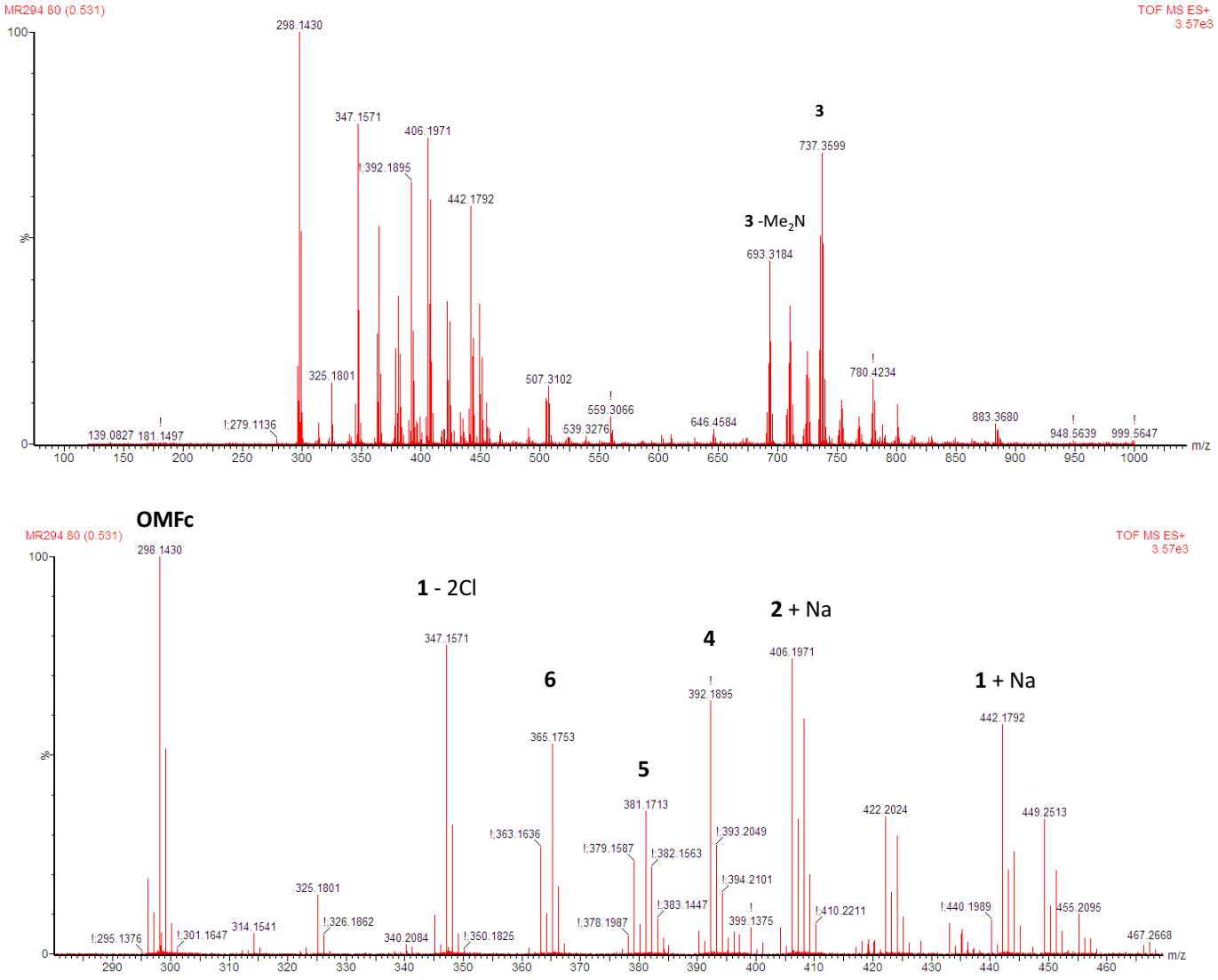


Figure S6. Mass spectrum (ESI+) of the complex mixture obtained from experiment A; **OMFc** = octamethylferrocene.

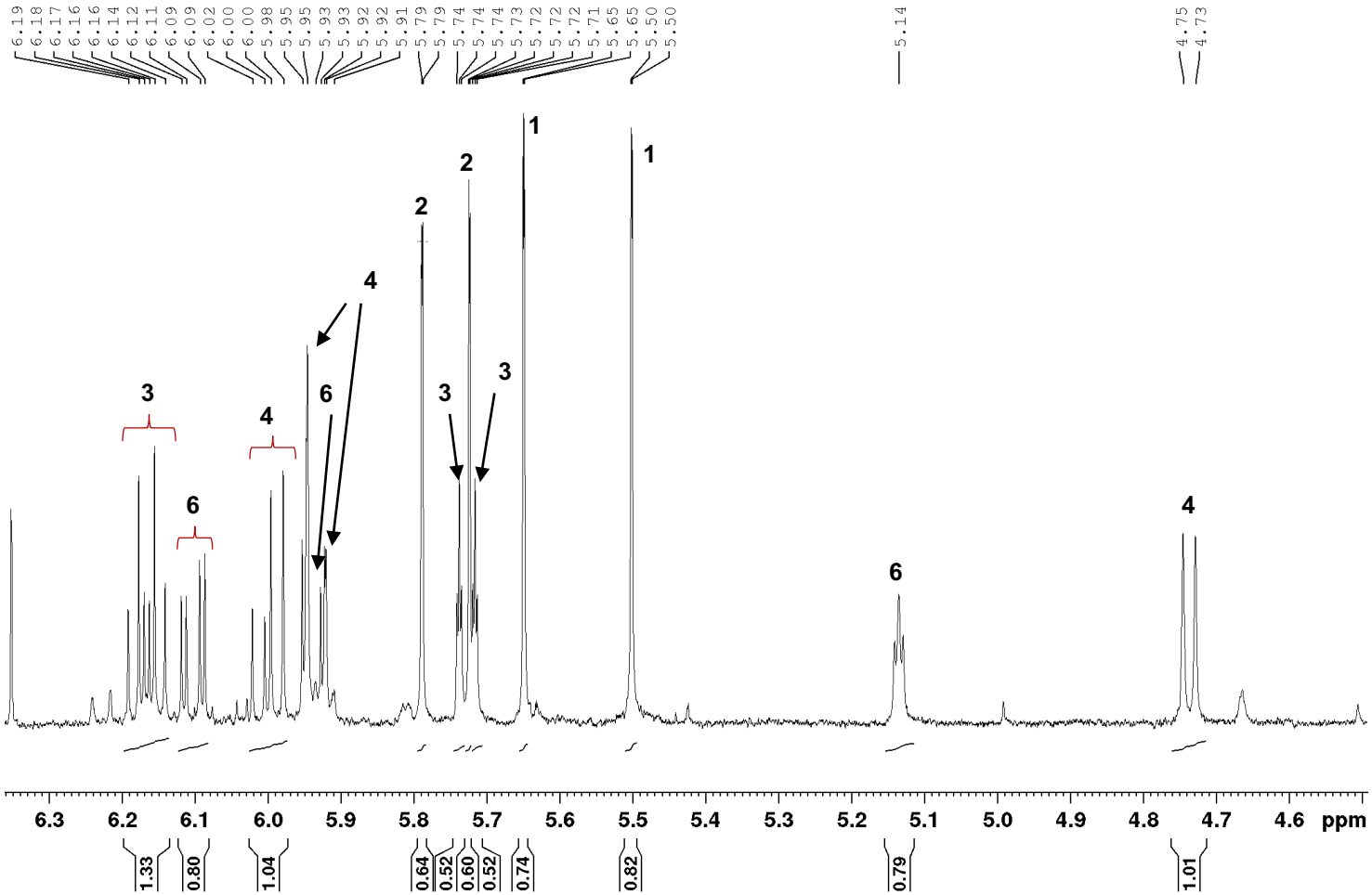


Figure S7. Selected range of the ^{1}H NMR spectrum (500 MHz) in C_6D_6 after aqueous work-up of experiment B.

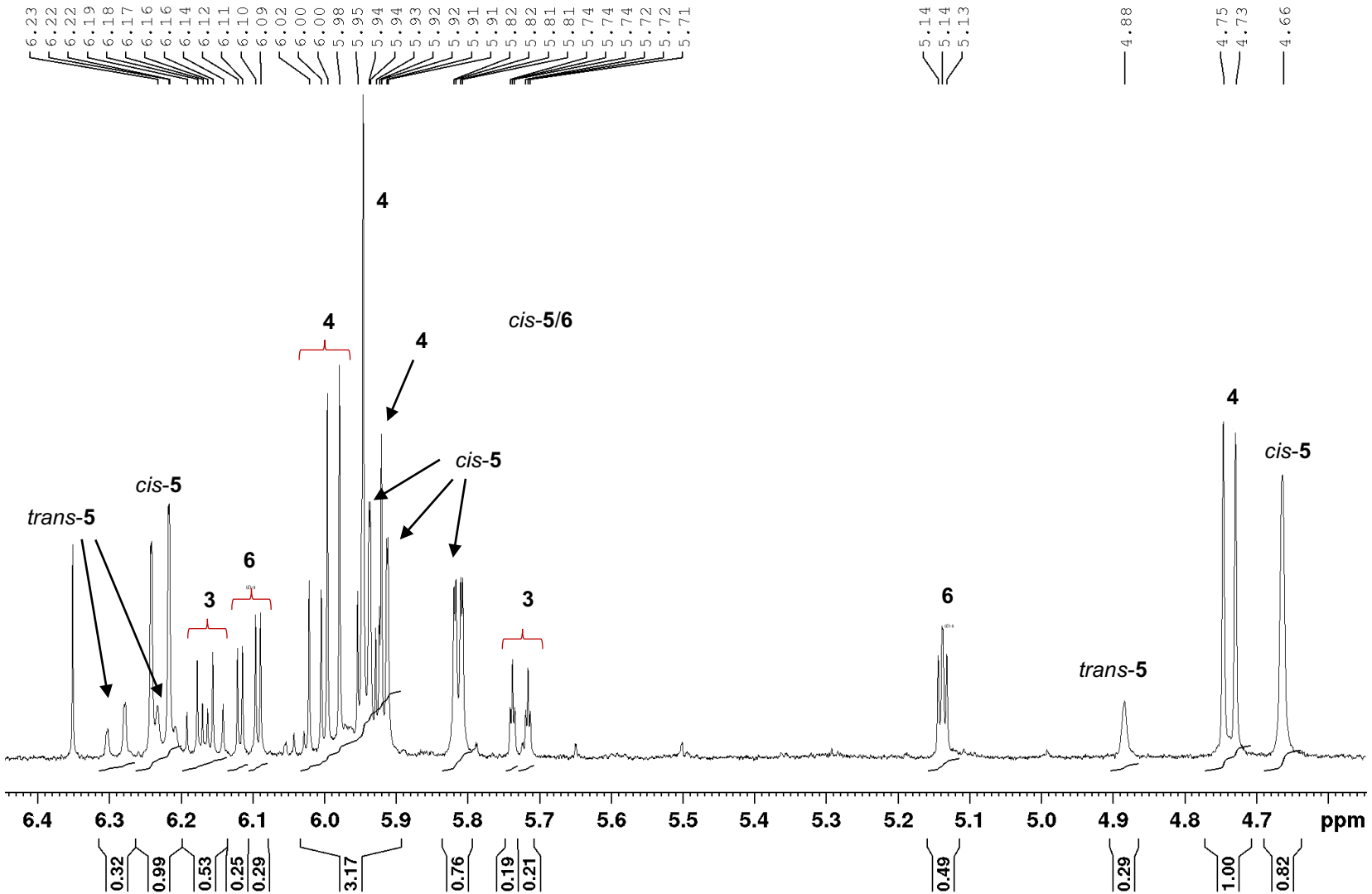


Figure S8. Selected range of the ^{1}H NMR spectrum (500 MHz) in C_6D_6 after aqueous work-up of experiment C.

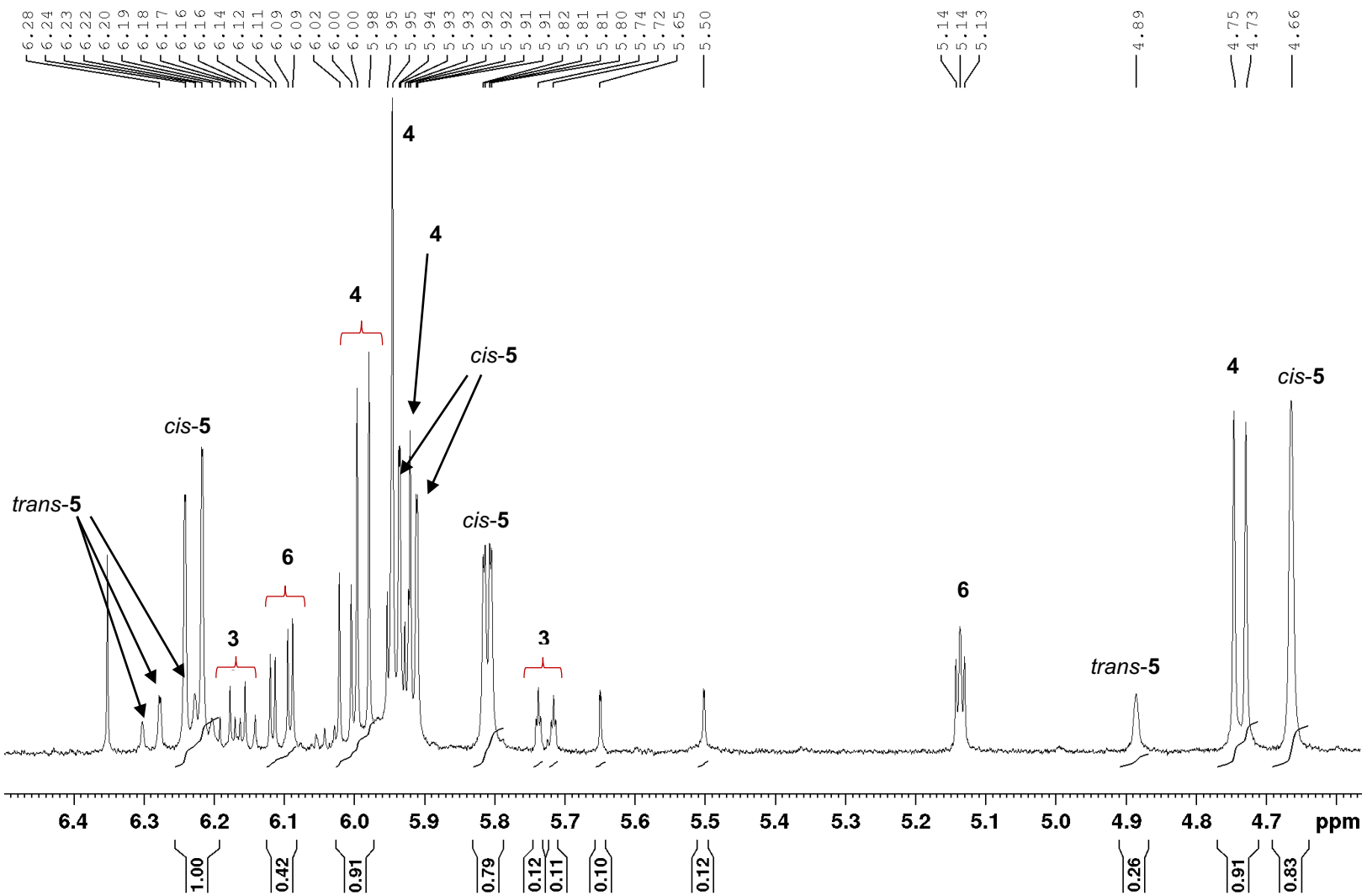


Figure S9. Selected range of the ^{1}H NMR spectrum (500 MHz) in C_6D_6 after aqueous work-up of experiment D.

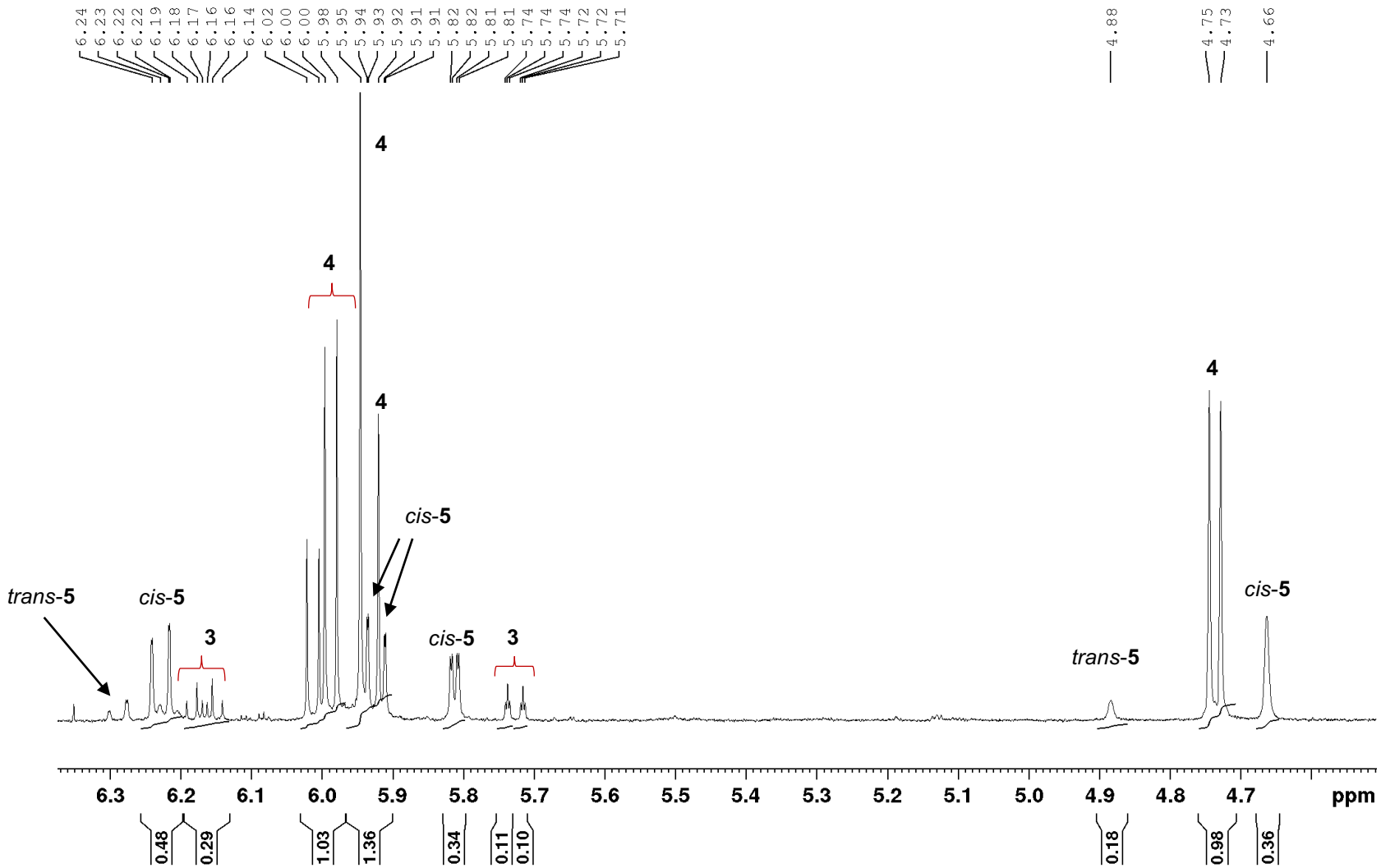


Figure S10. Selected range of the ^{1}H NMR spectrum (500 MHz) in C_6D_6 after aqueous work-up of experiment E.

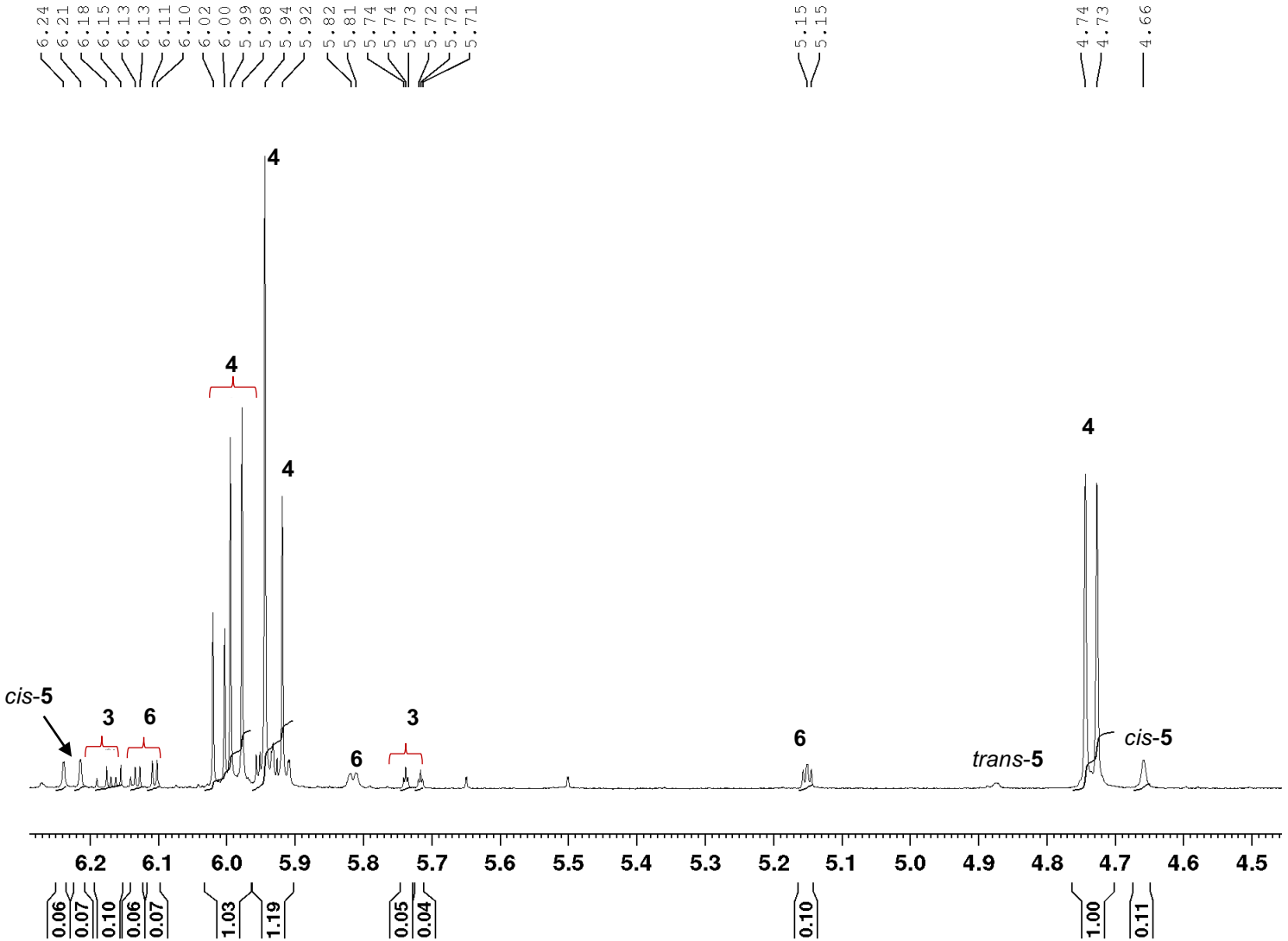


Figure S11. Selected range of the ^{1}H NMR spectrum (500 MHz) in C_6D_6 after aqueous work-up of experiment F.

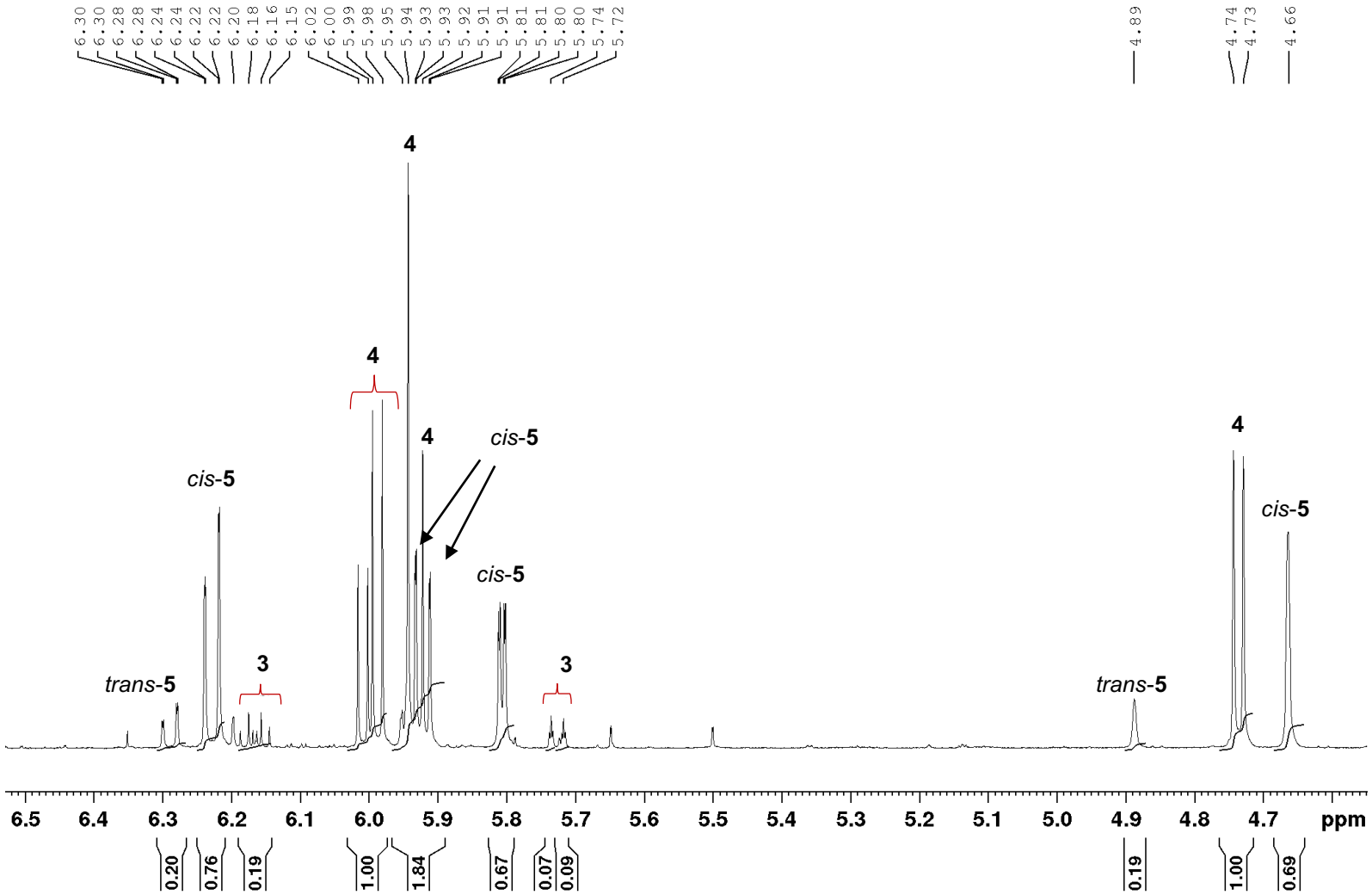


Figure S12. Selected range of the ^{1}H NMR spectrum (500 MHz) in C_6D_6 after aqueous work-up of experiment G.

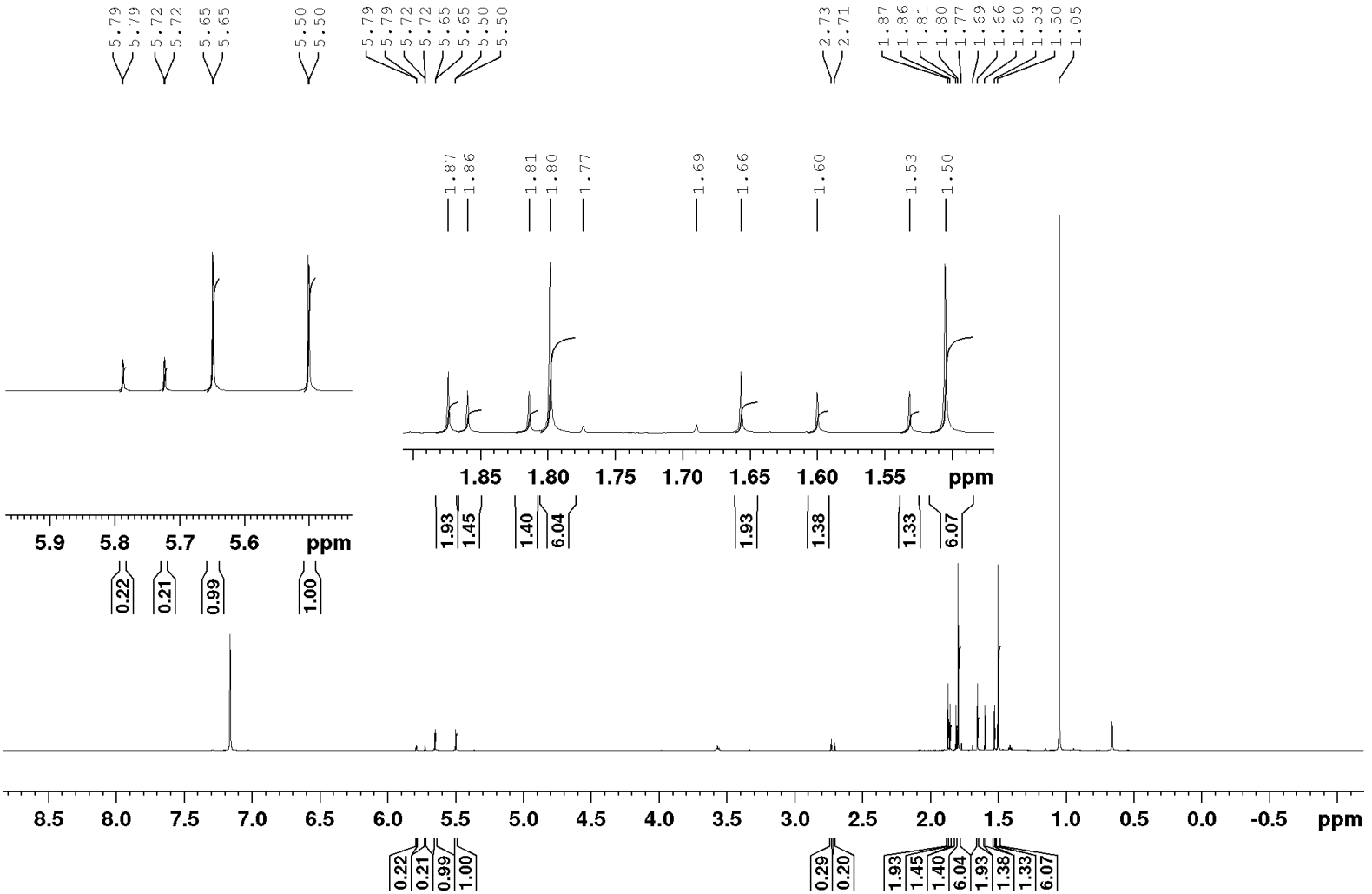


Figure S13. ^{1}H NMR spectrum (600 MHz) in C_6D_6 of the mixture of **1**, **2**, and 1,1'-diethynyloctamethylferrocene obtained from reaction of **1** with tBuOK.

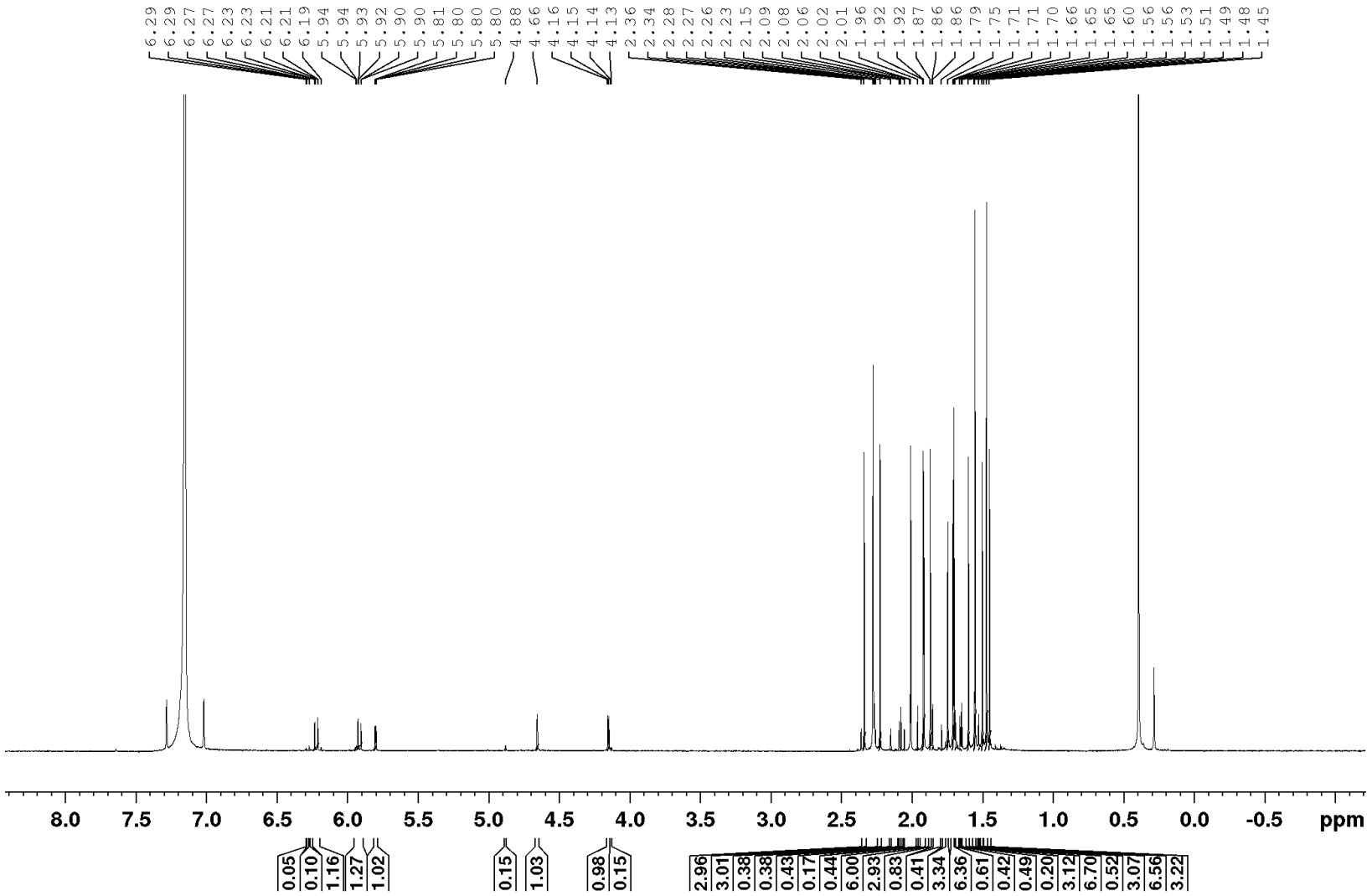


Figure S14. ^{1}H NMR spectrum (600 MHz) in C_6D_6 of compound *cis*-**5** with minor amount of *trans*-**5**.

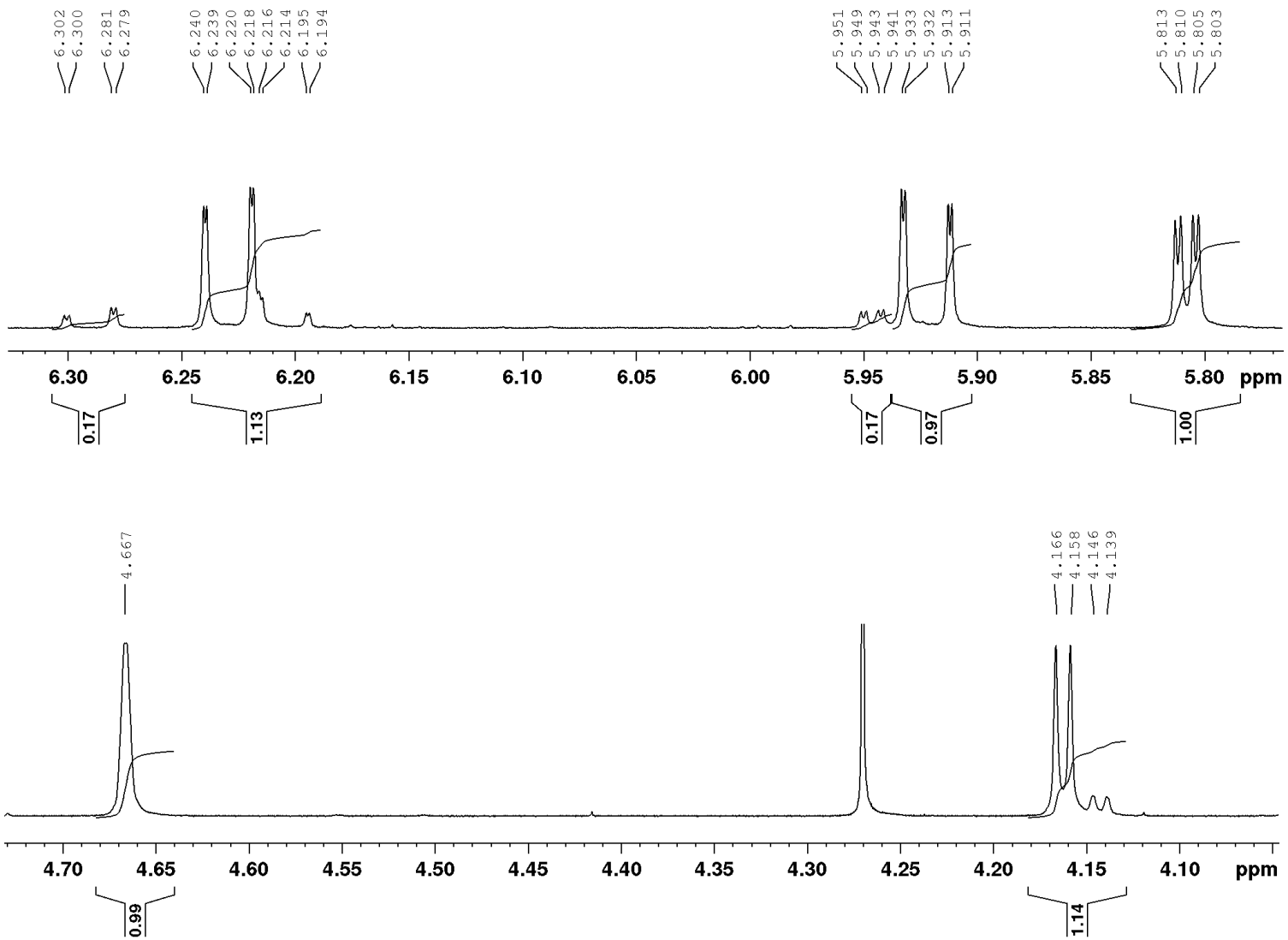


Figure S15. Selected ranges of the ^{1}H NMR spectrum in C_6D_6 of compound *cis*-**5** with minor amount of *trans*-**5** showing the proton resonances of the handle-ring systems.

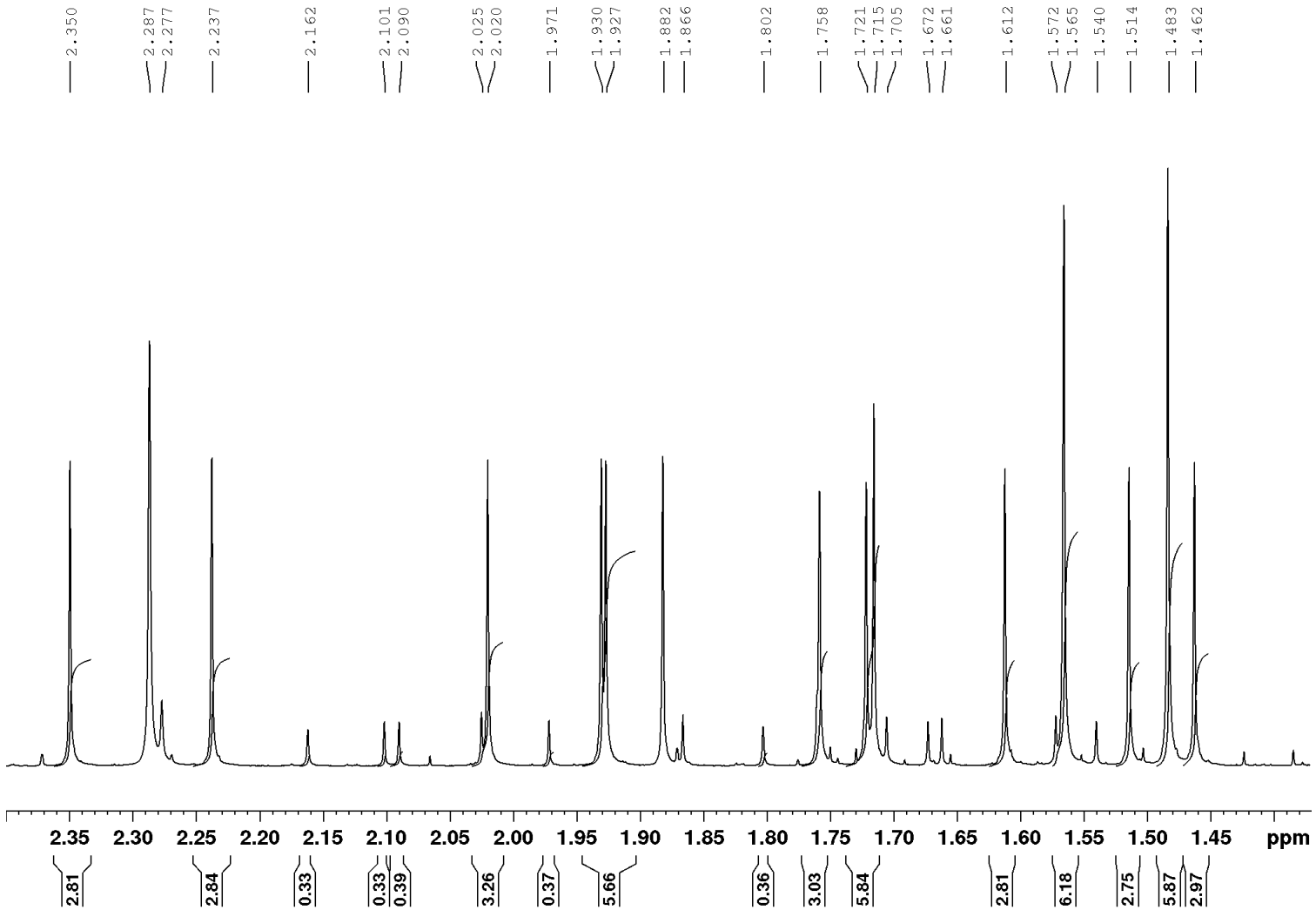


Figure S16. Selected range of the ^{1}H NMR spectrum in C_6D_6 of compound *cis*-**5** with minor amount of *trans*-**5** showing the proton resonances of the methyl groups.

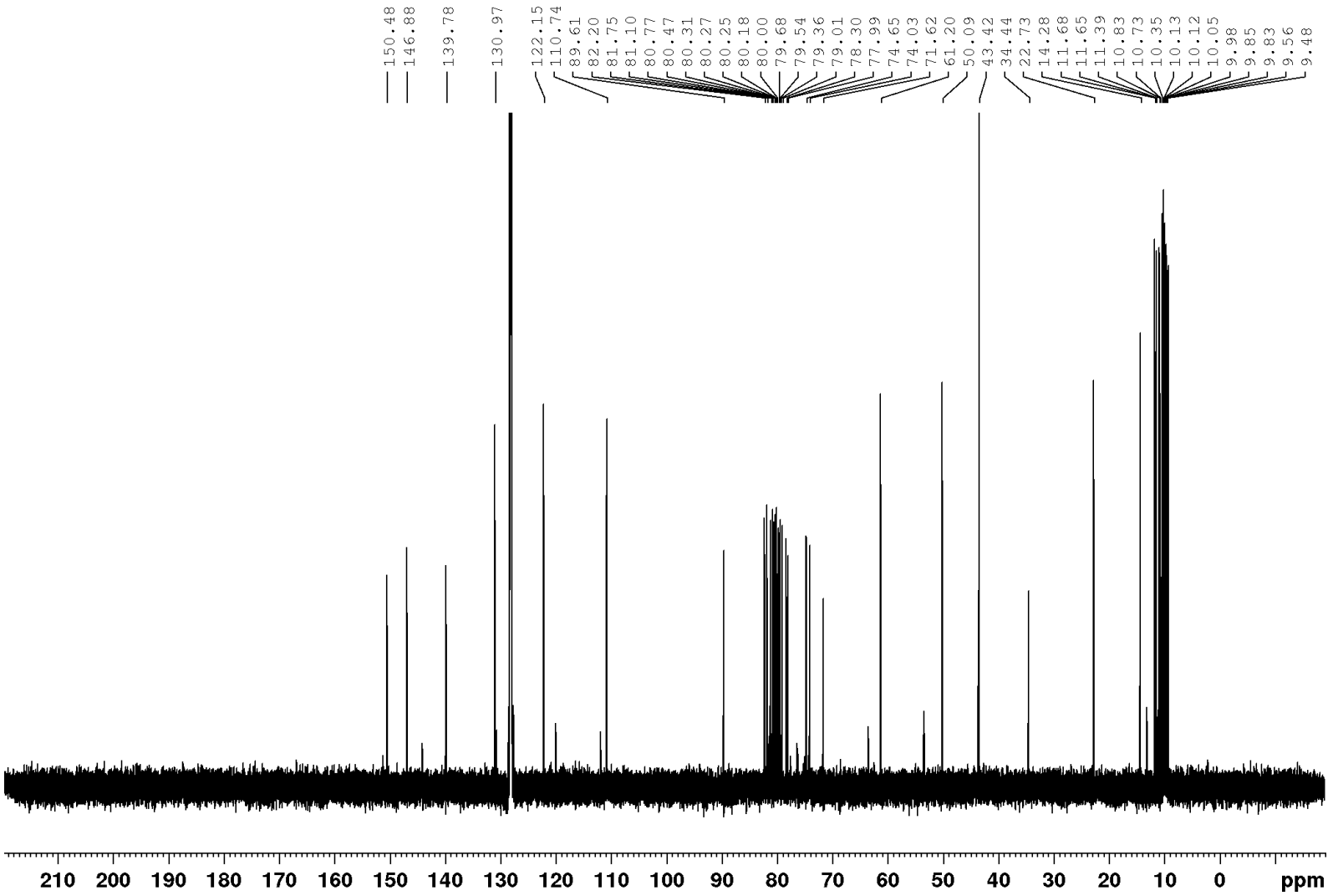


Figure S17. ^{13}C NMR spectrum (151 MHz) of compound *cis*-**5** with minor amount of *trans*-**5** in C_6D_6.

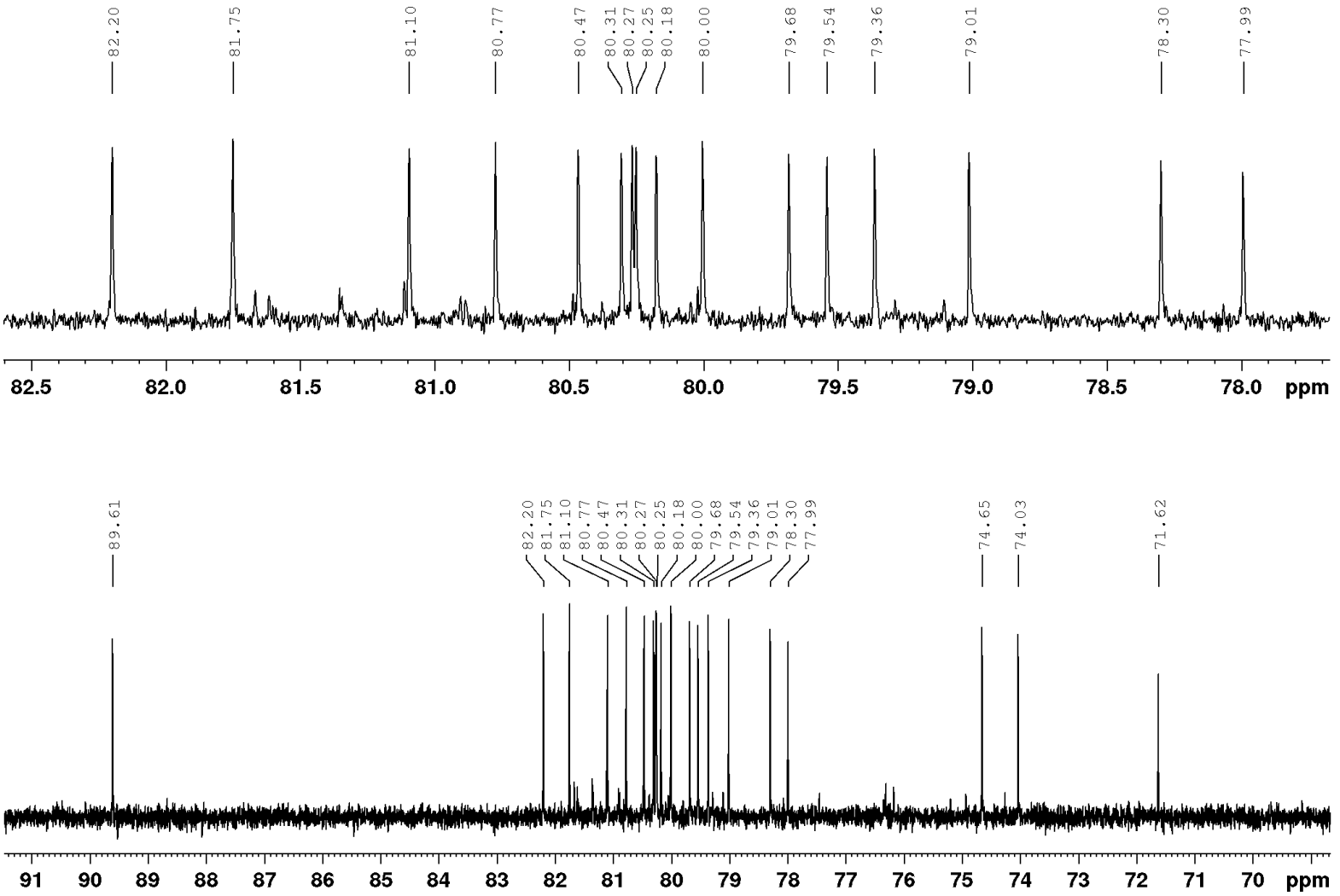


Figure S18. Selected ranges of the ^{13}C NMR spectrum of *cis*-**5** with minor amount of *trans*-**5** in C_6D_6 showing the ipso-C resonances.

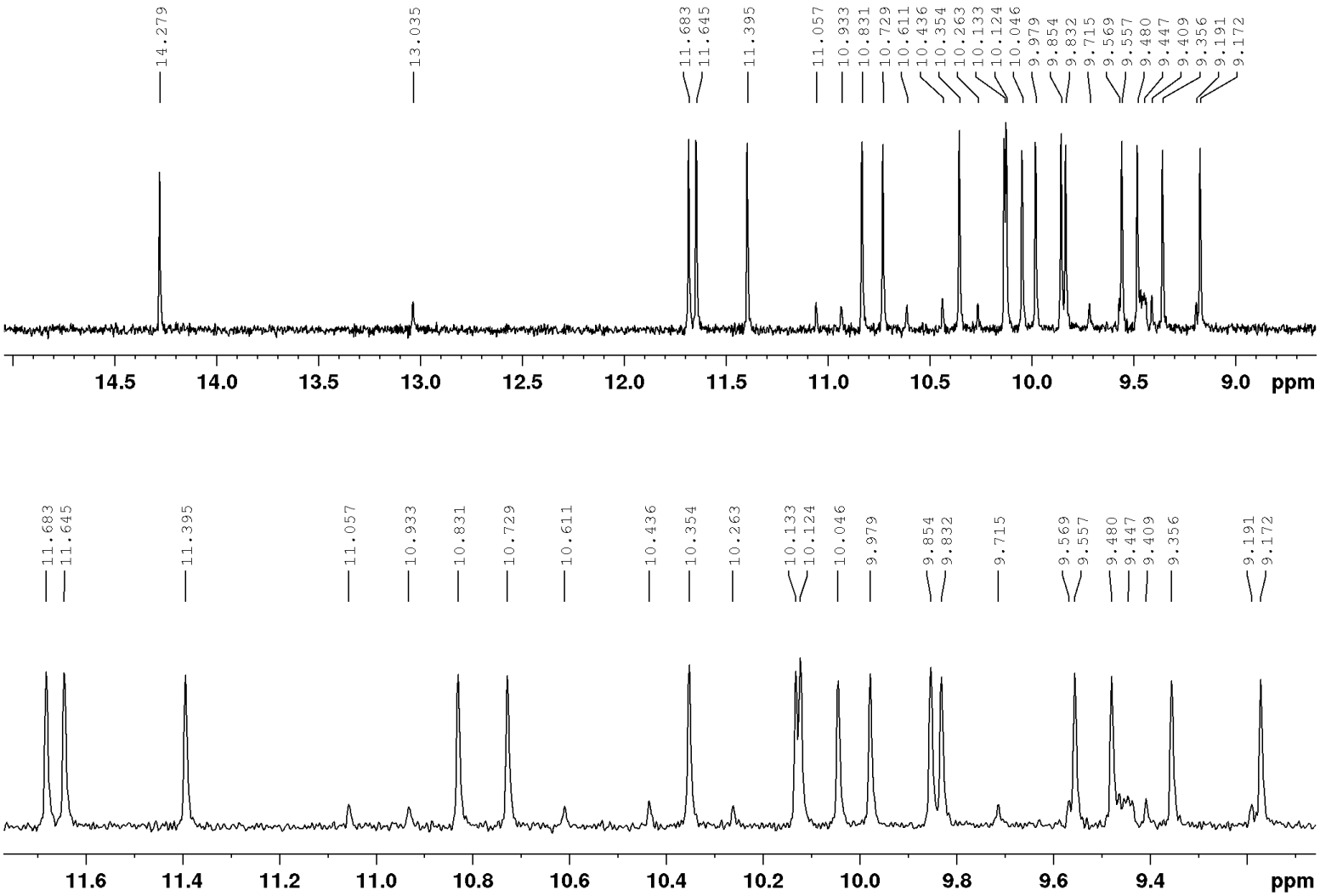


Figure S19. Selected range of ^{13}C NMR spectrum of *cis*-**5** with minor amount of *trans*-**5** in C_6D_6 showing Cp methyl C resonances.

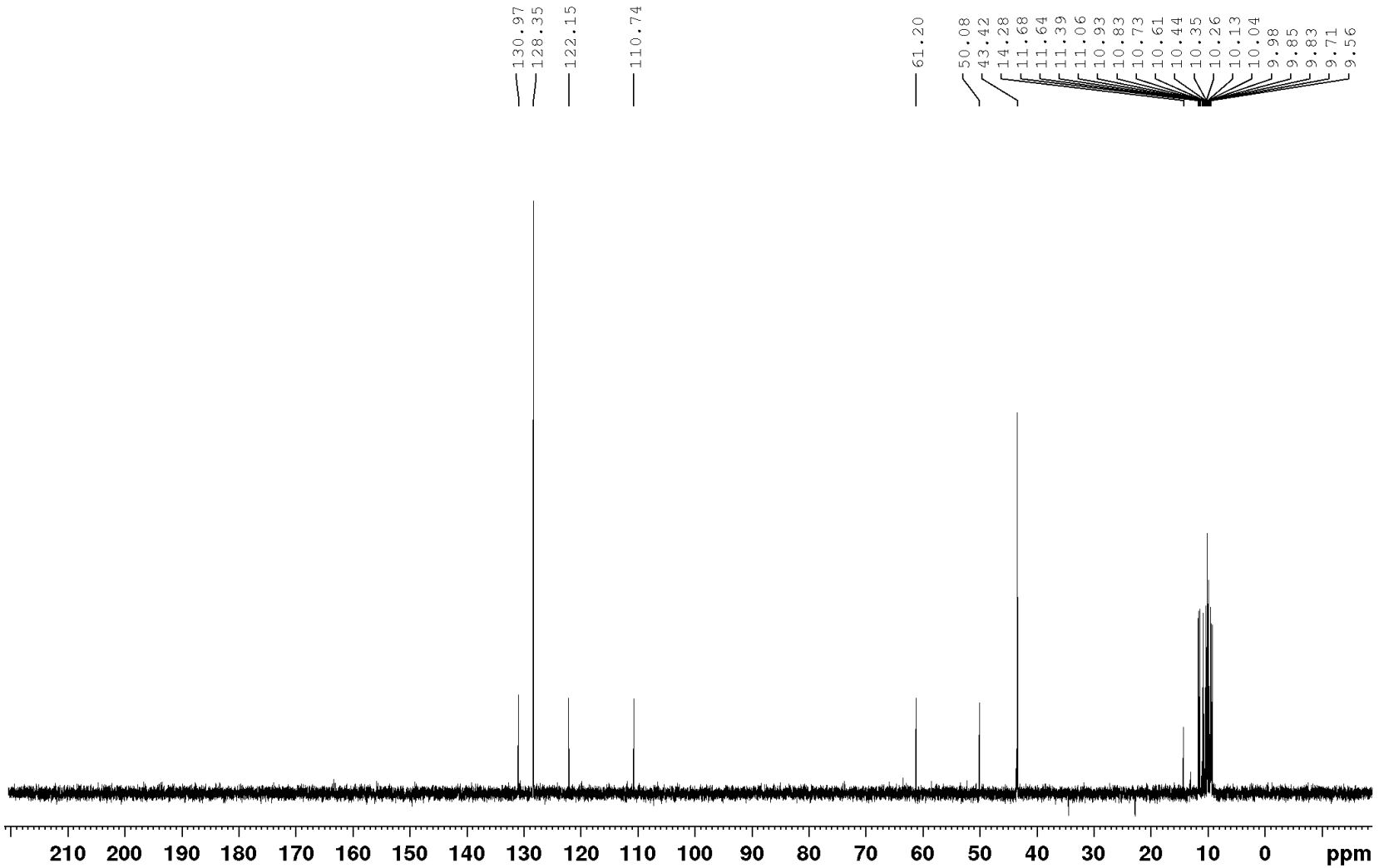


Figure S20. ^{13}C NMR DEPT spectrum of *cis*-**5** with minor amount of *trans*-**5** in C_6D_6.

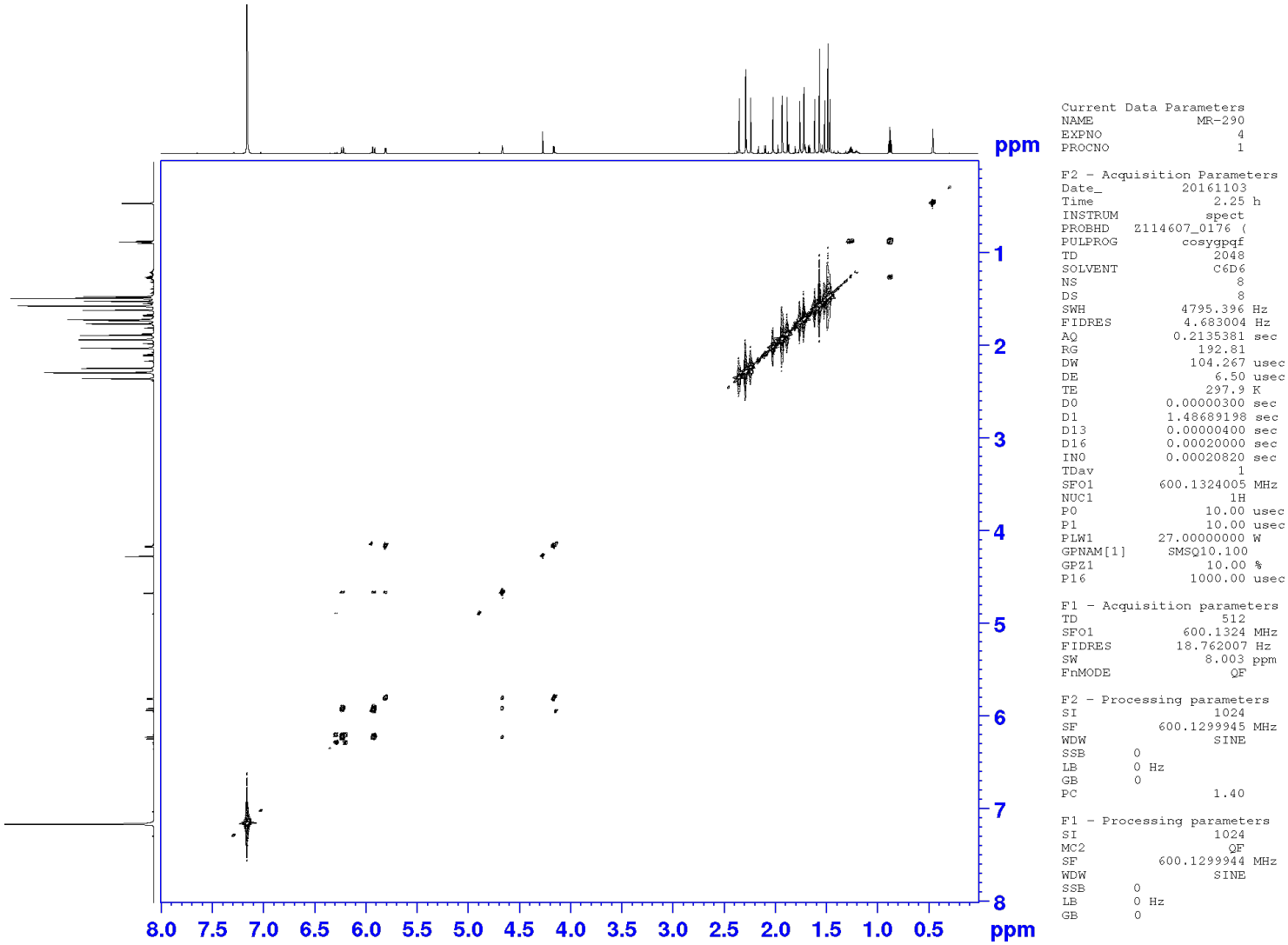
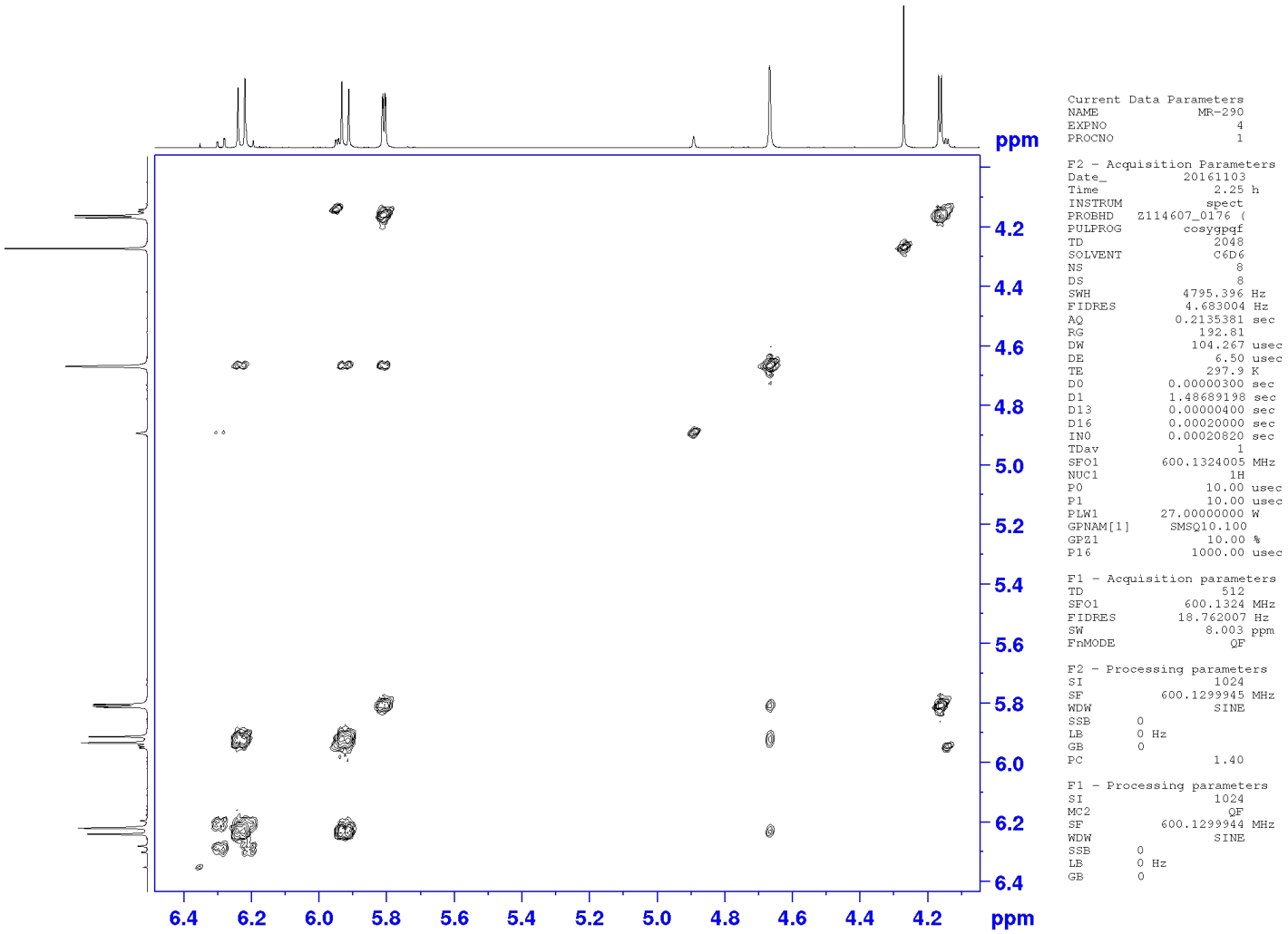


Figure S21. 2D COSY spectrum of *cis*-**5** with minor amount of *trans*-**5.**

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TD                      2048
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NS                         8
DS                         8
SWH                4795.396 Hz
FIDRES             4.683004 Hz
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RG                    192.81
DW                   104.267 usec
DE                     6.50 usec
TE                    297.9 K
D0                 0.00000300 sec
D1                 1.48689198 sec
D13                0.00000400 sec
D16                0.00020000 sec
IN0                0.00020820 sec
TDav                       1
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NUC1                      1H
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P1                     10.00 usec
PLW1           27.00000000 W
GPNAM[1]       SMSQ10.100
GPZ1                   10.00 %
P16                  1000.00 usec

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FIDRES           18.762007 Hz
SW                     8.003 ppm
FnMODE                    QF

F2 - Processing parameters
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SF              600.1299945 MHz
WDW                      SINE
SSB         0
LB          0 Hz
GB          0
PC                     1.40

F1 - Processing parameters
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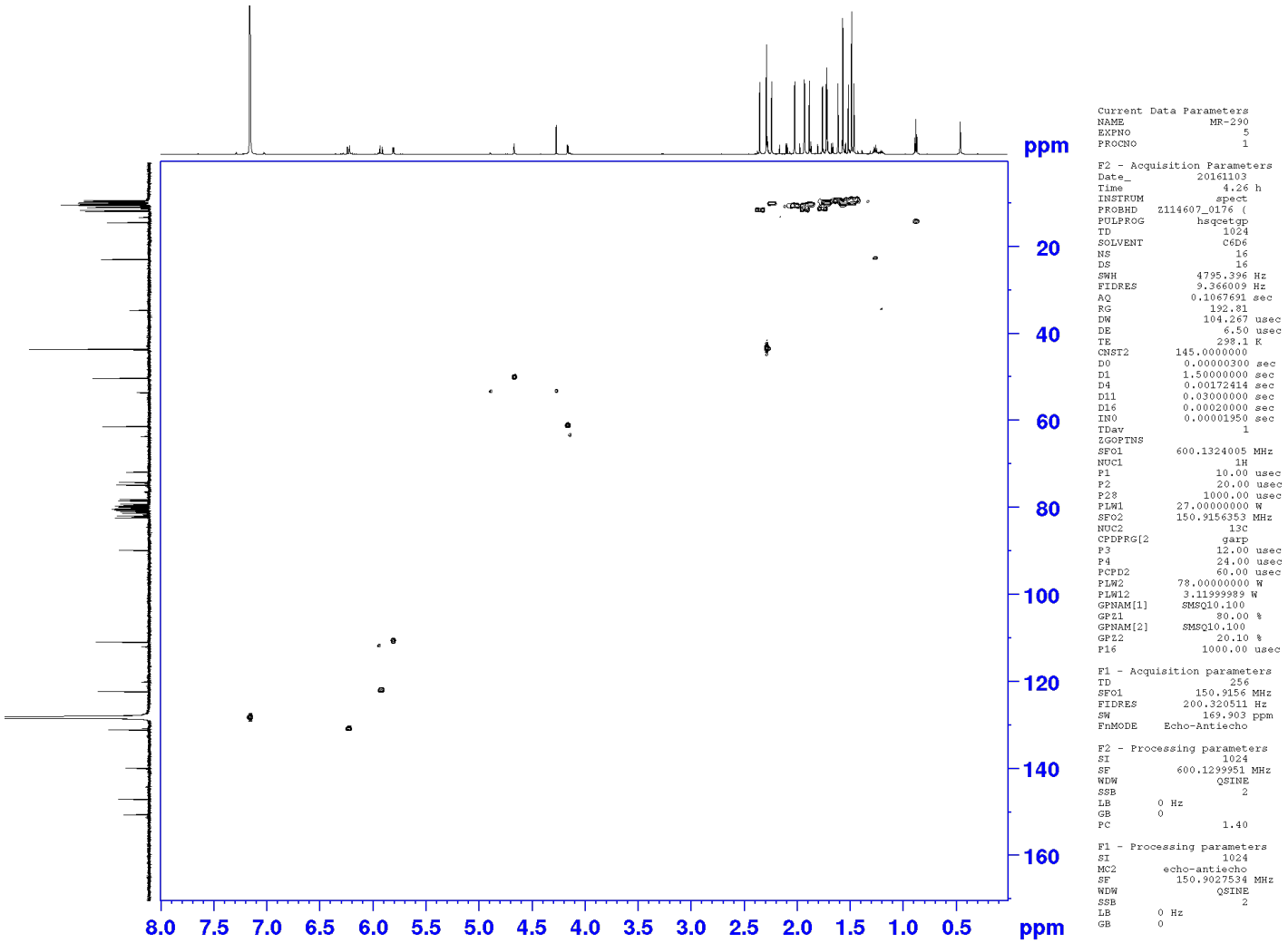
Figure S22. 2D COSY spectrum of *cis*-**5** with minor amount of *trans*-**5.**

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PROCNO                     1

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SOLVENT                C6D6
NS                       16
DS                       16
SWH                4795.396 Hz
FIDRES             9.366009 Hz
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RG                    192.81
DW                   104.267 usec
DE                      6.50 usec
TE                    299.1 K
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D1                1.50000000 sec
D4                0.00172414 sec
D11               0.03000000 sec
D16               0.00020000 sec
IN0               0.00001950 sec
TDav                       1
ZGOPTNS
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NUC1                      1H
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P2                     20.00 usec
P28                  1000.00 usec
PLW1            27.00000000 W
SFO2            150.9156353 MHz
NUC2                      13C
CPDPRG[2                garp
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P4                     24.00 usec
PCPD2                  60.00 usec
PLW2            78.00000000 W
PLW12            3.11999989 W
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GPZ1                   80.00 %
GPNAM[2]       SMSQ10.100
GPZ2                   20.10 %
P16                  1000.00 usec

F1 - Acquisition parameters
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SFO1               150.9156 MHz
FIDRES          200.320511 Hz
SW                 169.903 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
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SF              600.1299951 MHz
WDW                    QSINE
SSB                        2
LB          0 Hz
GB          0
PC                      1.40

F1 - Processing parameters
SI                     1024
MC2         echo-antiecho
SF            150.9027534 MHz
WDW                    QSINE
SSB                        2
LB          0 Hz
GB          0
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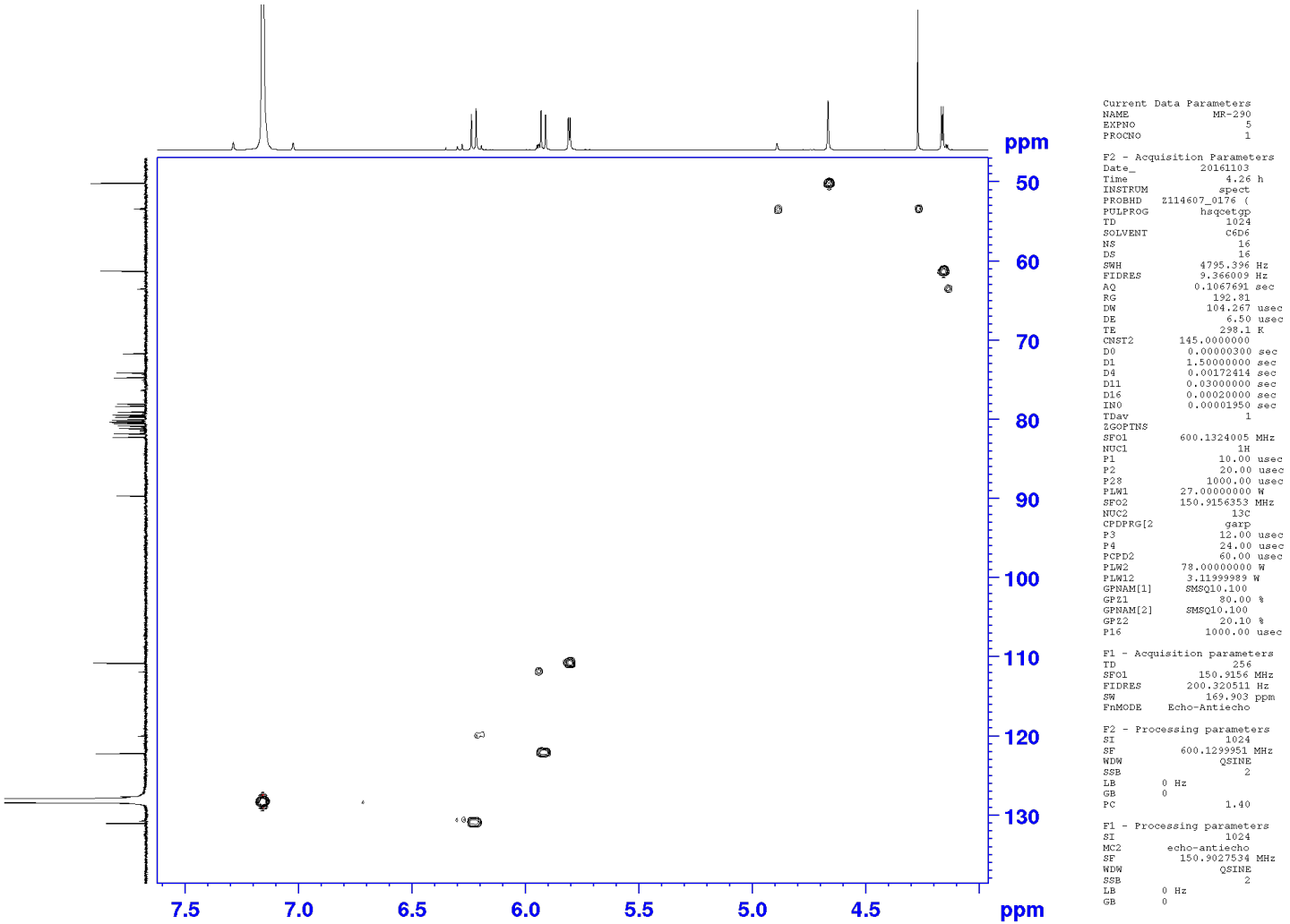
Figure S23. 2D HSQC spectrum of compound *trans*-**5** with minor amount of *cis*-**5.**

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Current Data Parameters
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EXPNO                      5
PROCNO                     1

F2 - Acquisition Parameters
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PULPROG             hsqcetgp
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SOLVENT                 C6D6
NS                        16
DS                        16
SWH                 4795.396 Hz
FIDRES              9.366009 Hz
AQ                  0.1067691 sec
RG                     192.81
DW                   104.267 usec
DE                      6.50 usec
TE                     298.1 K
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D0                  0.00000300 sec
D1                  1.50000000 sec
D4                  0.00172414 sec
D11                 0.03000000 sec
D16                 0.00020000 sec
IN0                 0.00001950 sec
TDav                       1
ZGOPTNS
SFO1               600.1324005 MHz
NUC1                       1H
P1                      10.00 usec
P2                      20.00 usec
P28                   1000.00 usec
PLW1               27.00000000 W
SFO2               150.9156353 MHz
NUC2                       13C
CPDPRG[2                 garp
P3                      12.00 usec
P4                      24.00 usec
PCPD2                   60.00 usec
PLW2               78.00000000 W
PLW12               3.11999989 W
GPNAM[1]           SMSQ10.100
GPZ1                   80.00 %
GPNAM[2]           SMSQ10.100
GPZ2                   20.10 %
P16                  1000.00 usec

F1 - Acquisition parameters
TD                        256
SFO1               150.9156 MHz
FIDRES             200.320511 Hz
SW                 169.903 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                       1024
SF                 600.1299951 MHz
WDW                     QSINE
SSB                         2
LB          0 Hz
GB          0
PC                       1.40

F1 - Processing parameters
SI                       1024
MC2          echo-antiecho
SF                 150.9027534 MHz
WDW                     QSINE
SSB                         2
LB          0 Hz
GB          0
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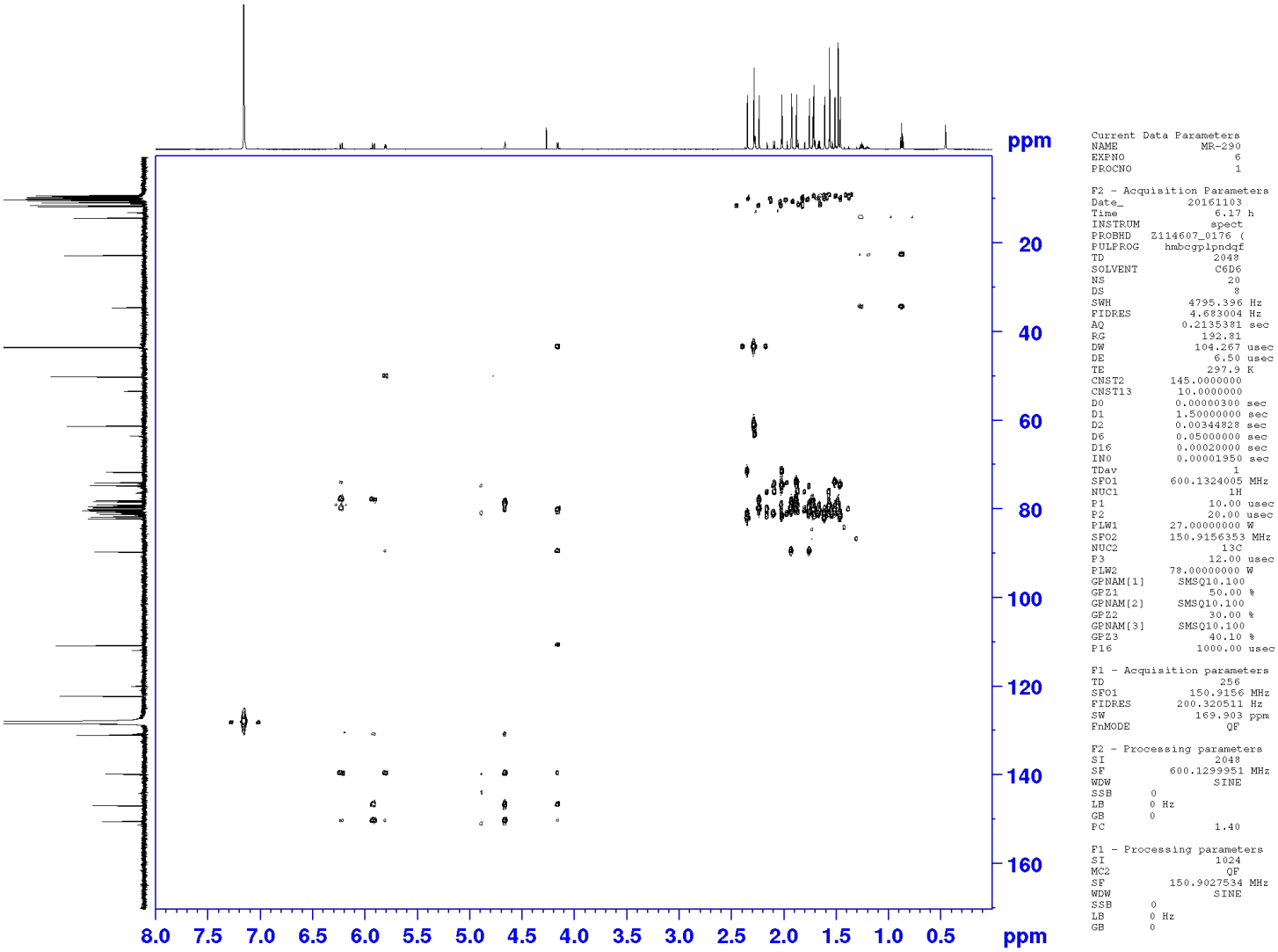
Figure S24. 2D HSQC spectrum of *cis*-**5** with minor amount of *trans*-**5.**

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Current Data Parameters
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EXPNO                      6
PROCNO                     1

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TD                      2048
SOLVENT                 C6D6
NS                        20
DS                         8
SWH                 4795.396 Hz
FIDRES              4.683004 Hz
AQ                  0.2135381 sec
RG                     192.81
DW                  104.267 usec
DE                      6.50 usec
TE                     297.9 K
CNST2              145.0000000
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D0                  0.00000300 sec
D1                  1.50000000 sec
D2                  0.00344828 sec
D6                  0.05000000 sec
D16                 0.00020000 sec
IN0                 0.00001950 sec
TDav                       1
SFO1               600.1324005 MHz
NUC1                      1H
P1                      10.00 usec
P2                      20.00 usec
PLW1               27.00000000 W
SFO2               150.9156353 MHz
NUC2                      13C
P3                      12.00 usec
PLW2               78.00000000 W
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GPZ1                    50.00 %
GPNAM[2]            SMSQ10.100
GPZ2                    30.00 %
GPNAM[3]            SMSQ10.100
GPZ3                    40.10 %
P16                   1000.00 usec

F1 - Acquisition parameters
TD                       256
SFO1                150.9156 MHz
FIDRES              200.320511 Hz
SW                  169.903 ppm
FnMODE                    QF

F2 - Processing parameters
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SF                 600.1299951 MHz
WDW                     SINE
SSB          0
LB           0 Hz
GB           0
PC                      1.40

F1 - Processing parameters
SI                      1024
MC2                       QF
SF                 150.9027534 MHz
WDW                     SINE
SSB          0
LB           0 Hz
GB           0
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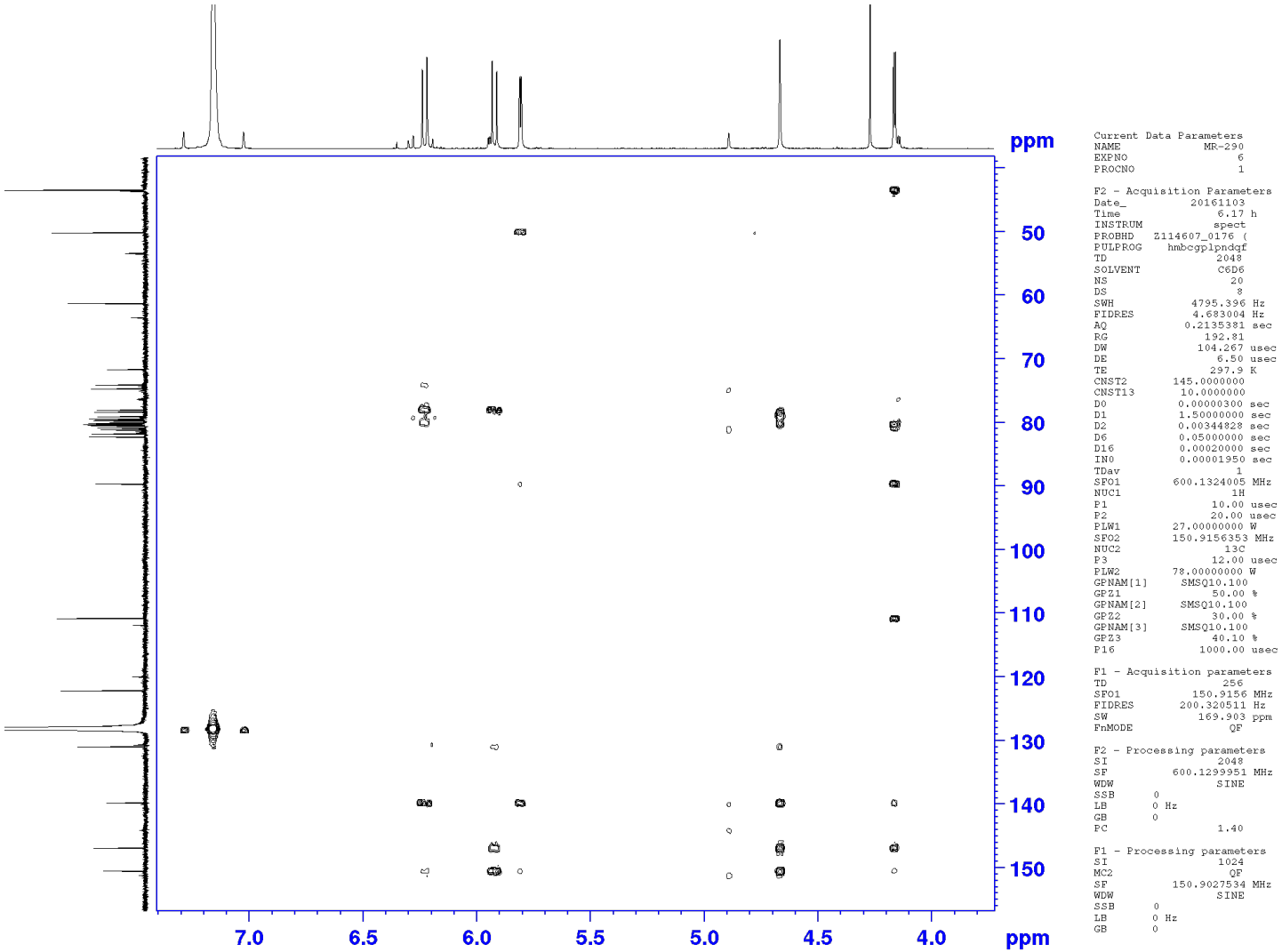
Figure S25. 2D HMBC spectrum of compound *cis*-**5** with minor amount of *trans*-**5.**

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EXPNO                      6
PROCNO                     1

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NS                        20
DS                         8
SWH                 4795.396 Hz
FIDRES              4.683004 Hz
AQ                0.2135381 sec
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DW                  104.267 usec
DE                    6.50 usec
TE                   297.9 K
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CNST13             10.0000000
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D2                 0.00344828 sec
D6                 0.05000000 sec
D16                0.00020000 sec
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P2                    20.00 usec
PLW1              27.00000000 W
SFO2              150.9156353 MHz
NUC2                      13C
P3                    12.00 usec
PLW2              78.00000000 W
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GPNAM[2]           SMSQ10.100
GPZ2                  30.00 %
GPNAM[3]           SMSQ10.100
GPZ3                  40.10 %
P16                 1000.00 usec

F1 - Acquisition parameters
TD                       256
SFO1              150.9156 MHz
FIDRES            200.320511 Hz
SW                  169.903 ppm
FnMODE                   QF

F2 - Processing parameters
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SF                600.1299951 MHz
WDW                     SINE
SSB          0
LB           0 Hz
GB           0
PC                      1.40

F1 - Processing parameters
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MC2                       QF
SF                150.9027534 MHz
WDW                     SINE
SSB          0
LB           0 Hz
GB           0
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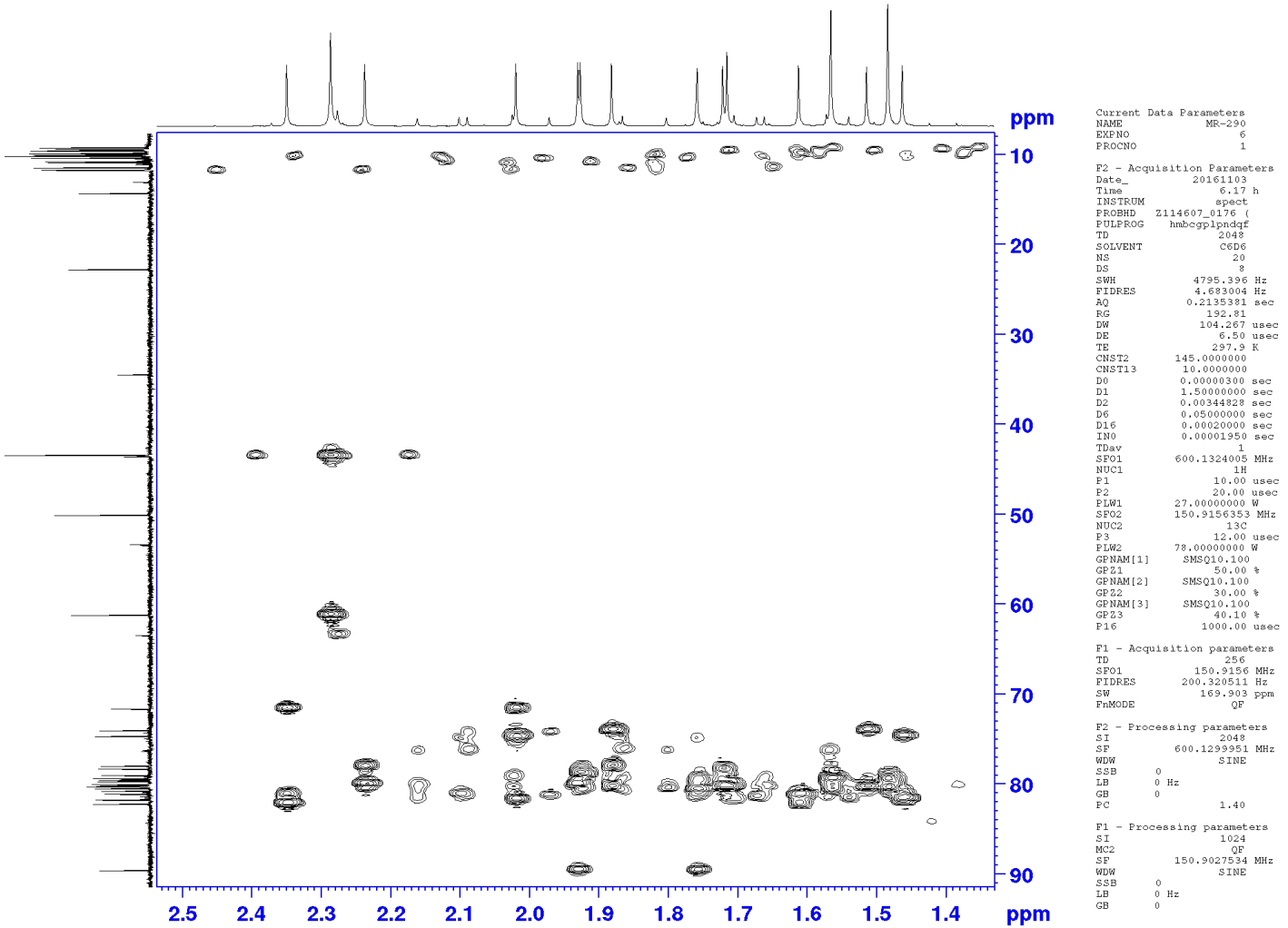
Figure S26. 2D HMBC spectrum of *cis*-**5** with minor amount of *trans*-**5.**

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Current Data Parameters
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PROCNO                     1

F2 - Acquisition Parameters
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PULPROG     hmbcgplpndqf
TD                      2048
SOLVENT                 C6D6
NS                        20
DS                         8
SWH                 4795.396 Hz
FIDRES              4.683004 Hz
AQ                  0.2135381 sec
RG                     192.81
DW                  104.267 usec
DE                    6.50 usec
TE                    297.9 K
CNST2              145.0000000
CNST13              10.0000000
D0                  0.00000300 sec
D1                  1.50000000 sec
D2                  0.00344828 sec
D6                  0.05000000 sec
D16                 0.00020000 sec
IN0                 0.00001950 sec
TDav                       1
SFO1               600.1324005 MHz
NUC1                      1H
P1                       10.00 usec
P2                       20.00 usec
PLW1               27.00000000 W
SFO2               150.9156353 MHz
NUC2                      13C
P3                       12.00 usec
PLW2               78.00000000 W
GPNAM[1]            SMSQ10.100
GPZ1                     50.00 %
GPNAM[2]            SMSQ10.100
GPZ2                     30.00 %
GPNAM[3]            SMSQ10.100
GPZ3                     40.10 %
P16                    1000.00 usec

F1 - Acquisition parameters
TD                        256
SFO1                150.9156 MHz
FIDRES              200.320511 Hz
SW                    169.903 ppm
FnMODE                     QF

F2 - Processing parameters
SI                       2048
SF                 600.1299951 MHz
WDW                      SINE
SSB          0
LB           0 Hz
GB           0
PC                       1.40

F1 - Processing parameters
SI                       1024
MC2                        QF
SF                 150.9027534 MHz
WDW                      SINE
SSB          0
LB           0 Hz
GB           0
```

Figure S27. 2D HMBC spectrum of *cis*-**5** with minor amount of *trans*-**5.**

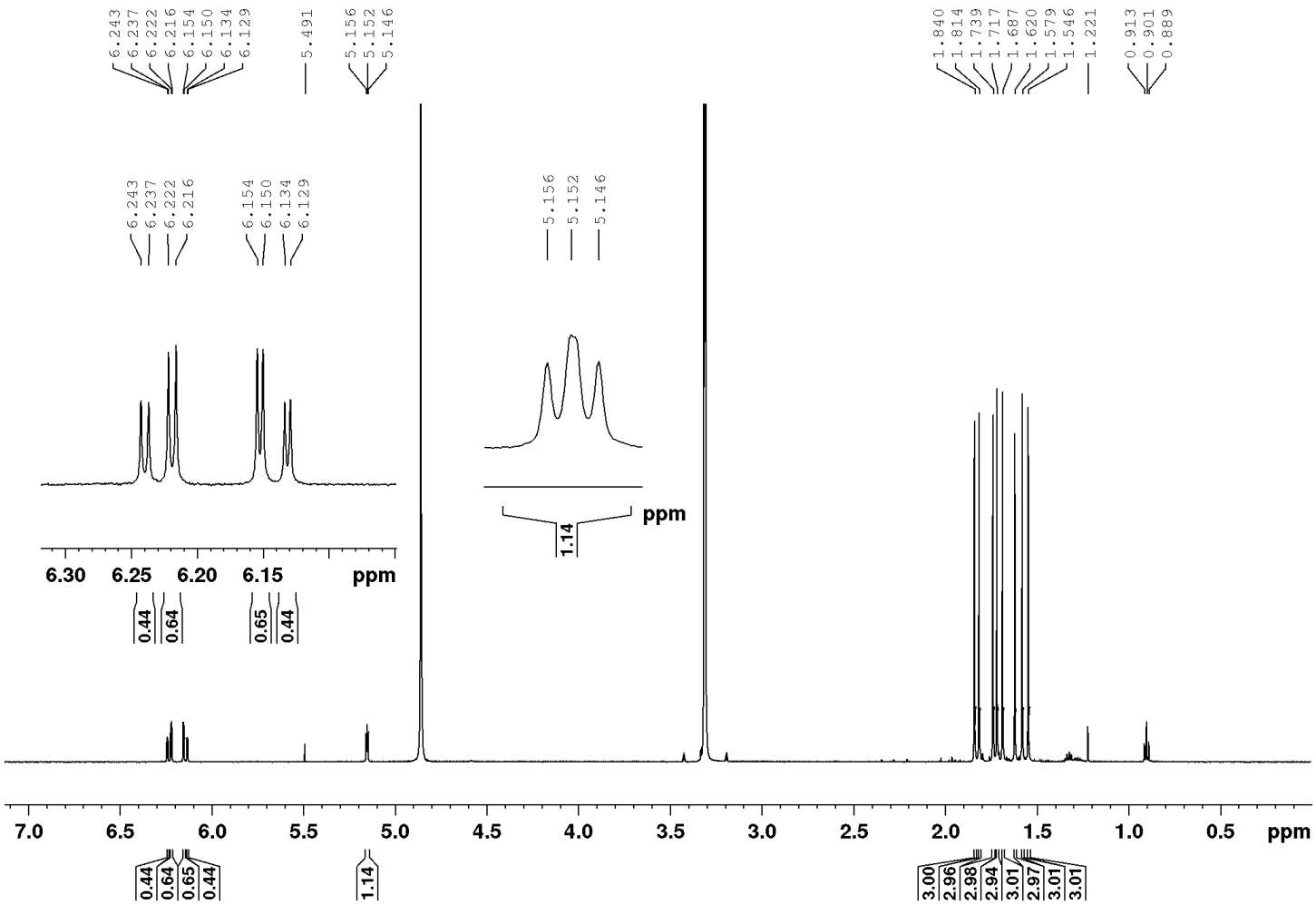

Figure S28. [1]H NMR spectrum (600 MHz) of compound **6** in methanol-*d*.

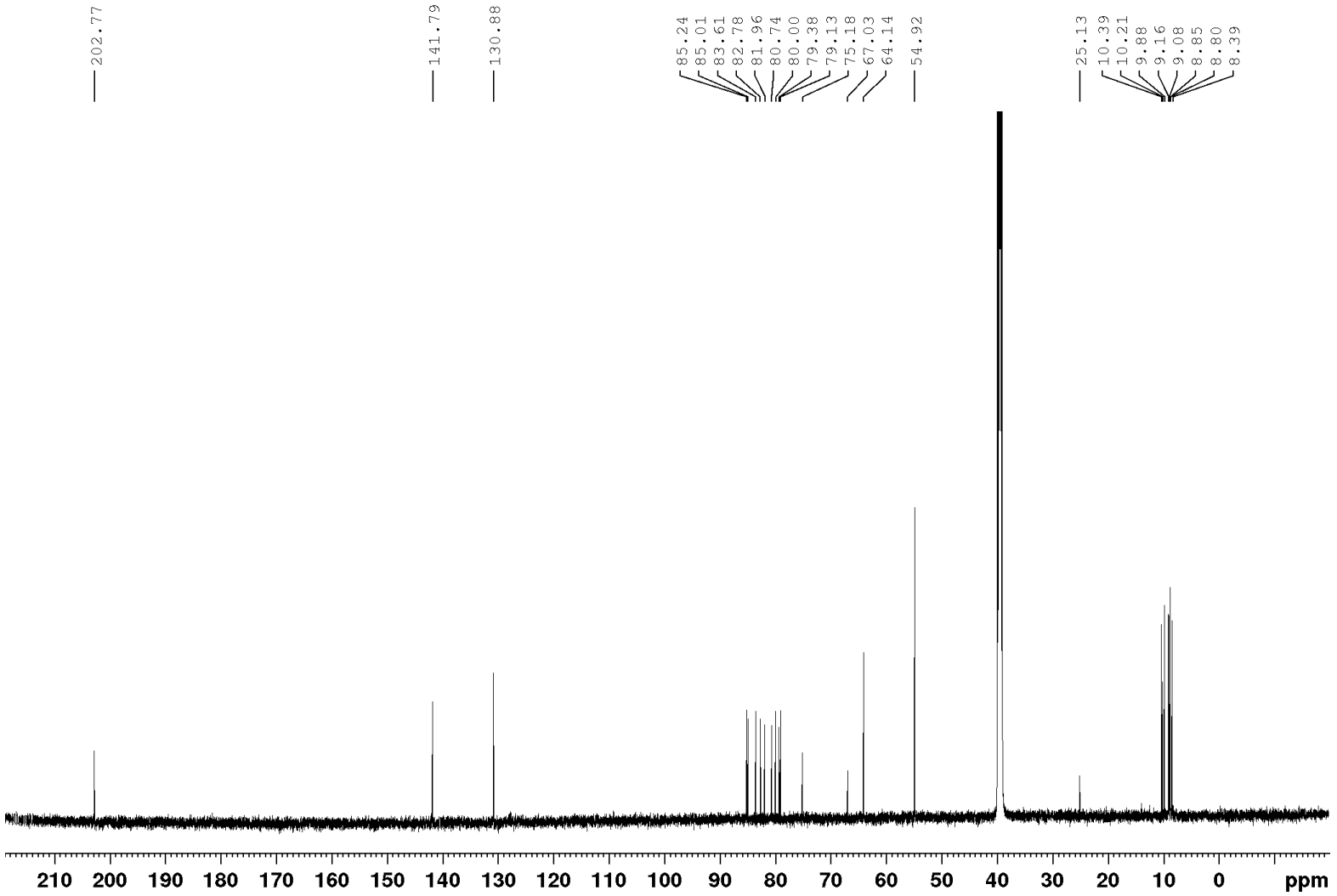

Figure S29. ^{13}C NMR spectrum (600 MHz) of compound **6** in DMSO-d^6.

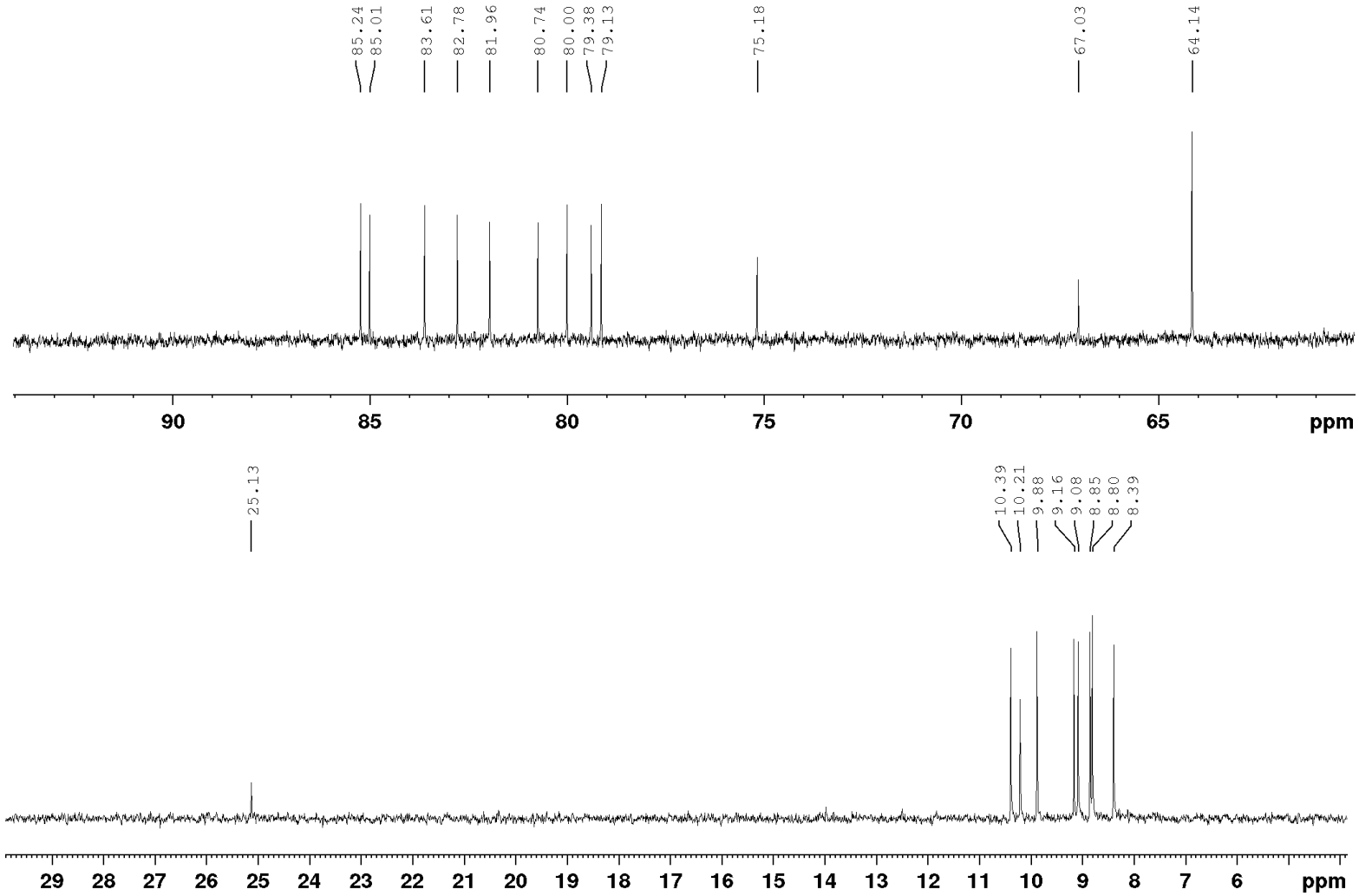

Figure S30. Selected ranges of the ^{13}C NMR spectrum of compound **6**.

The following data represent Cartesian coordinates for the intermediates along the proposed mechanism, in units of angstrom:

Point A1				Point A2			
C	-1.595803	-0.312391	0.280078	C	0.098109	-2.070111	-0.097750
C	-0.927715	-0.340015	1.560530	C	0.565865	-1.643944	1.238347
C	-0.032296	-1.455367	1.552067	C	1.773658	-0.948864	1.033618
C	-0.140179	-2.113830	0.278913	C	2.062592	-0.887954	-0.387329
C	-1.105399	-1.410697	-0.509099	C	1.040941	-1.545450	-1.103749
C	-2.729676	0.557274	-0.063825	C	-1.203124	-2.306511	-0.357062
C	-1.199204	0.572626	2.721377	C	-0.078196	-2.028074	2.534685
C	0.817998	-1.905453	2.706342	C	2.667277	-0.419002	2.114482
C	0.575408	-3.369778	-0.129260	C	3.304171	-0.292296	-0.981218
C	-1.578474	-1.782464	-1.885075	C	0.958646	-1.814914	-2.574613
Fe	0.459781	-0.117283	0.006776	Fe	0.089030	-0.021422	-0.020539
C	0.182755	1.776042	-2.636973	C	-1.867605	0.858911	-2.476722
C	1.011097	1.215835	-1.517809	C	-1.161153	1.188301	-1.196210
C	0.648747	3.057467	0.216832	C	-3.031497	0.560632	0.425870
C	1.197815	1.819922	-0.218039	C	-1.724324	1.033254	0.137031
C	1.845913	0.058284	-1.571417	C	0.094190	1.839014	-1.045324
C	2.034213	-0.830078	-2.767801	C	0.988091	2.286418	-2.163520
C	2.140434	1.019787	0.525202	C	-0.798472	1.558978	1.092851
C	2.539446	-0.063357	-0.317499	C	0.338652	2.037162	0.361039
C	2.668007	1.349115	1.890699	C	-1.030025	1.650457	2.570309
C	3.571998	-1.100778	0.019376	C	1.501306	2.779151	0.952070
Cl	-4.293999	-0.339470	-0.191896	H	-0.081726	-1.886472	-2.905432
H	-1.926282	-0.902858	-2.436021	H	1.450227	-2.765445	-2.819296
H	-2.415863	-2.491239	-1.835642	H	1.450950	-1.031480	-3.156821
H	-0.784094	-2.255078	-2.470987	H	3.631104	0.600860	-0.442397
H	1.545252	-3.465328	0.367712	H	3.166909	-0.029201	-2.032555
H	0.748960	-3.404591	-1.209428	H	4.124770	-1.019990	-0.930659
H	-0.015320	-4.258065	0.134505	H	2.041051	2.295925	-1.870856
H	2.270421	-1.858889	-2.478811	H	0.725440	3.308982	-2.464785
H	2.863107	-0.469650	-3.392803	H	0.883580	1.651630	-3.048019
H	1.140022	-0.855328	-3.397878	H	2.109268	-0.194611	3.027421
H	1.146690	-1.062484	3.321798	H	3.198710	0.483886	1.805100
H	1.711390	-2.439967	2.369213	H	3.423722	-1.172162	2.371500
H	0.257775	-2.588101	3.360306	H	1.706245	2.468632	1.979817
H	3.642455	-1.264070	1.099031	H	1.283820	3.855086	0.976242
H	4.566374	-0.788616	-0.328794	H	2.415986	2.649767	0.366474
H	3.349941	-2.063173	-0.451034	H	-0.102690	1.536352	3.139498
H	2.895395	0.448161	2.468451	H	-1.741859	0.891777	2.906485
H	1.946565	1.945080	2.458055	H	-1.450064	2.631638	2.827095
H	3.595306	1.934648	1.820987	H	0.344386	-2.969750	2.908676
H	-0.305099	0.716862	3.335798	H	-1.155445	-2.174065	2.412920
H	-1.979100	0.155023	3.373464	H	-2.566201	0.028373	-2.344189
H	-0.620241	2.413141	-2.256394	H	-1.167370	0.594403	-3.274129
H	-0.272189	0.983407	-3.239967	C	-2.429404	-2.673649	-0.567144
C	-2.773362	1.880364	-0.208663	H	-3.237123	-1.945103	-0.625590
H	-1.539677	1.555763	2.385814	H	-2.684721	-3.728827	-0.664201
H	0.798899	2.387283	-3.311111	H	0.077825	-1.267691	3.304693
C	0.207283	4.127880	0.579046	H	-2.450579	1.722166	-2.823057
H	-0.169280	5.076977	0.890120	C	-4.159814	0.188911	0.662007
H	-3.702652	2.410200	-0.388634	H	-5.170310	-0.080245	0.880077
H	-1.859115	2.458922	-0.131696				

Point A3				Point A4			
C	-1.716617	-0.591702	0.301872	C	-1.832174	-0.398509	0.355032
C	-1.058090	-0.421459	1.575796	C	-1.164076	-0.012152	1.572310
C	0.005299	-1.376797	1.644080	C	-0.150184	-0.985432	1.862336
C	0.015271	-2.133280	0.423068	C	-0.186164	-1.984736	0.831982
C	-1.048025	-1.654630	-0.407612	C	-1.215317	-1.618026	-0.098095
C	-2.982709	0.043294	-0.127905	C	-3.103572	0.185938	-0.241269
C	-1.478577	0.501364	2.683652	C	-1.516561	1.144605	2.470358
C	0.900813	-1.607755	2.828114	C	0.710725	-1.010821	3.094099
C	0.925798	-3.285193	0.106375	C	0.633832	-3.243412	0.791889
C	-1.425892	-2.196950	-1.759423	C	-1.614978	-2.425311	-1.301642
Fe	0.286035	-0.094231	0.006944	Fe	0.255141	-0.126403	0.012069
C	-0.399406	1.708364	-2.619418	C	-0.403350	1.747926	-2.591177
C	0.563728	1.278179	-1.552706	C	0.588303	1.143976	-1.639905
C	0.032892	3.071209	0.189136	C	0.642318	3.024835	0.088135
C	0.732518	1.921117	-0.269500	C	1.044408	1.757315	-0.413500
C	1.548058	0.246200	-1.643959	C	1.323896	-0.070070	-1.805133
C	1.796919	-0.629320	-2.839073	C	1.240229	-0.997686	-2.984909
C	1.816457	1.271551	0.426651	C	2.063940	0.916014	0.167891
C	2.316412	0.240832	-0.427757	C	2.231823	-0.209269	-0.697008
C	2.364141	1.684084	1.760956	C	2.868246	1.246960	1.390704
C	3.501481	-0.635012	-0.135936	C	3.260938	-1.291578	-0.532154
H	-1.968803	-1.454589	-2.351635	H	-2.119127	-1.801081	-2.041337
H	-2.069428	-3.083577	-1.670383	H	-2.320551	-3.220698	-1.024689
H	-0.541638	-2.500013	-2.327683	H	-0.749175	-2.906139	-1.770443
H	1.897744	-3.182135	0.597666	H	1.609595	-3.111032	1.270065
H	1.104069	-3.378086	-0.969657	H	0.812783	-3.579389	-0.234882
H	0.487428	-4.233998	0.446211	H	0.123305	-4.064355	1.316387
H	2.136285	-1.628823	-2.548603	H	1.453110	-2.034000	-2.702586
H	2.573697	-0.196855	-3.484857	H	1.966570	-0.716851	-3.760938
H	0.896215	-0.746618	-3.448562	H	0.247634	-0.981212	-3.444673
H	1.011661	-0.702928	3.432981	H	0.947332	-0.000625	3.443232
H	1.901704	-1.933179	2.526286	H	1.658899	-1.529621	2.916587
H	0.489024	-2.388602	3.482721	H	0.206870	-1.532552	3.921146
H	3.598310	-0.841370	0.934855	H	3.498046	-1.468288	0.522107
H	4.433286	-0.150755	-0.459863	H	4.200017	-1.021201	-1.035953
H	3.436699	-1.594898	-0.656573	H	2.925113	-2.241416	-0.958982
H	2.704434	0.823274	2.344556	H	3.157308	0.348027	1.943866
H	1.608828	2.216267	2.347237	H	2.304400	1.894241	2.070228
H	3.223197	2.358841	1.640933	H	3.792960	1.778490	1.123732
H	-2.078297	-0.037142	3.430946	H	-1.462221	0.849022	3.525756
H	-2.084523	1.326362	2.303789	H	-2.533059	1.485421	2.252173
H	-1.325411	2.094355	-2.184191	H	-1.341143	2.000186	-2.081847
H	-0.661736	0.879234	-3.283921	H	-0.642345	1.055613	-3.404615
C	-3.258923	1.354248	-0.176570	C	-3.269863	1.559535	-0.280360
H	-2.495932	2.091626	0.034220	H	-2.506878	2.252646	0.053218
H	-4.256280	1.695520	-0.438164	H	-4.205864	1.974723	-0.654043
H	-0.615536	0.926046	3.206306	H	-0.852104	2.006665	2.333115
H	0.035455	2.502474	-3.242417	H	-0.001552	2.663370	-3.047680
C	-0.536014	4.071867	0.572177	C	0.326146	4.116922	0.514007
H	-1.029284	4.959495	0.900790	H	0.056328	5.084243	0.874879
O	-3.980187	-0.848674	-0.478958	O	-3.966415	-0.684978	-0.629895
H	-3.699783	-1.741796	-0.223965				

Point A5				Point A6			
C	-1.181068	1.366445	0.241929	C	-1.273570	0.461681	-0.145869
C	-0.373666	1.777407	-0.884363	C	-0.606303	0.909418	-1.342897
C	0.957170	1.986343	-0.408984	C	0.355435	1.901301	-0.959174
C	0.975969	1.742854	1.005739	C	0.274533	2.082133	0.464280
C	-0.336071	1.352813	1.423272	C	-0.739886	1.204526	0.968489
C	-2.589919	0.936944	0.108382	C	-2.463598	-0.426574	-0.081871
C	-0.847168	1.980774	-2.294721	C	-0.936872	0.482331	-2.744251
C	2.122183	2.462109	-1.230140	C	1.237855	2.674013	-1.899463
C	2.153575	1.954875	1.914353	C	1.070658	3.065098	1.276046
C	-0.742337	1.216765	2.866151	C	-1.211500	1.107789	2.391045
Fe	0.334689	0.004808	0.005849	Fe	0.725236	0.084157	0.011801
C	-0.325177	-2.399992	2.131269	C	0.646524	-1.901842	2.568972
C	0.201123	-1.916211	0.809363	C	1.272621	-1.464925	1.276030
C	-1.972614	-2.121926	-0.641223	C	-0.130169	-2.941347	-0.349484
C	-0.540863	-1.819882	-0.423310	C	0.908087	-1.943715	-0.033683
C	1.569771	-1.600501	0.520745	C	2.379539	-0.565558	1.121964
C	2.701617	-1.643426	1.507669	C	3.107213	0.131259	2.237458
C	0.382917	-1.475544	-1.471604	C	1.822656	-1.368822	-0.985806
C	1.683017	-1.331108	-0.885039	C	2.718892	-0.506202	-0.272543
C	0.044490	-1.369625	-2.930786	C	1.857846	-1.678706	-2.454912
C	2.956522	-1.038676	-1.626461	C	3.861265	0.265124	-0.871258
H	-1.688811	0.691223	3.001555	H	-1.597670	0.108375	2.611515
H	-0.860247	2.211086	3.318486	H	-2.019377	1.825276	2.590504
H	0.017397	0.686928	3.449592	H	-0.404298	1.319843	3.100155
H	3.100264	1.765876	1.398884	H	2.051933	3.256996	0.830065
H	2.116070	1.298798	2.789127	H	1.237054	2.704045	2.295857
H	2.183488	2.989938	2.282836	H	0.552111	4.031443	1.351544
H	3.483687	-0.918728	1.260402	H	3.524478	1.089981	1.913386
H	3.170675	-2.637366	1.524816	H	3.942861	-0.479662	2.607983
H	2.358712	-1.428298	2.524769	H	2.447478	0.328389	3.088880
H	2.033036	2.156470	-2.277106	H	1.498748	2.086128	-2.785742
H	3.071845	2.072018	-0.851547	H	2.172681	2.980509	-1.419544
H	2.189135	3.558846	-1.214664	H	0.737270	3.587401	-2.251141
H	2.777122	-0.433957	-2.520887	H	3.653094	0.557731	-1.905458
H	3.440655	-1.969427	-1.954048	H	4.782938	-0.334324	-0.880970
H	3.676759	-0.501158	-1.001663	H	4.075416	1.178470	-0.306280
H	0.671019	-0.633099	-3.443425	H	2.161936	-0.812504	-3.052380
H	-1.000928	-1.081202	-3.078556	H	0.875247	-2.004592	-2.809052
H	0.194267	-2.333500	-3.437617	H	2.571043	-2.487472	-2.670375
H	-0.039877	1.814951	-3.014427	H	-0.050904	0.472054	-3.386864
H	-1.211185	3.007132	-2.437019	H	-1.663355	1.168822	-3.202193
H	-1.416915	-2.460862	2.124459	H	-0.371081	-2.269342	2.404710
H	-0.024688	-1.754342	2.963397	H	0.599567	-1.087868	3.299463
C	-3.066250	-0.329594	0.833267	C	-2.486582	-1.785131	-0.268389
H	-1.672152	1.309647	-2.542442	H	-1.376333	-0.519256	-2.756200
H	0.054921	-3.407252	2.350369	H	1.221938	-2.718794	3.027728
O	-3.365229	1.516140	-0.649369	N	-3.644663	0.264079	0.230974
C	-3.050949	-1.518740	-0.116147	C	-1.477799	-2.828823	-0.435706
H	-4.028573	-1.894738	-0.411028	H	-1.964044	-3.777255	-0.672709
H	-4.092674	-0.154161	1.169208	H	0.258027	-3.945542	-0.536200
H	-2.452143	-0.539251	1.708518	C	-3.868747	1.605921	-0.305548
H	-2.164562	-2.942332	-1.335268	C	-4.876779	-0.474568	0.453746
				H	-3.480901	-2.218999	-0.306490
				H	-5.301729	-0.899008	-0.471659
				H	-5.617962	0.204842	0.884566
				H	-4.705122	-1.292368	1.159487
				H	-4.285919	1.577270	-1.326029
				H	-2.937284	2.169839	-0.329663
				H	-4.579251	2.136668	0.336400

Point B2				Point B3			
C	0.183964	-0.00187	-0.06692	C	0.00462	0.00108	-0.0023
C	-0.47374	0.049983	1.214934	C	-0.02272	0.020158	1.439099
C	0.534415	0.031439	2.231169	C	1.330849	0.014927	1.906933
C	1.816537	-0.06293	1.593457	C	2.201733	-0.0386	0.767103
C	1.608815	-0.09119	0.174946	C	1.390522	-0.05415	-0.41465
C	-0.46511	-0.02943	-1.40513	C	-1.16223	-0.02774	-0.92468
C	-1.95452	-0.00743	1.471467	C	-1.23946	-0.0714	2.318441
C	0.270185	0.02322	3.711179	C	1.747435	-0.01025	3.350704
C	3.139876	-0.17976	2.296988	C	3.702062	-0.12515	0.808797
C	2.695208	-0.23097	-0.85451	C	1.911231	-0.1549	-1.82097
Fe	0.823072	1.663008	0.942374	Fe	0.994152	1.669686	0.663075
C	1.269171	3.112413	-1.90311	C	0.194739	3.195761	-2.06743
C	1.037163	3.207667	-0.42144	C	0.601759	3.246559	-0.62211
C	-1.61714	3.197272	-0.30349	C	-1.76467	3.189044	0.584349
C	-0.23015	3.282857	0.261949	C	-0.26809	3.279634	0.526298
C	2.075055	3.303914	0.564525	C	1.954527	3.343797	-0.15388
C	3.552176	3.32899	0.286472	C	3.183703	3.404527	-1.01636
C	0.042022	3.443144	1.671931	C	0.562909	3.413563	1.700693
C	1.463846	3.445896	1.853524	C	1.931727	3.444771	1.276624
C	-0.96368	3.634898	2.773967	C	0.099819	3.556336	3.124469
C	2.193675	3.647107	3.152462	C	3.131971	3.623768	2.163952
H	2.402689	0.210527	-1.80891	H	1.222855	0.299245	-2.53625
H	2.925931	-1.2884	-1.04537	H	2.040272	-1.20438	-2.12058
H	3.62125	0.249247	-0.52151	H	2.886062	0.334553	-1.92047
H	3.141463	0.362887	3.248083	H	4.11065	0.36897	1.696348
H	3.959699	0.216418	1.689532	H	4.159289	0.342078	-0.06943
H	3.379857	-1.22915	2.521139	H	4.040089	-1.17113	0.834346
H	4.129439	2.922116	1.123109	H	4.055422	2.979507	-0.50841
H	3.905663	4.356363	0.117329	H	3.434261	4.442989	-1.27697
H	3.80794	2.747926	-0.60493	H	3.050206	2.859028	-1.95551
H	-0.60723	0.626795	3.967551	H	1.028375	0.522438	3.981437
H	1.120636	0.418474	4.276264	H	2.727337	0.455527	3.497794
H	0.083085	-0.9967	4.077304	H	1.81582	-1.04002	3.730262
H	1.616423	3.278696	4.006606	H	2.97951	3.174337	3.150502
H	2.396219	4.712569	3.333708	H	3.355988	4.688586	2.322204
H	3.158188	3.128981	3.15813	H	4.026205	3.166474	1.728537
H	-0.58964	3.244563	3.725907	H	0.862609	3.205298	3.826894
H	-1.91132	3.128233	2.567947	H	-0.81194	2.985596	3.325471
H	-1.19209	4.699723	2.925179	H	-0.1131	4.606099	3.372634
H	-2.30917	0.829881	2.082701	H	-1.26765	0.71659	3.079307
H	-2.21358	-0.92984	2.009197	H	-1.25587	-1.03242	2.851111
H	0.461369	2.576218	-2.4041	H	-0.75418	2.67307	-2.20133
H	2.206471	2.592872	-2.12672	H	0.948626	2.687936	-2.67751
C	-1.38473	0.850353	-1.87539	C	-2.2007	0.844608	-0.94742
H	-2.51502	-0.00473	0.534435	H	-2.15665	-0.00684	1.729481
H	1.34092	4.109783	-2.35873	H	0.078	4.208603	-2.47785
N	0.03222	-1.0768	-2.23604	N	-1.065	-1.06994	-1.89455
C	-2.11274	2.040369	-1.29569	C	-2.62383	2.023517	-0.1024
C	-0.33371	-1.0778	-3.6416	C	-1.99978	-1.07216	-3.00593
C	-0.0032	-2.4223	-1.66338	C	-0.84098	-2.41589	-1.3675
H	0.654566	-3.08138	-2.24054	H	-0.49922	-3.07146	-2.17591
H	-1.01923	-2.85659	-1.67656	H	-1.75834	-2.85555	-0.93586
H	0.347873	-2.40331	-0.63048	H	-0.07337	-2.39577	-0.59211
H	-0.11916	-0.10191	-4.08731	H	-2.00454	-0.09382	-3.49586
H	-1.3991	-1.31185	-3.82237	H	-3.03803	-1.31511	-2.71318
H	0.264896	-1.8356	-4.15803	H	-1.67602	-1.82393	-3.73353
C	-2.98896	6.514919	-4.78628	C	-4.69871	6.662279	-2.96232
C	-1.56606	6.570017	-4.57049	C	-3.29426	6.570147	-3.2859
C	-1.23837	7.908586	-4.19096	C	-2.71837	7.858125	-3.06056
C	-2.45	8.680564	-4.16439	C	-3.75493	8.745353	-2.602

C	-3.53675	7.826154	-4.53003	C	-4.98099	8.013494	-2.53847
C	-3.72019	5.412823	-5.42547	C	-5.65627	5.623335	-3.11654
C	-0.59778	5.444833	-4.79231	C	-2.62117	5.358165	-3.85721
C	0.145816	8.440203	-3.9502	C	-1.29287	8.248124	-3.33013
C	-2.5518	10.15611	-3.90161	C	-3.59734	10.21401	-2.32844
C	-4.96385	8.246684	-4.73237	C	-6.34017	8.549053	-2.19713
Fe	-2.59446	7.08171	-2.80633	Fe	-3.57038	7.123227	-1.27852
C	-5.05626	5.34223	-1.43064	C	-5.53441	5.253279	0.522182
C	-3.78362	6.136228	-1.34795	C	-4.28447	6.079309	0.387806
C	-2.11811	4.171471	-1.3978	C	-2.69159	4.154486	-0.19684
C	-2.43525	5.606177	-1.31799	C	-2.97638	5.580861	0.013931
C	-3.71499	7.539237	-1.08682	C	-4.15485	7.467972	0.705557
C	-4.89424	8.46082	-0.95242	C	-5.24233	8.365752	1.226318
C	-1.54992	6.701641	-1.02091	C	-2.05204	6.6824	0.102539
C	-2.33892	7.889427	-0.88321	C	-2.77989	7.841893	0.524195
C	-0.06428	6.621463	-0.81977	C	-0.57105	6.633299	-0.14384
C	-1.82691	9.244091	-0.48333	C	-2.19058	9.192012	0.819639
Cl	-3.17448	5.097831	-7.12156	H	-6.99682	7.749729	-1.83958
H	-5.64202	7.39014	-4.68656	H	-6.81784	8.998747	-3.07882
H	-5.09667	8.721431	-5.71474	H	-6.29176	9.320339	-1.42242
H	-5.2835	8.970993	-3.97675	H	-2.59664	10.45281	-1.9559
H	-1.77336	10.50359	-3.21619	H	-4.32226	10.56724	-1.58796
H	-3.52148	10.42322	-3.46962	H	-3.75414	10.80166	-3.24389
H	-2.44345	10.7262	-4.83506	H	-5.07107	9.410804	0.948422
H	-4.63507	9.492238	-1.21197	H	-5.29159	8.326434	2.32363
H	-5.27131	8.47029	0.080146	H	-6.22669	8.080762	0.843641
H	-5.72261	8.153234	-1.59843	H	-0.62148	7.385814	-3.28043
H	0.824605	7.658445	-3.59713	H	-0.93357	8.989234	-2.60879
H	0.151819	9.24655	-3.20984	H	-1.18767	8.6888	-4.33131
H	0.572005	8.847948	-4.8776	H	-1.29551	9.384905	0.21987
H	-0.80945	9.421737	-0.84525	H	-1.89572	9.268743	1.875814
H	-1.80188	9.341094	0.611345	H	-2.90278	9.998559	0.621245
H	-2.46225	10.0484	-0.86517	H	-0.20002	7.582141	-0.54457
H	0.432735	7.550259	-1.1155	H	-0.30872	5.842475	-0.84918
H	0.373735	5.804014	-1.39584	H	-0.02264	6.431531	0.785964
H	0.178988	6.440869	0.235774	H	-1.54165	5.376188	-3.68302
H	0.273376	5.53452	-4.13621	H	-2.77798	5.299982	-4.9436
H	-0.23156	5.436966	-5.82781	H	-5.88053	4.85485	-0.43688
H	-4.87625	4.338083	-1.82155	H	-5.36068	4.397184	1.186426
H	-5.50071	5.228838	-0.43151	C	-6.47782	4.741779	-3.26095
C	-4.75549	4.697241	-4.9881	H	-3.01571	4.439677	-3.41368
H	-1.06156	4.473608	-4.59647	H	-6.3498	5.84434	0.950376
H	-5.80969	5.829686	-2.05895	C	-3.37212	3.15352	-0.78765
C	-2.47919	3.179522	-2.23272	H	-2.03893	3.221849	1.646201
H	-5.26017	3.968113	-5.61244	H	-4.25576	3.138353	-1.42166
H	-5.11897	4.842436	-3.97895	H	-2.98877	0.618941	-1.6635
H	-2.30786	3.229117	0.548046	H	-3.26732	1.613968	0.6972
H	-2.99422	3.176122	-3.19079	H	-7.2045	3.975005	-3.41298
H	-1.7887	0.628899	-2.86154				
H	-3.04432	1.645862	-0.85181				

Point B4				Point B5			
C	-0.11883	-0.59511	0.630406	C	0.353588	-0.38891	0.205174
C	-0.83439	0.124802	1.680494	C	-0.47461	-0.20139	1.370335
C	0.14449	0.580873	2.613626	C	0.384132	0.062116	2.485626
C	1.447659	0.193429	2.152201	C	1.744046	0.009403	2.030594
C	1.303282	-0.53831	0.936313	C	1.734235	-0.2773	0.625876
C	-0.72256	-1.23761	-0.52716	C	-0.09361	-0.71094	-1.17708
C	-2.32126	0.191409	1.886647	C	-1.96527	-0.37992	1.456121
C	-0.14341	1.300304	3.900531	C	-0.07689	0.272035	3.900887
C	2.743224	0.466815	2.861272	C	2.964902	0.163291	2.893641
C	2.440481	-1.11268	0.138418	C	2.958643	-0.46263	-0.22596
Fe	0.472671	1.3441	0.665646	Fe	0.694443	1.481553	0.9721
C	1.359053	1.286934	-2.44375	C	1.469337	2.488954	-1.98582
C	0.921293	2.056968	-1.22938	C	0.9877	2.802297	-0.59697
C	-1.71661	2.012189	-1.55957	C	-1.64295	2.502233	-0.86033
C	-0.43315	2.366958	-0.83844	C	-0.37579	2.838953	-0.1281
C	1.796679	2.681592	-0.2834	C	1.839508	3.173135	0.496869
C	3.298298	2.664164	-0.32601	C	3.334037	3.322016	0.435245
C	-0.38108	3.204857	0.330488	C	-0.35033	3.252827	1.256989
C	0.997658	3.380103	0.682344	C	1.017115	3.446886	1.639092
C	-1.54888	3.828665	1.041806	C	-1.53039	3.499068	2.15641
C	1.521038	4.208627	1.821344	C	1.498828	3.927037	2.979376
H	2.154327	-1.31442	-0.89717	H	2.76575	-0.2024	-1.26822
H	2.801643	-2.05177	0.576761	H	3.296162	-1.50834	-0.21228
H	3.288924	-0.42301	0.117655	H	3.78932	0.152304	0.136234
H	2.710049	1.409933	3.414739	H	2.779165	0.832231	3.740466
H	3.584867	0.516881	2.164455	H	3.811235	0.569007	2.330558
H	2.964269	-0.33018	3.584265	H	3.283846	-0.80412	3.307651
H	3.734121	2.746391	0.674008	H	3.796884	3.170651	1.41578
H	3.678018	3.508386	-0.9176	H	3.617891	4.328195	0.094649
H	3.685323	1.749098	-0.78413	H	3.786426	2.605888	-0.25786
H	-1.06938	1.879913	3.845841	H	-1.05267	0.767857	3.933654
H	0.665976	1.986929	4.16583	H	0.627435	0.887326	4.470393
H	-0.25151	0.586325	4.728295	H	-0.17843	-0.68448	4.433661
H	0.838956	4.200976	2.676707	H	0.848631	3.582403	3.789948
H	1.65144	5.255842	1.515742	H	1.52225	5.025394	3.025491
H	2.493821	3.848266	2.169175	H	2.511285	3.571576	3.195895
H	-1.28607	4.104949	2.066988	H	-1.28449	3.278698	3.200443
H	-2.40992	3.155475	1.09707	H	-2.39426	2.882691	1.890493
H	-1.8763	4.740511	0.525738	H	-1.85459	4.548755	2.111984
H	-2.60774	1.112628	2.402567	H	-2.46134	0.471231	1.935649
H	-2.6585	-0.64811	2.509633	H	-2.21098	-1.27119	2.050371
H	0.680118	0.462714	-2.67892	H	0.785892	1.814215	-2.50572
H	2.359659	0.865418	-2.31135	H	2.457207	2.017524	-1.96827
C	-1.79587	-0.66639	-1.34638	C	-1.00283	-0.0291	-1.91893
H	-2.87442	0.146596	0.946579	H	-2.40464	-0.51617	0.466001
H	1.391989	1.93997	-3.32535	H	1.561954	3.402917	-2.58417
N	-0.3656	-2.48297	-0.8383	N	0.606024	-1.82475	-1.72939
C	-2.1579	0.579647	-1.73746	C	-1.90893	1.15131	-1.66658
C	-0.72407	-3.11879	-2.11761	C	0.464152	-2.10164	-3.14779
C	0.284697	-3.41054	0.099193	C	0.59497	-3.05006	-0.93081
H	1.28999	-3.66058	-0.24613	H	1.386489	-3.72134	-1.2817
H	-0.31603	-4.32484	0.121916	H	-0.36706	-3.5891	-1.00309
H	0.325949	-2.97911	1.095969	H	0.778943	-2.81941	0.119734
H	-0.80231	-2.37382	-2.90744	H	0.664044	-1.19699	-3.72995
H	-1.66793	-3.66657	-2.02239	H	-0.53656	-2.47822	-3.42906
H	0.067517	-3.82632	-2.37228	H	1.196645	-2.86549	-3.42958
C	-2.72153	4.815655	-5.81752	C	-3.52981	3.800053	-5.33802
C	-2.18642	6.15192	-5.8437	C	-2.60317	4.718516	-5.94903
C	-3.24107	7.053411	-5.48184	C	-3.26701	5.981417	-6.0956
C	-4.43277	6.282441	-5.26088	C	-4.60588	5.844763	-5.59392
C	-4.12159	4.899803	-5.48233	C	-4.77592	4.494876	-5.13838

C	-1.98414	3.601958	-6.20661	C	-3.32337	2.347234	-5.16536
C	-0.7881	6.526744	-6.24384	C	-1.22906	4.368172	-6.44302
C	-3.13471	8.550857	-5.41159	C	-2.68843	7.205027	-6.74817
C	-5.79037	6.834944	-4.92784	C	-5.66883	6.906773	-5.62087
C	-5.08734	3.750265	-5.46009	C	-6.04828	3.876444	-4.63272
Fe	-2.91538	5.634043	-3.96917	Fe	-3.22583	5.400913	-4.0852
C	-4.68567	3.853445	-1.94409	C	-4.77841	4.511353	-1.38382
C	-3.47518	4.705342	-2.20393	C	-3.63771	5.218133	-2.05798
C	-1.84172	2.81092	-2.88621	C	-2.03831	3.214613	-2.16414
C	-2.19275	4.235698	-2.67144	C	-2.36112	4.630246	-2.39305
C	-3.37228	6.118059	-1.98267	C	-3.5882	6.606758	-2.40598
C	-4.4624	7.005847	-1.45186	C	-4.68066	7.611182	-2.16684
C	-1.29249	5.362003	-2.70503	C	-1.52289	5.673752	-2.92842
C	-2.02897	6.522055	-2.29212	C	-2.28656	6.887981	-2.94076
C	0.171223	5.309751	-3.03447	C	-0.09258	5.534134	-3.35871
C	-1.46865	7.908894	-2.14722	C	-1.78379	8.242256	-3.3547
H	-4.56749	2.803313	-5.2868	H	-5.84275	2.983251	-4.0349
H	-5.61763	3.665457	-6.41929	H	-6.69397	3.570572	-5.46839
H	-5.84551	3.867296	-4.67956	H	-6.62769	4.569919	-4.01409
H	-5.7216	7.73692	-4.3111	H	-5.24656	7.906921	-5.47716
H	-6.39994	6.106826	-4.38279	H	-6.41766	6.748124	-4.8385
H	-6.34286	7.104102	-5.83934	H	-6.19933	6.911978	-6.5838
H	-4.37391	8.028717	-1.83236	H	-4.65329	8.423309	-2.90042
H	-4.42788	7.062095	-0.35463	H	-4.58612	8.068481	-1.17157
H	-5.45455	6.634542	-1.7269	H	-5.67298	7.151359	-2.2192
H	-2.11812	8.871319	-5.163	H	-1.60015	7.244338	-6.63685
H	-3.80795	8.969394	-4.65608	H	-3.0994	8.127111	-6.32432
H	-3.39664	9.012848	-6.37411	H	-2.90567	7.217355	-7.82589
H	-0.67637	8.101997	-2.87794	H	-1.00412	8.172913	-4.11967
H	-1.03613	8.061034	-1.14821	H	-1.35283	8.78123	-2.49894
H	-2.24059	8.67191	-2.28744	H	-2.58803	8.865441	-3.75858
H	0.511611	6.229929	-3.51959	H	0.171449	6.272288	-4.12285
H	0.397552	4.473667	-3.7026	H	0.099395	4.541576	-3.7729
H	0.771142	5.174976	-2.12431	H	0.593547	5.680437	-2.51304
H	-0.41908	7.390952	-5.68155	H	-0.51812	5.189608	-6.30845
H	-0.74133	6.789311	-7.31038	H	-1.24931	4.127564	-7.51555
H	-4.66099	2.935535	-2.53965	H	-4.74294	4.654897	-0.29458
H	-4.75148	3.562552	-0.88578	H	-5.7493	4.882269	-1.72767
C	-1.54779	2.553692	-5.47435	C	-2.79181	1.64688	-4.13856
H	-0.094	5.697249	-6.07908	H	-0.83593	3.49163	-5.91907
H	-5.61472	4.379647	-2.18807	H	-4.74391	3.434294	-1.5747
C	-1.58999	2.174658	-4.05516	C	-2.25646	2.06497	-2.85152
H	-2.526	2.40358	-0.92429	H	-2.4564	2.61524	-0.1322
H	-2.46754	-1.4349	-1.71987	H	-1.23283	-0.4678	-2.88759
H	-3.07537	0.56423	-2.32524	H	-2.85472	0.737969	-1.27322
H	-1.30886	1.127668	-3.94116	H	-2.77195	0.565232	-4.27962
H	-1.06491	1.774887	-6.06552	H	-3.66625	1.747759	-6.01259
H	-1.7701	3.532244	-7.27578				

Point B6			
C	0.000297	0.000289	0.000241
C	0.001871	0.001389	1.443251
C	1.367639	0.002024	1.882798
C	2.207986	-0.00107	0.719342
C	1.367324	-0.01145	-0.44336
C	-1.24756	-0.11329	-0.85969
C	-1.19729	-0.06971	2.347236
C	1.839666	-0.0737	3.307757
C	3.709667	-0.06612	0.716494
C	1.845679	-0.13935	-1.86189
Fe	0.965523	1.688862	0.713521
C	1.649113	3.337734	-1.9558
C	1.229293	3.337377	-0.5112
C	-1.41102	3.186479	-0.7285
C	-0.11145	3.311913	0.026172
C	2.141828	3.414409	0.595408
C	3.637153	3.534968	0.498505
C	-0.01163	3.379152	1.461119
C	1.378543	3.432185	1.809496
C	-1.15438	3.462778	2.434635
C	1.933811	3.580539	3.19843
H	1.134926	0.298492	-2.56686
H	1.970758	-1.1968	-2.13417
H	2.814167	0.349661	-2.01025
H	4.136683	0.40371	1.608371
H	4.135136	0.438864	-0.1566
H	4.062596	-1.10715	0.695608
H	4.132967	3.135999	1.389137
H	3.944334	4.585836	0.397991
H	4.036227	2.996892	-0.36727
H	1.132561	0.398496	3.996905
H	2.808663	0.417927	3.441965
H	1.958039	-1.11828	3.629893
H	1.296325	3.09682	3.945388
H	2.018838	4.639969	3.479909
H	2.933003	3.141729	3.286067
H	-0.87192	3.073531	3.417977
H	-2.0278	2.895178	2.099065
H	-1.47658	4.504067	2.57682
H	-0.98749	0.379502	3.323052
H	-1.50125	-1.11069	2.52569
H	0.955755	2.774198	-2.58213
H	2.642367	2.893302	-2.07639
C	-1.35253	0.876869	-2.02042
H	-2.06121	0.45348	1.926549
H	1.704612	4.35845	-2.35682
N	-1.41486	-1.49151	-1.41091
C	-1.45758	2.205109	-1.91266
C	-2.78202	-1.68863	-1.89452
C	-1.09476	-2.55686	-0.46187
H	-1.21834	-3.52203	-0.96561
H	-1.7513	-2.55913	0.429765
H	-0.05951	-2.47756	-0.12545
H	-3.04629	-0.93254	-2.63798
H	-3.5305	-1.63635	-1.07864
H	-2.86527	-2.67347	-2.36676
C	-2.49284	5.728973	-4.92891
C	-1.41732	6.688423	-4.89043
C	-1.99983	7.999239	-4.86686
C	-3.42842	7.856363	-4.90553

C	-3.73464	6.456401	-4.95667
C	-2.35791	4.270495	-5.12634
C	0.046763	6.363681	-4.971
C	-1.24142	9.297154	-4.87615
C	-4.42806	8.977234	-4.96381
C	-5.1004	5.846602	-5.09328
Fe	-2.65013	6.873499	-3.22703
C	-4.81245	5.079167	-1.61601
C	-3.63708	6.01435	-1.61782
C	-1.79133	4.240842	-1.79847
C	-2.24358	5.627066	-1.66192
C	-3.69009	7.440154	-1.49183
C	-4.94069	8.262659	-1.35537
C	-1.4481	6.822019	-1.52962
C	-2.34461	7.937172	-1.43982
C	0.048666	6.885762	-1.43738
C	-1.94625	9.37309	-1.24563
H	-5.11098	4.815964	-4.72597
H	-5.41874	5.825109	-6.14534
H	-5.85762	6.40996	-4.53767
H	-4.0683	9.869412	-4.44058
H	-5.38319	8.690898	-4.51191
H	-4.63391	9.270416	-6.00317
H	-4.81393	9.2663	-1.7735
H	-5.22171	8.382384	-0.29935
H	-5.78954	7.796317	-1.86603
H	-0.26113	9.195009	-4.39915
H	-1.78454	10.08748	-4.3481
H	-1.06932	9.648678	-5.9034
H	-0.9704	9.588029	-1.69187
H	-1.87912	9.624555	-0.1776
H	-2.6734	10.05696	-1.69513
H	0.442258	7.824819	-1.84047
H	0.512466	6.064086	-1.98675
H	0.382909	6.813711	-0.39315
H	0.654518	7.067012	-4.39324
H	0.400079	6.40728	-6.0112
H	-5.14495	4.86862	-0.58964
H	-5.66758	5.499727	-2.15457
C	-2.05246	3.288186	-4.2512
H	0.250449	5.355125	-4.59859
H	-4.55914	4.122215	-2.08213
C	-1.77685	3.329281	-2.82159
H	-2.22465	3.015461	-0.01136
H	-1.99729	2.282923	-4.66977
H	-2.5256	3.944357	-6.15562
H	-2.09914	0.091734	-0.18303
H	-1.41696	0.427783	-3.01045