

Supplementary data for article:

Milenković, M. R.; Bacchi, A.; Cantoni, G.; Vilipić, J.; Sladić, D.; Vujčić, M.; Gligorijević, N.; Jovanovic, K.; Radulović, S. S. Synthesis, Characterization and Biological Activity of Three Square-Planar Complexes of Ni(II) with Ethyl (2E)-2-[2-(Diphenylphosphino) Benzylidene]Hydrazinecarboxylate and Monodentate Pseudohalides. *European Journal of Medicinal Chemistry* **2013**, 68, 111–120. <https://doi.org/10.1016/j.ejmech.2013.07.039>

## Supplementary data

### **Synthesis, characterization and biological activity of three square-planar complexes of Ni(II) with ethyl (2E)-2-[2-(diphenylphosphino)benzylidene]hydrazinecarboxylate and monodentate pseudohalides**

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- 1. NMR spectra of ligand HL: Fig. S1 – Fig. S5.**
- 2. NMR spectra of complex 1: Fig. S6 – Fig. S9.**
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- 4. NMR spectra of complex 3: Fig. S14 – Fig. S17.**

Fig. S1. <sup>1</sup>H NMR spectrum of ligand HL.

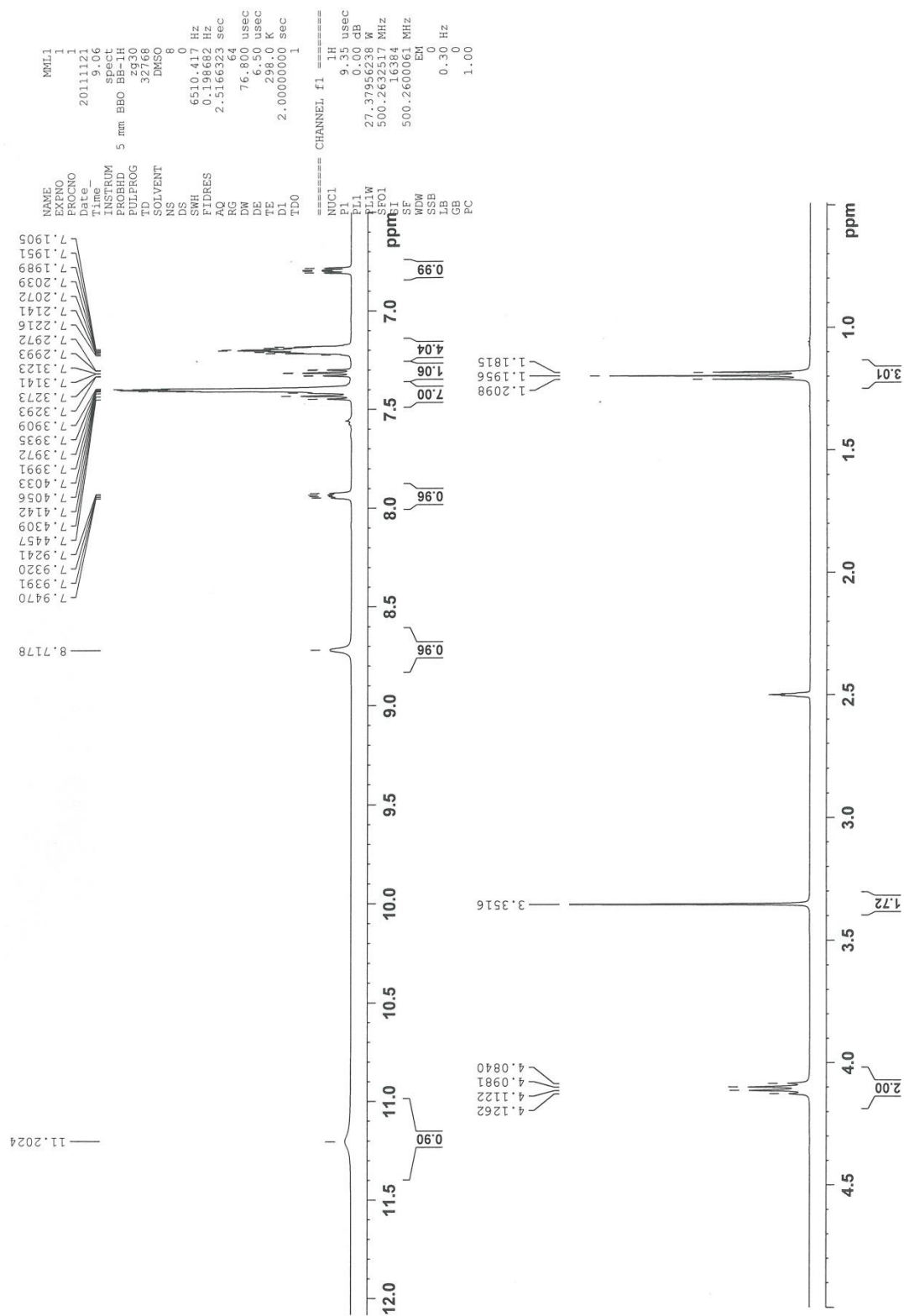




Fig. S2.  $^{13}\text{C}$  NMR spectrum of ligand HL.

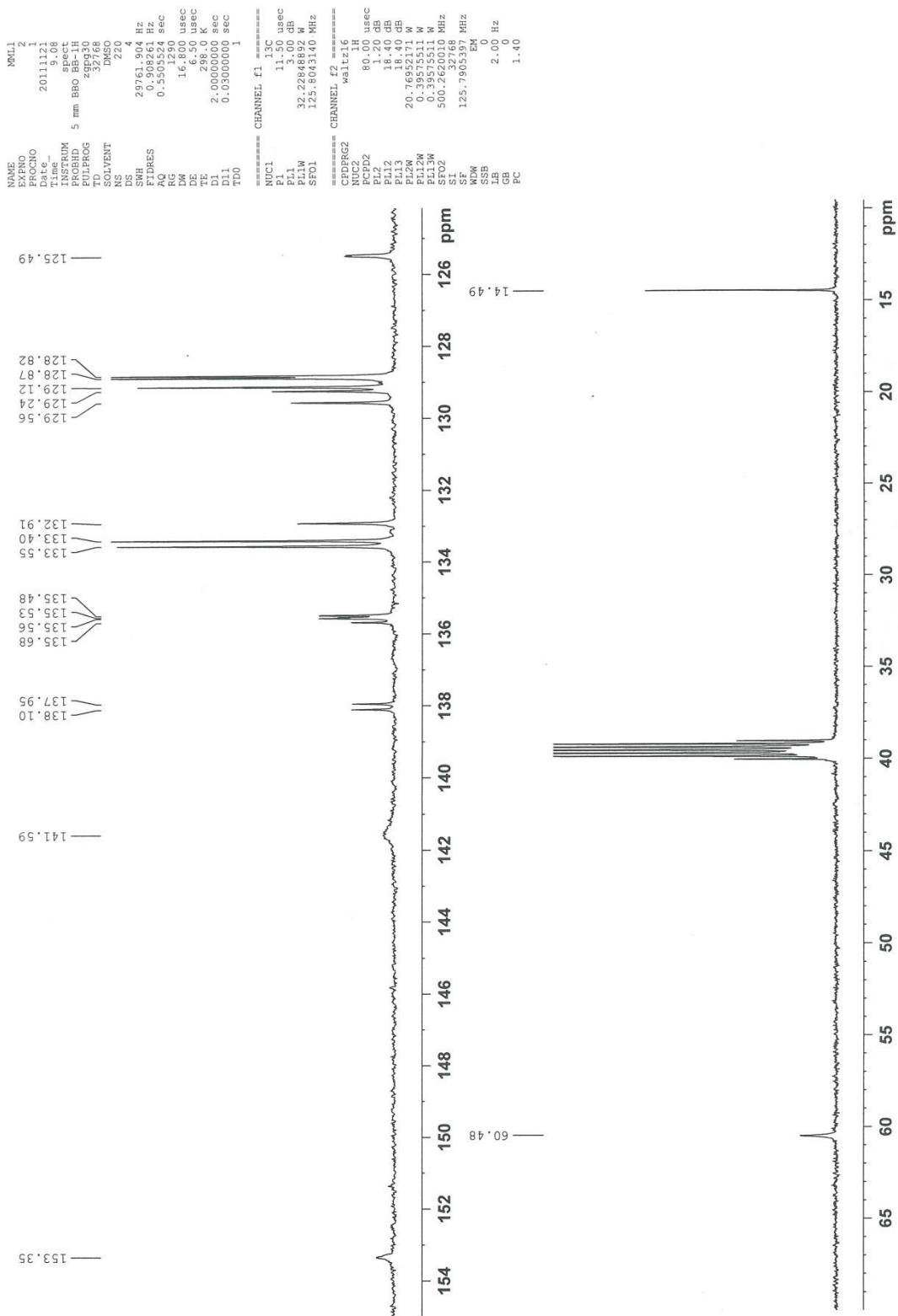


Fig. S3. COSY spectrum of ligand HL.

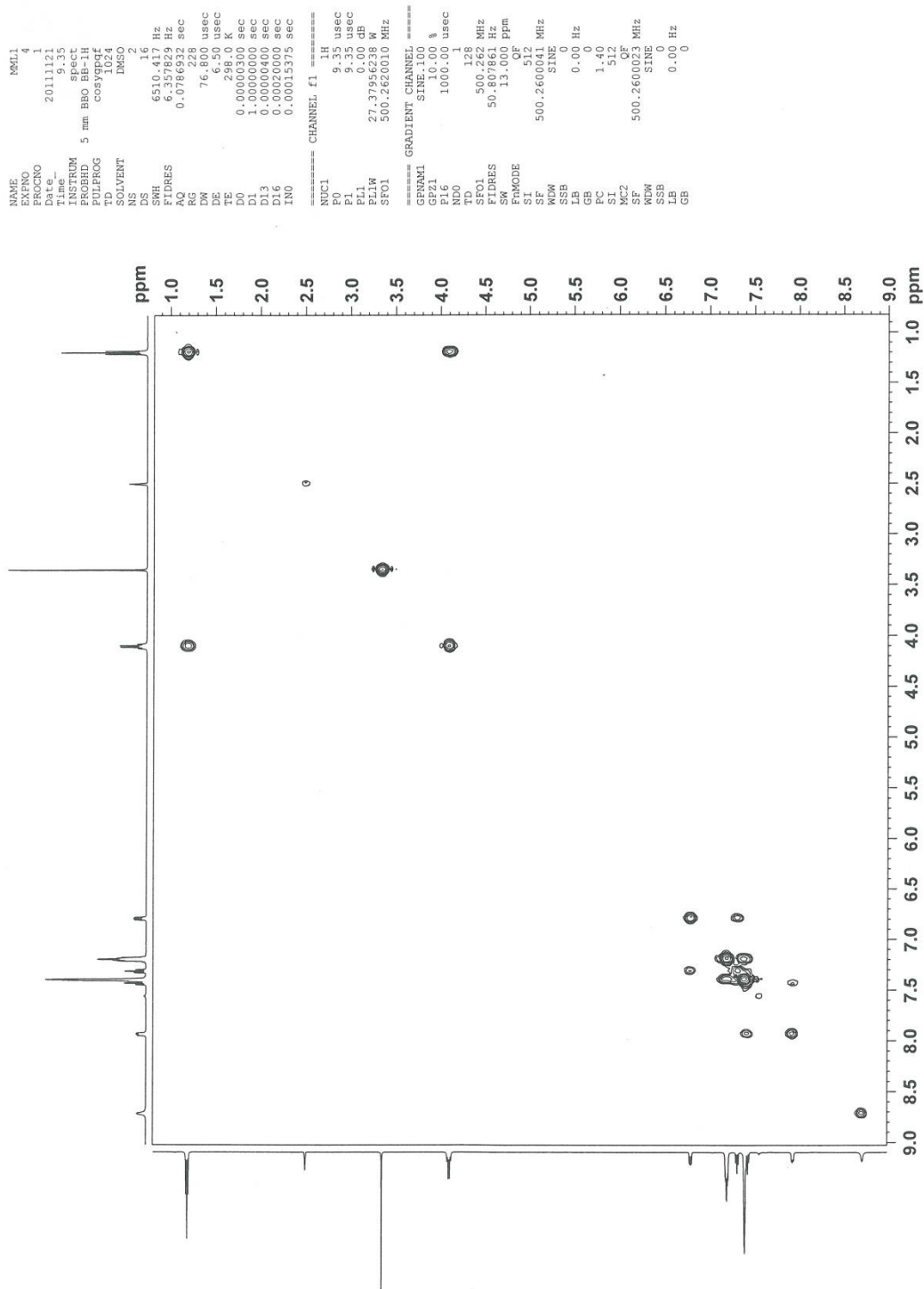




Fig. S4. DEPT spectrum of ligand HL.

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EXPNO         8
PROCNO        1
Date_         2011121
Time          9.44
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       dept135
TD            32768
SOLVENT       DMSO
NS            270
DS            8
SWH           22727.273 Hz
FWDRES        0.593581 Hz
AQ            0.7209360 sec
RG            32800
DW            22.000 usec
DE            6.50 usec
TE            298.0 K
CNST2         145.0000000
D1            2.0000000 sec
D2            0.0034828 sec
D12           0.00002000 sec
TD0           1
===== CHANNEL f1 =====
NUC1          13C
P1            11.50 usec
P2            23.00 usec
PL1           3.00 dB
PL1W          32.22848892 W
SFO1          125.8005402 MHz
===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
P3            11.00 usec
P4            22.00 usec
PCPD2         80.00 usec
PL2           1.20 dB
PL12          18.40 dB
PL2W          20.76952171 W
PL12W         0.39575511 W
SFO2          500.2618755 MHz
SI            32768
SF            125.7905399 MHz
WDW           EM
SSB           0
LB            1.50 Hz
GB            0
PC            1.40
  
```

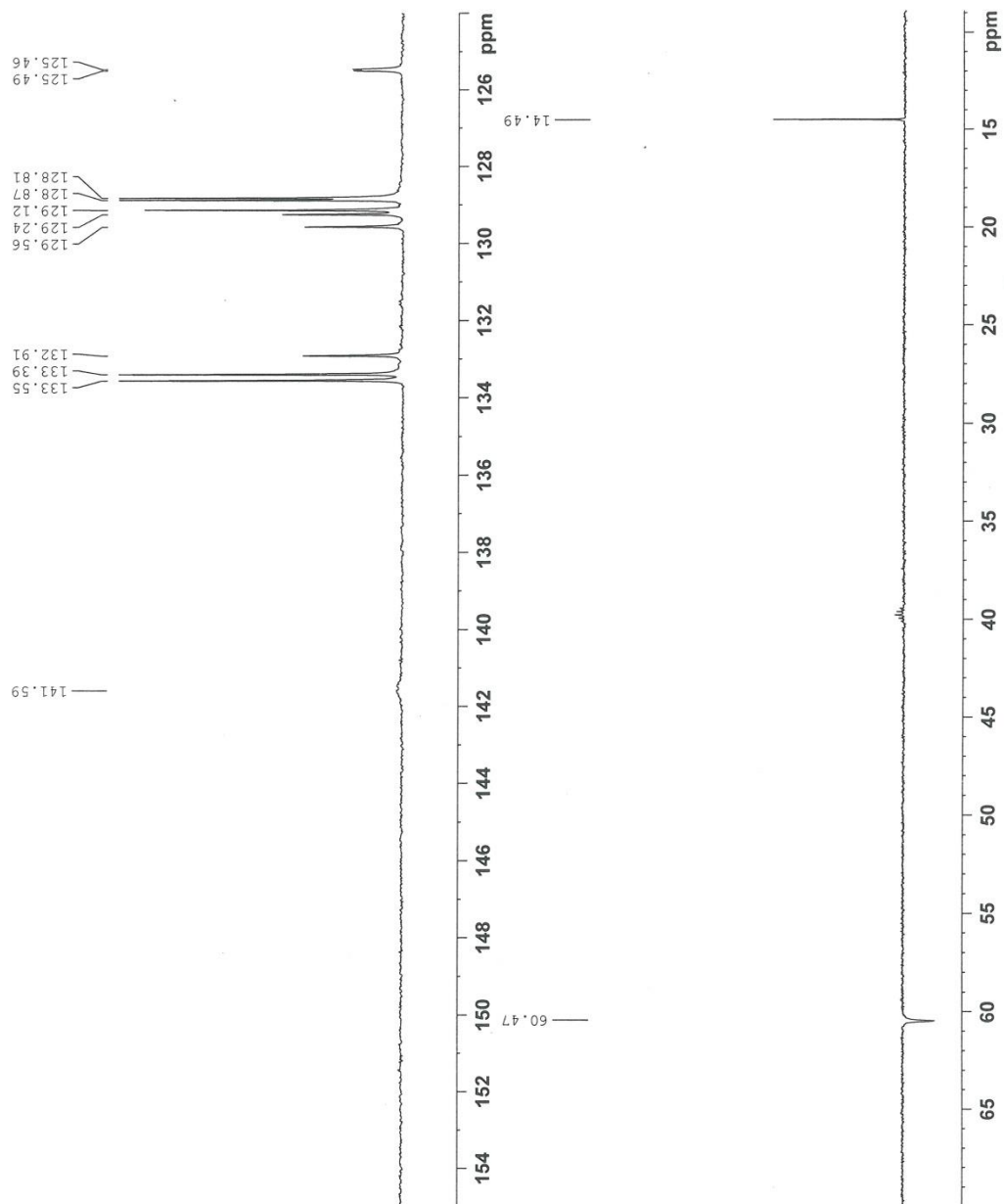








Fig. S5b. HSQC spectrum of ligand HL.

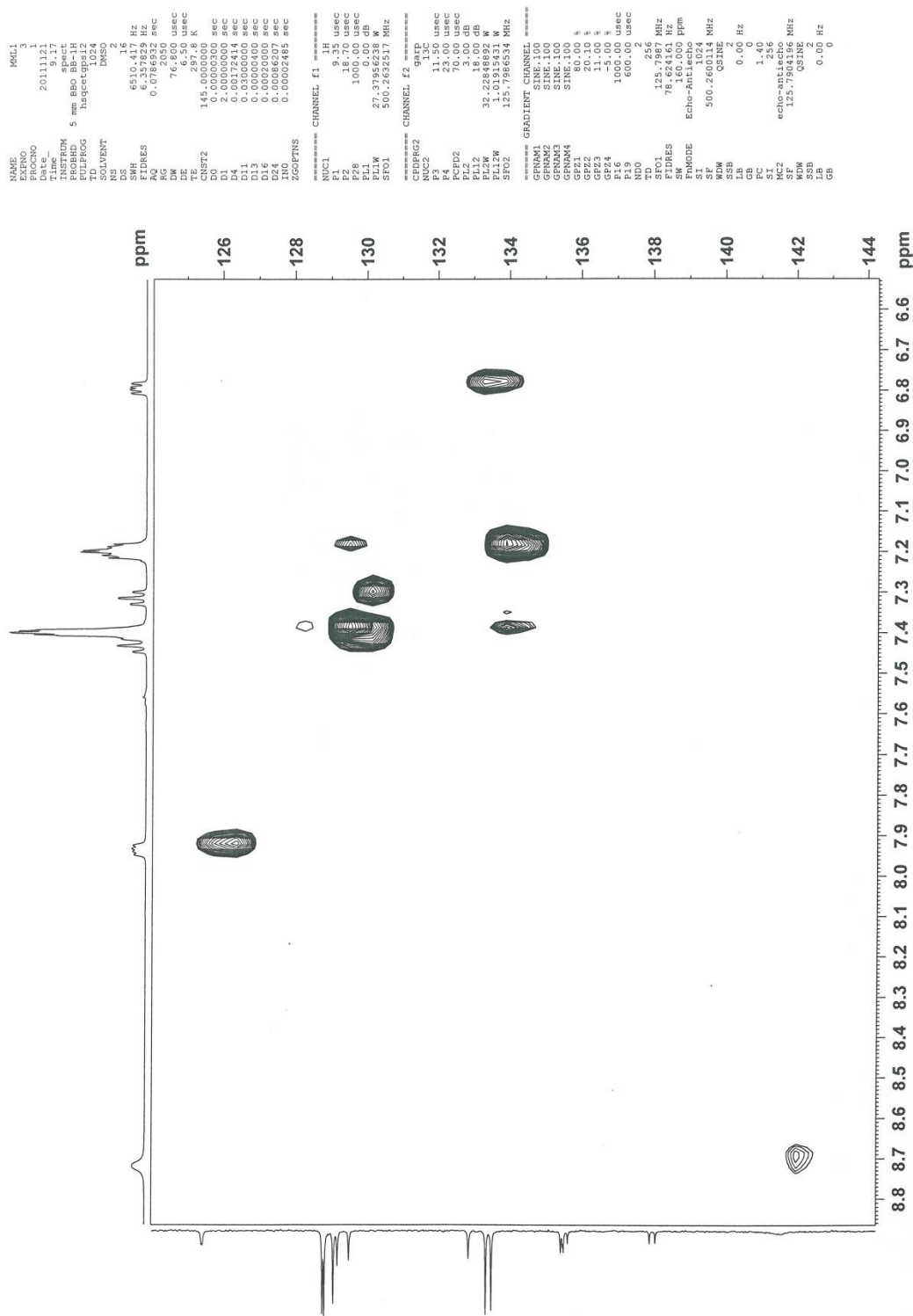


Fig. S6. <sup>1</sup>H NMR spectrum of complex 1.

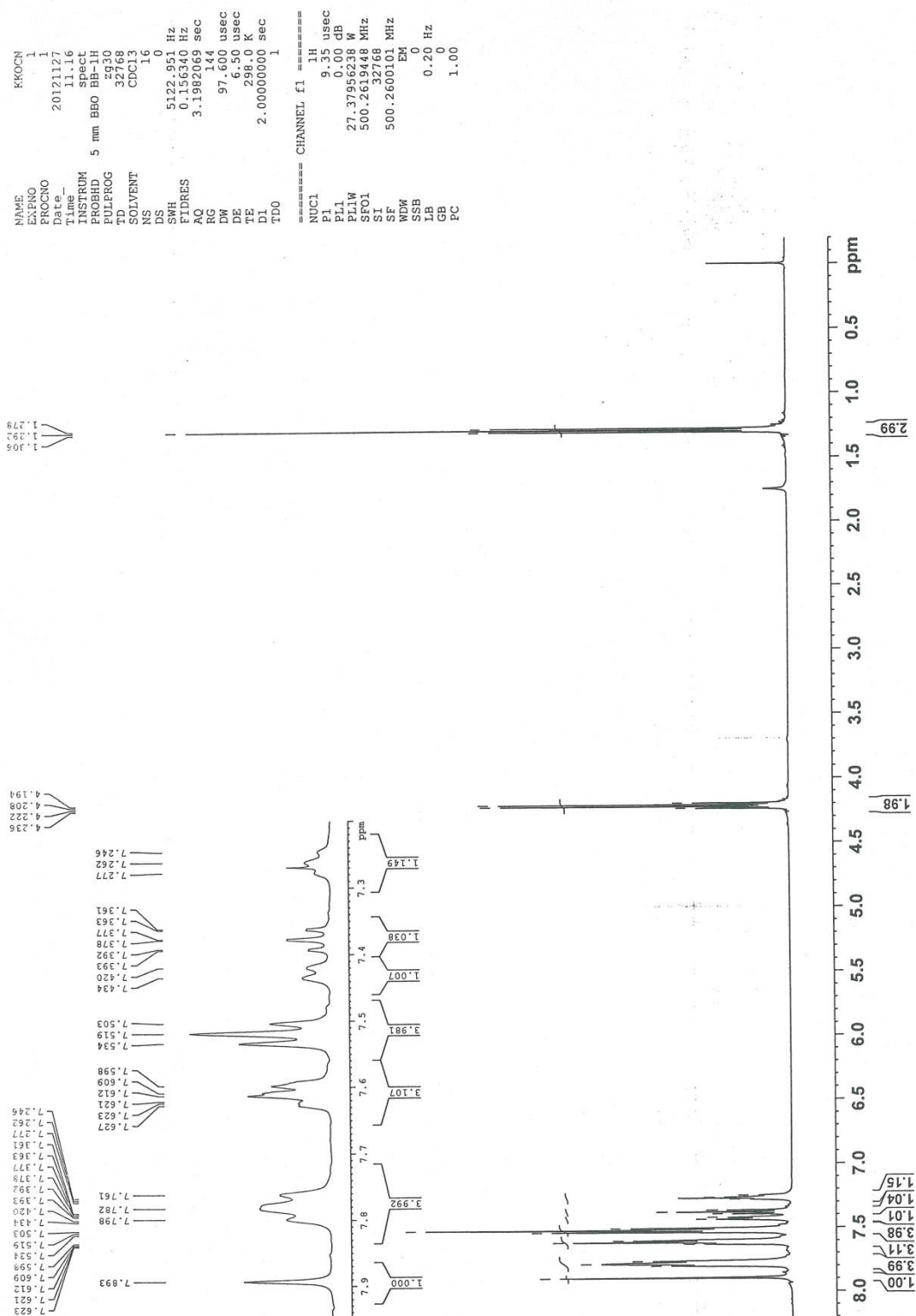


Fig. S7.  $^{13}\text{C}$  NMR spectrum of complex 1.

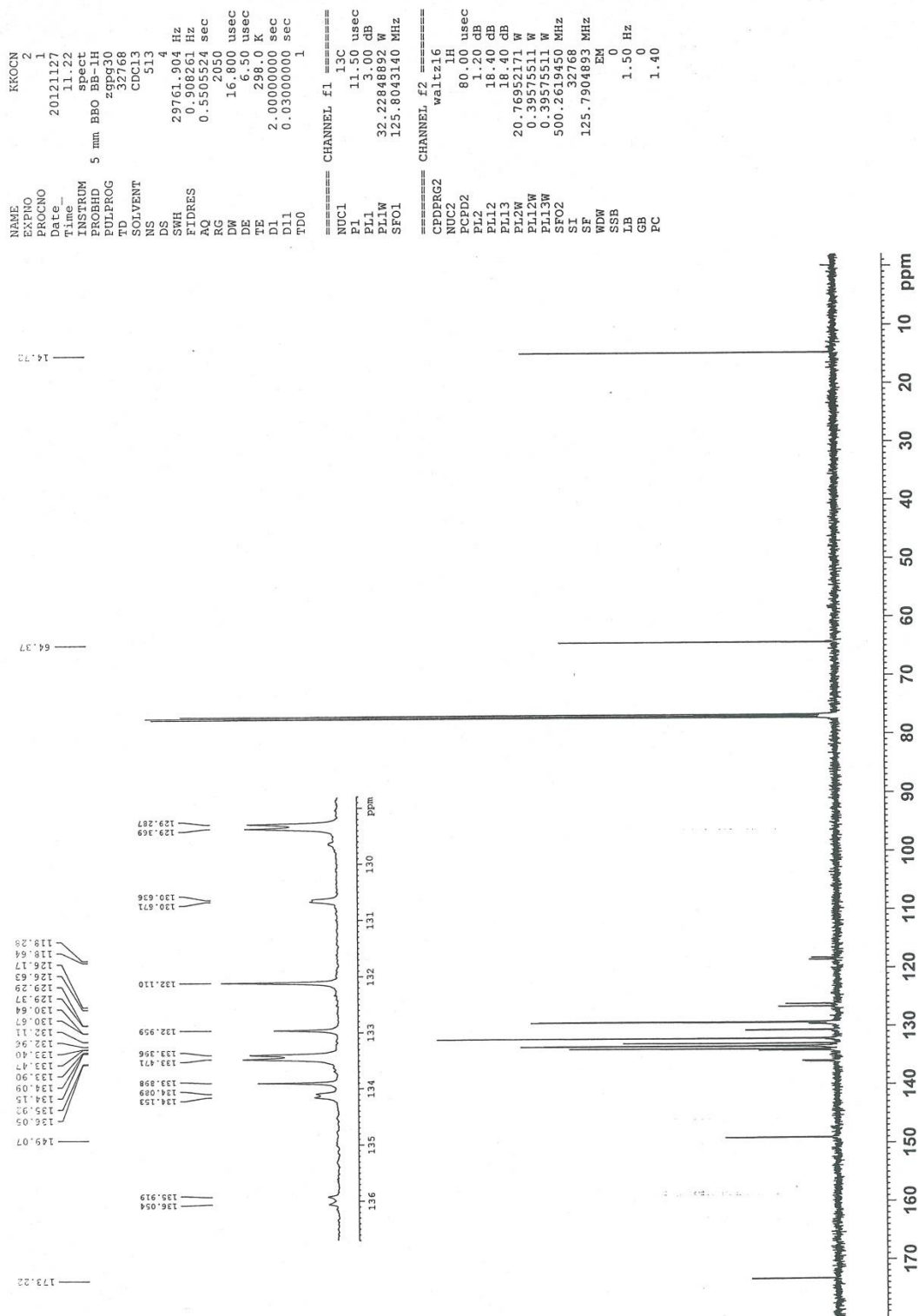


Fig. S8. COSY spectrum of complex 1.

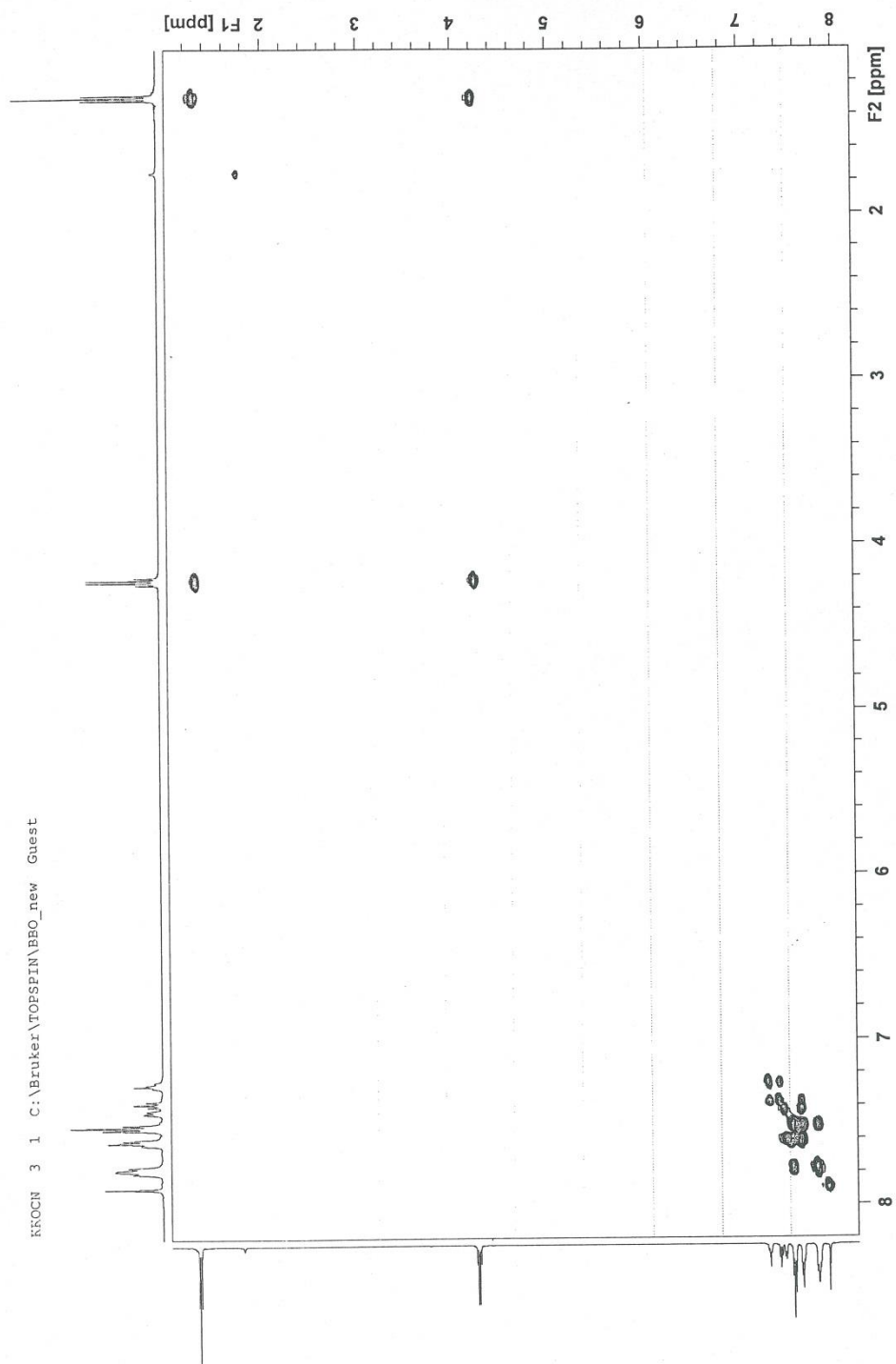


Fig. S9a. HSQC spectrum of complex 1.

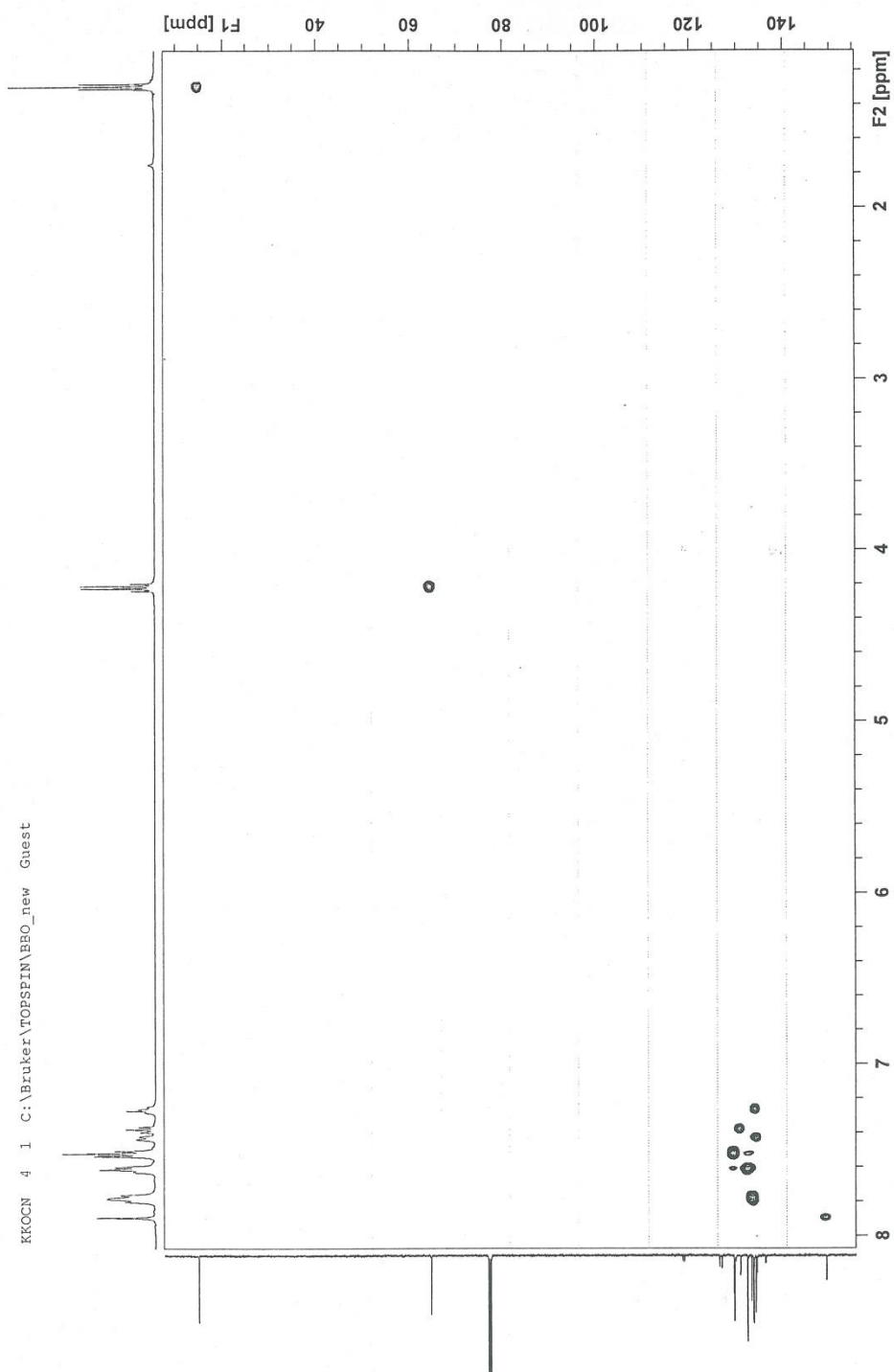


Fig. S9b. HSQC spectrum of complex 1.

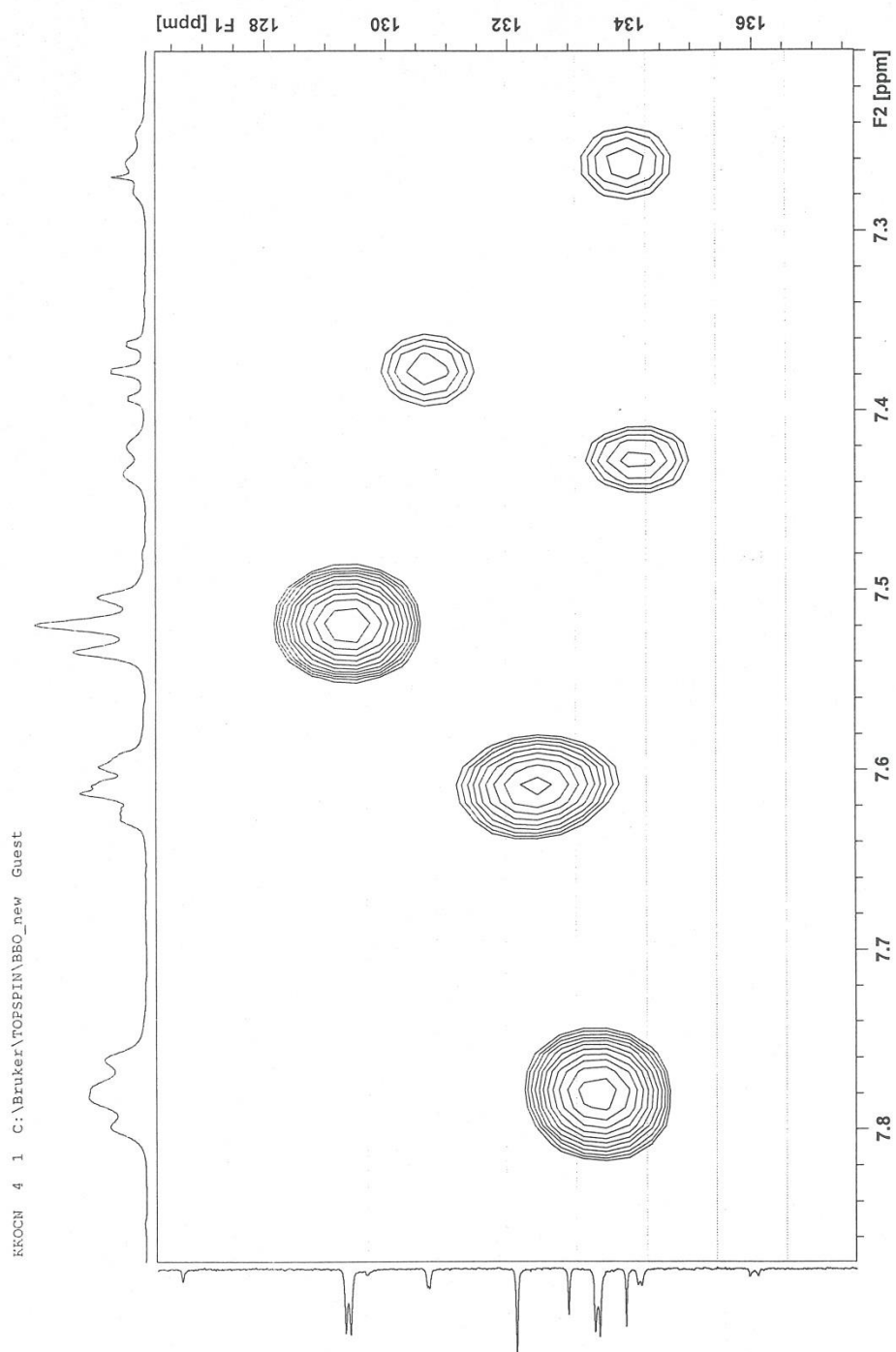






Fig. S11.  $^{13}\text{C}$  NMR spectrum of complex 2.

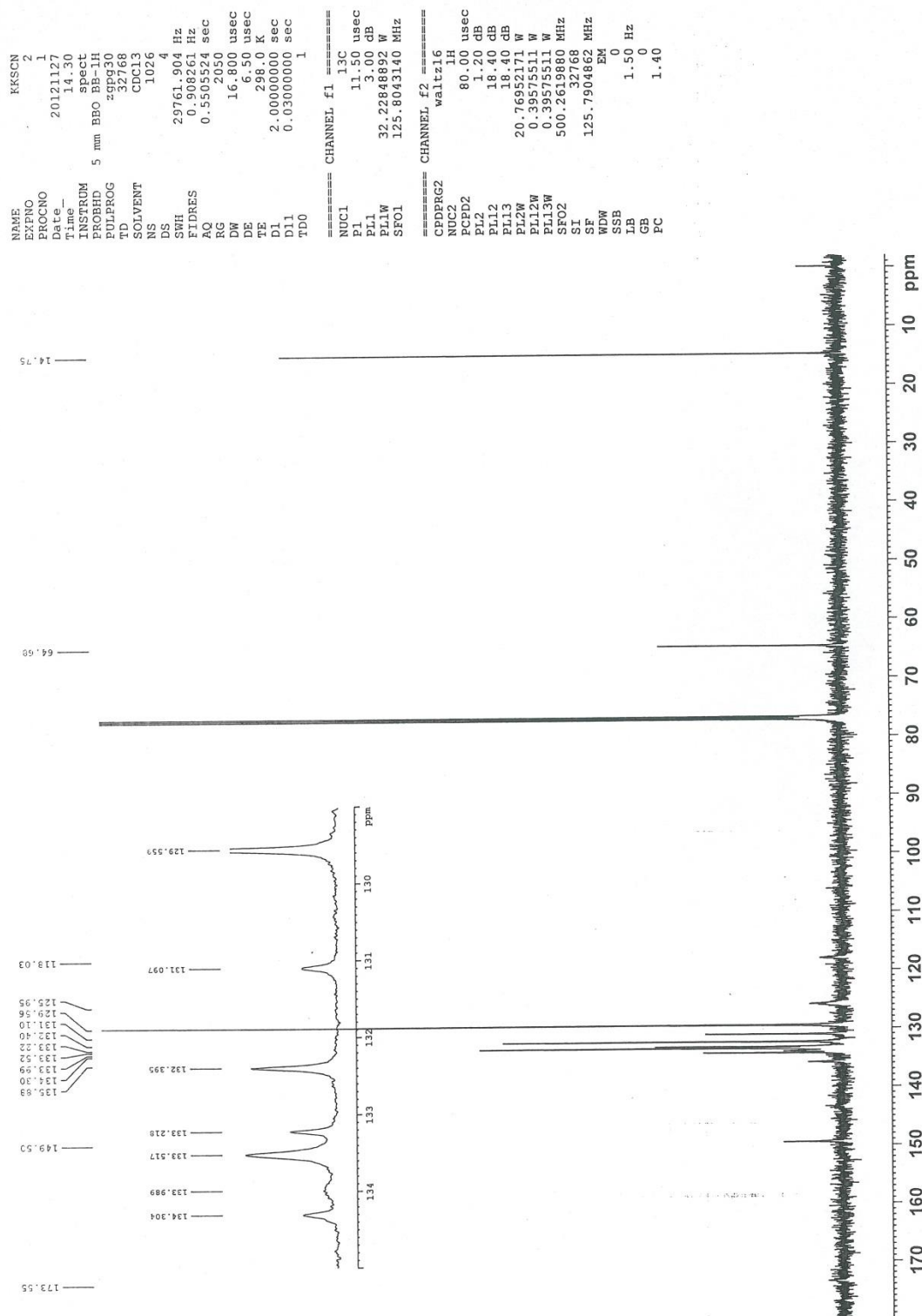


Fig. S12. COSY spectrum of complex 2.

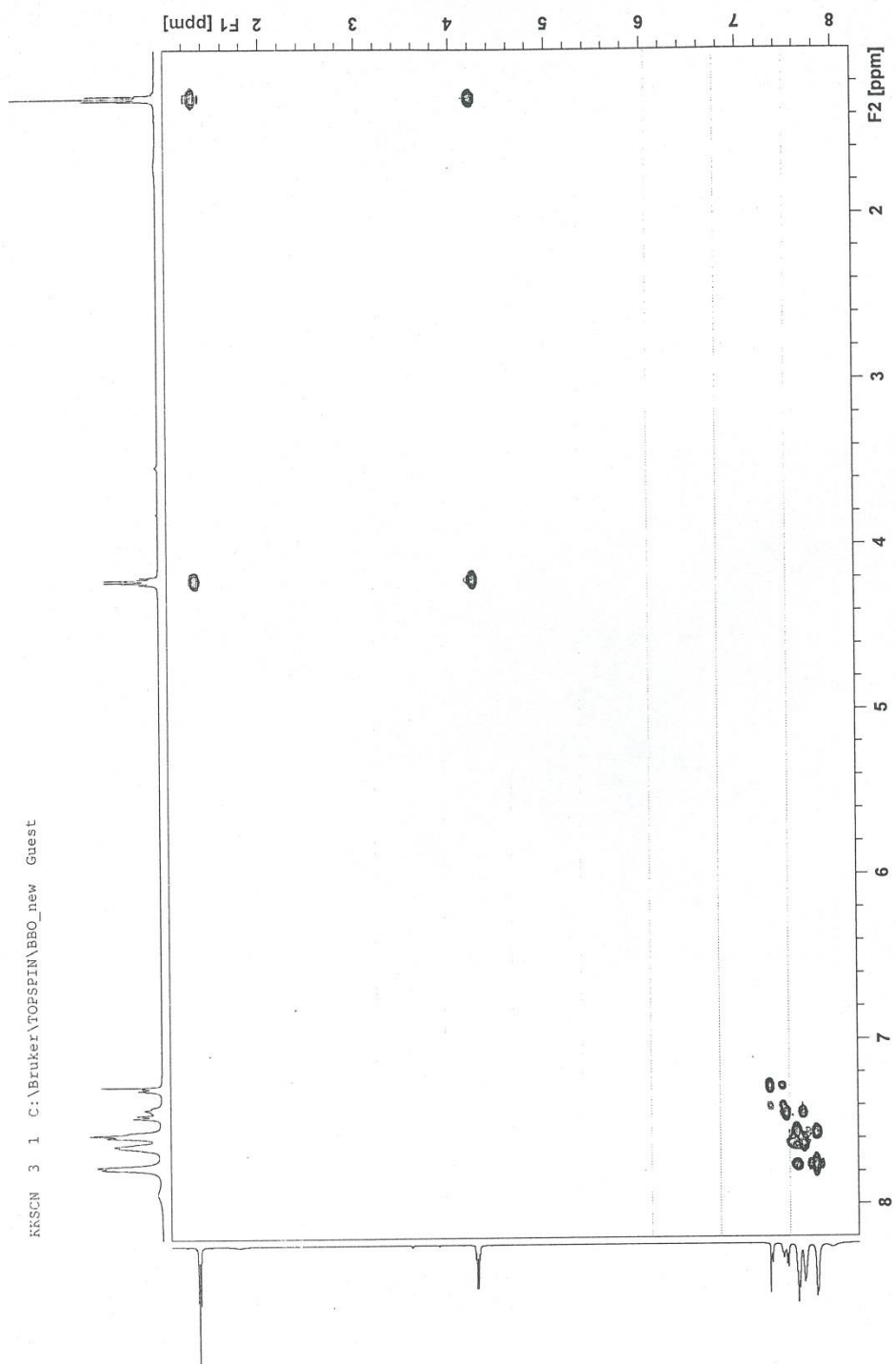


Fig. S13a. HSQC spectrum of complex 2.

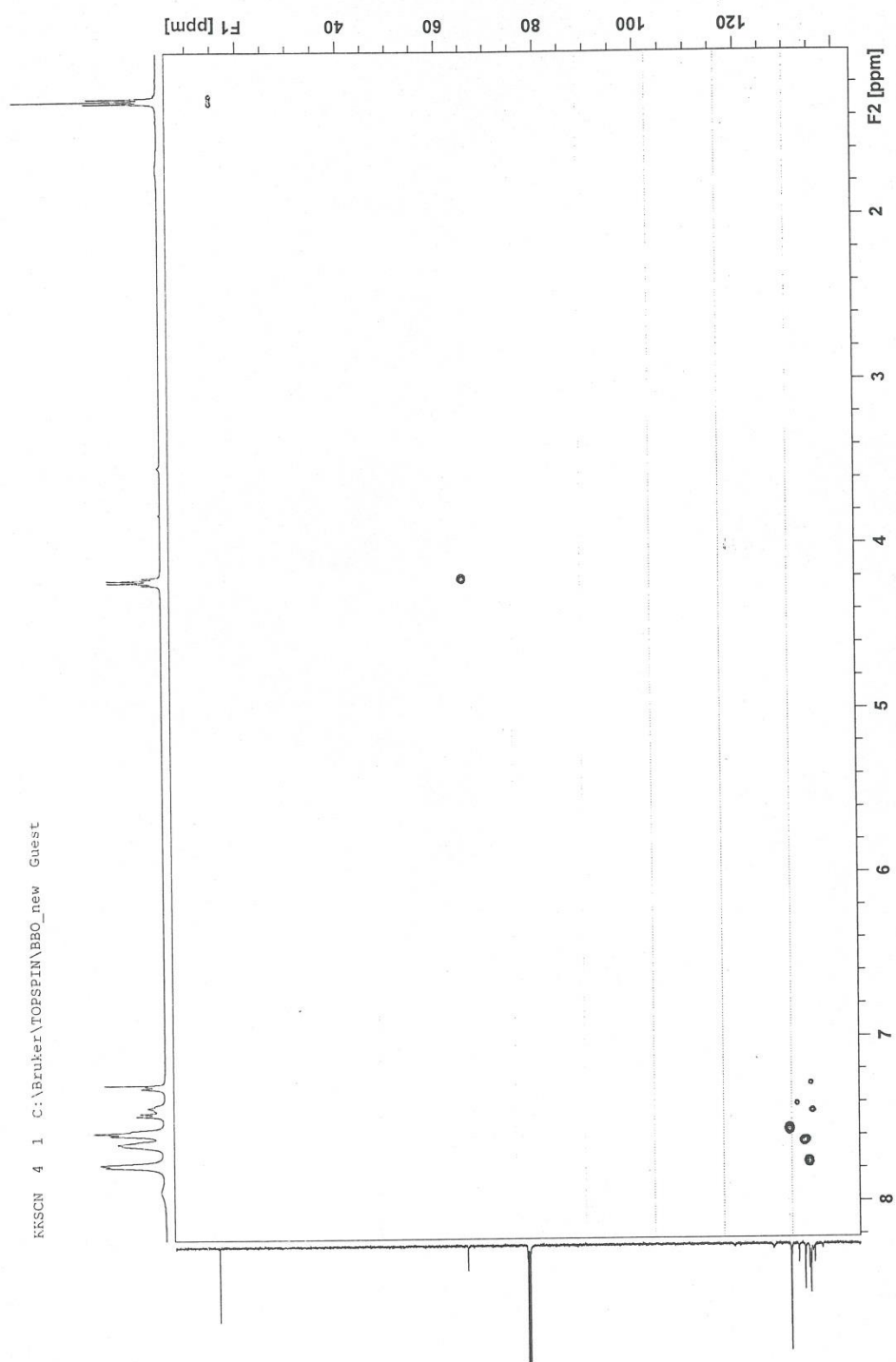
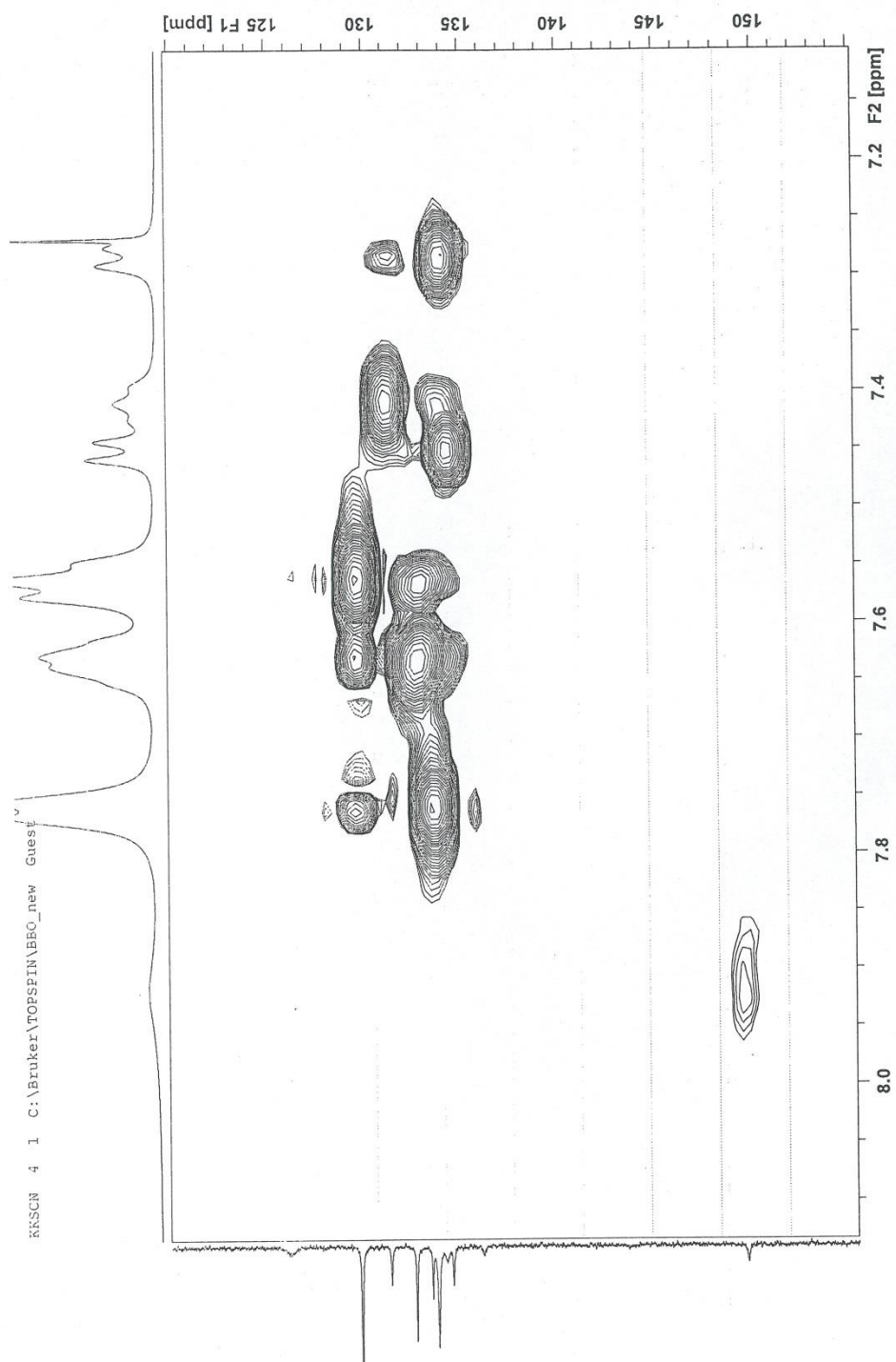


Fig. S13b. HSQC spectrum of complex 2.



**Fig. S14.**  $^1\text{H}$  NMR spectrum of complex **3**.

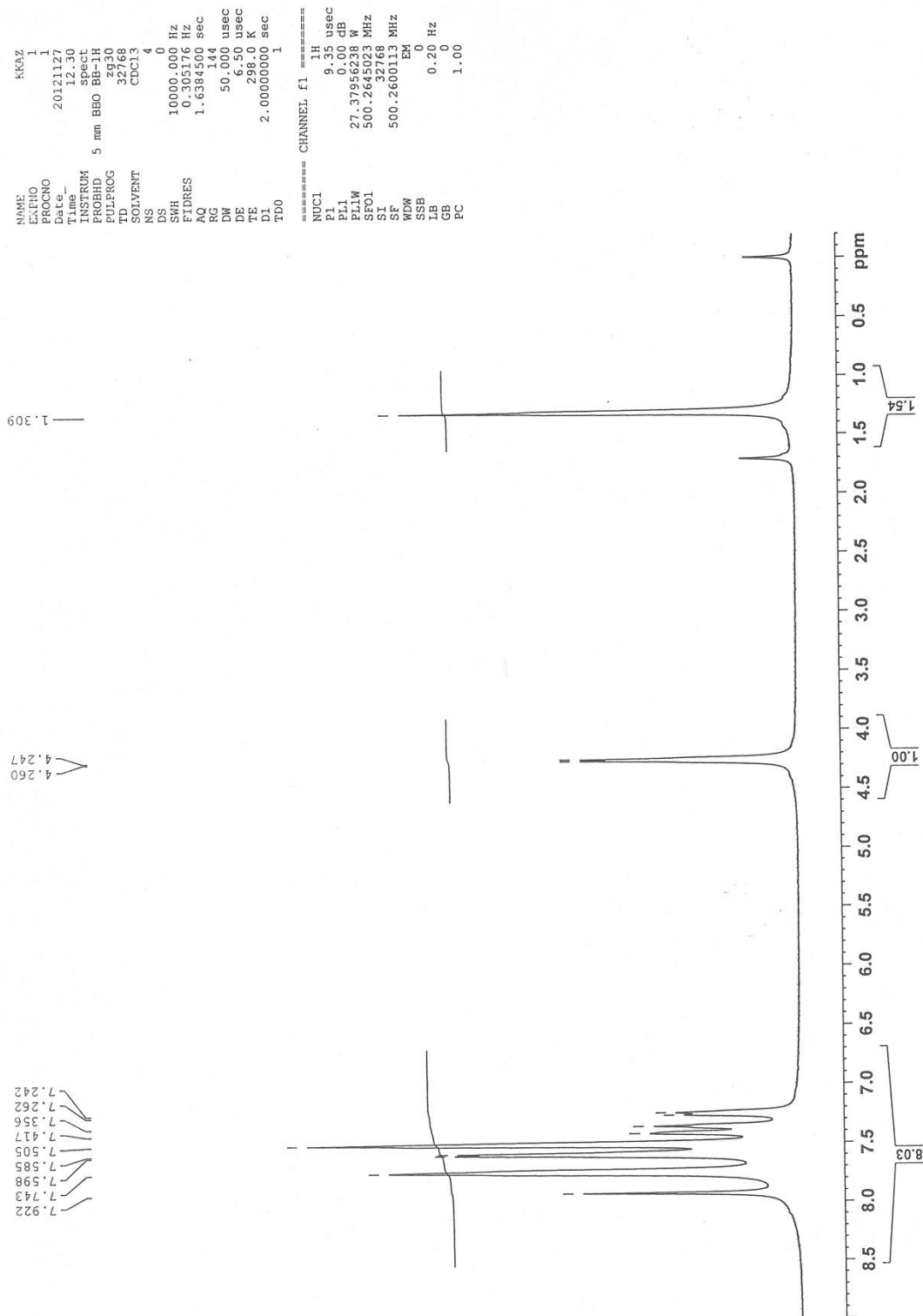


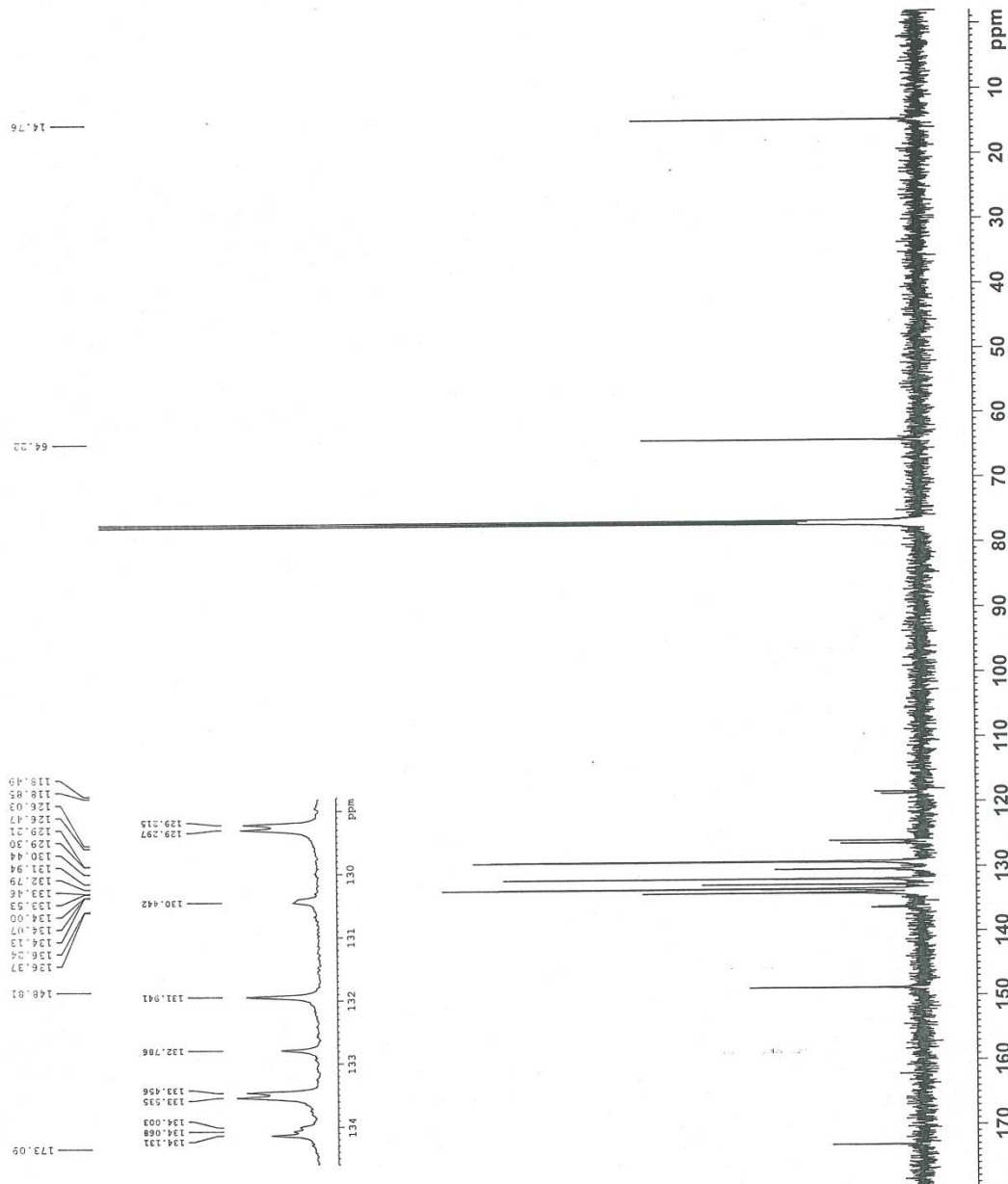
Fig. S15.  $^{13}\text{C}$  NMR spectrum of complex 3.

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NAME          KKAZ
EXPNO         2
PROCNO        1
Date_         20121127
Time_        12.39
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            643
DS            4
SWH           29761.904 Hz
FIDRES       0.908261 Hz
AQ           0.5505524 sec
RG           2050
DW           16.800 usec
DE           6.50 usec
TE           298.0 K
D1           2.0000000 sec
D11          0.0300000 sec
TD0          1

===== CHANNEL f1 =====
NUC1          13C
P1           11.50 usec
PL1          3.00 dB
PL1W         32.22848892 W
SF01         125.8043140 MHz

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        80.00 usec
PL2          1.20 dB
PL12         18.40 dB
PL13         18.40 dB
PL1W         20.76952171 W
PL2W         0.39575511 W
PL13W        0.39575511 W
SF02         500.2617509 MHz
SI           32768
WDW          EM
SSB          0
LB           1.50 Hz
GB           0
PC           1.40
  
```



**Fig. S16.** COSY spectrum of complex **3**.

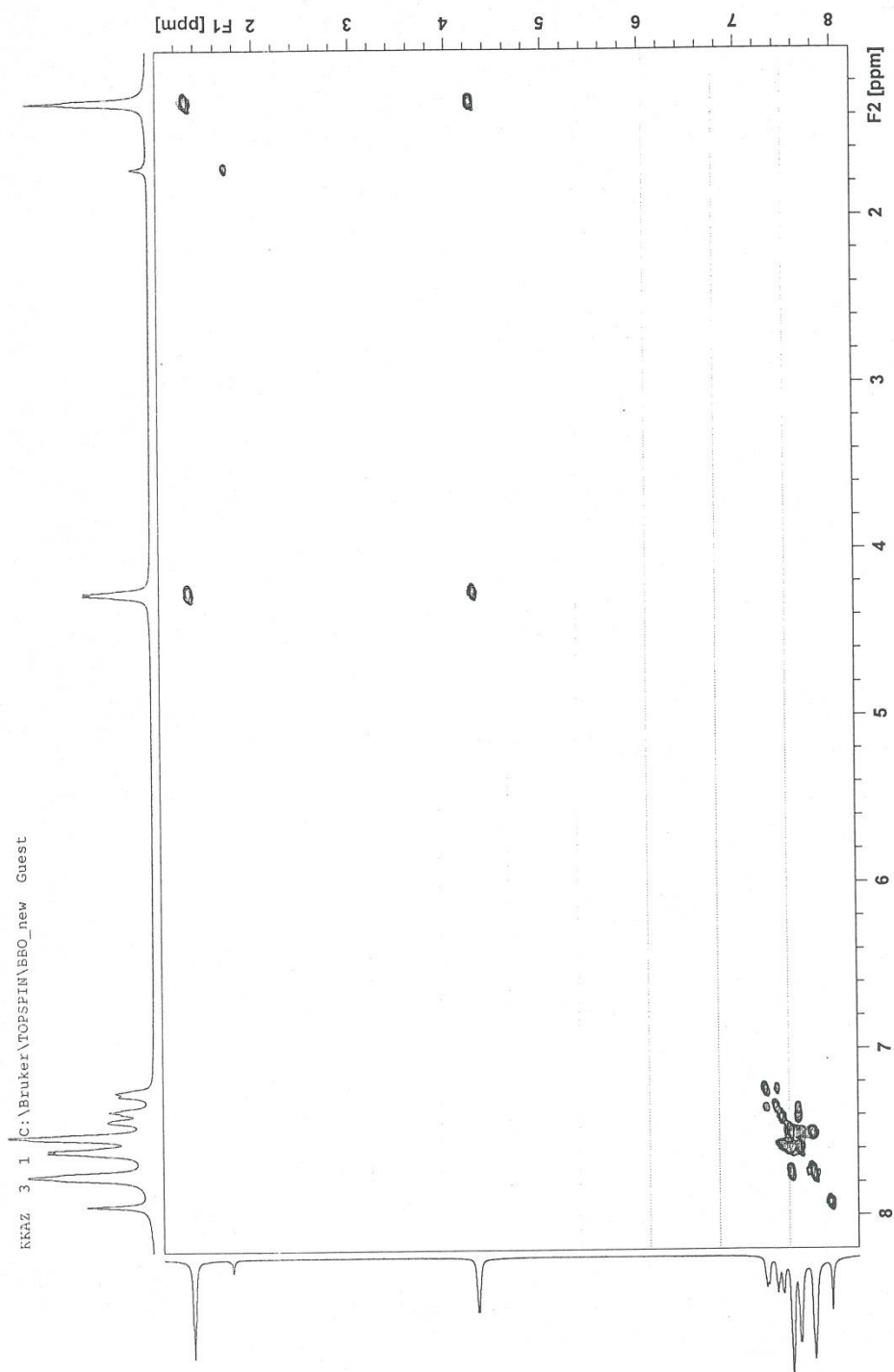
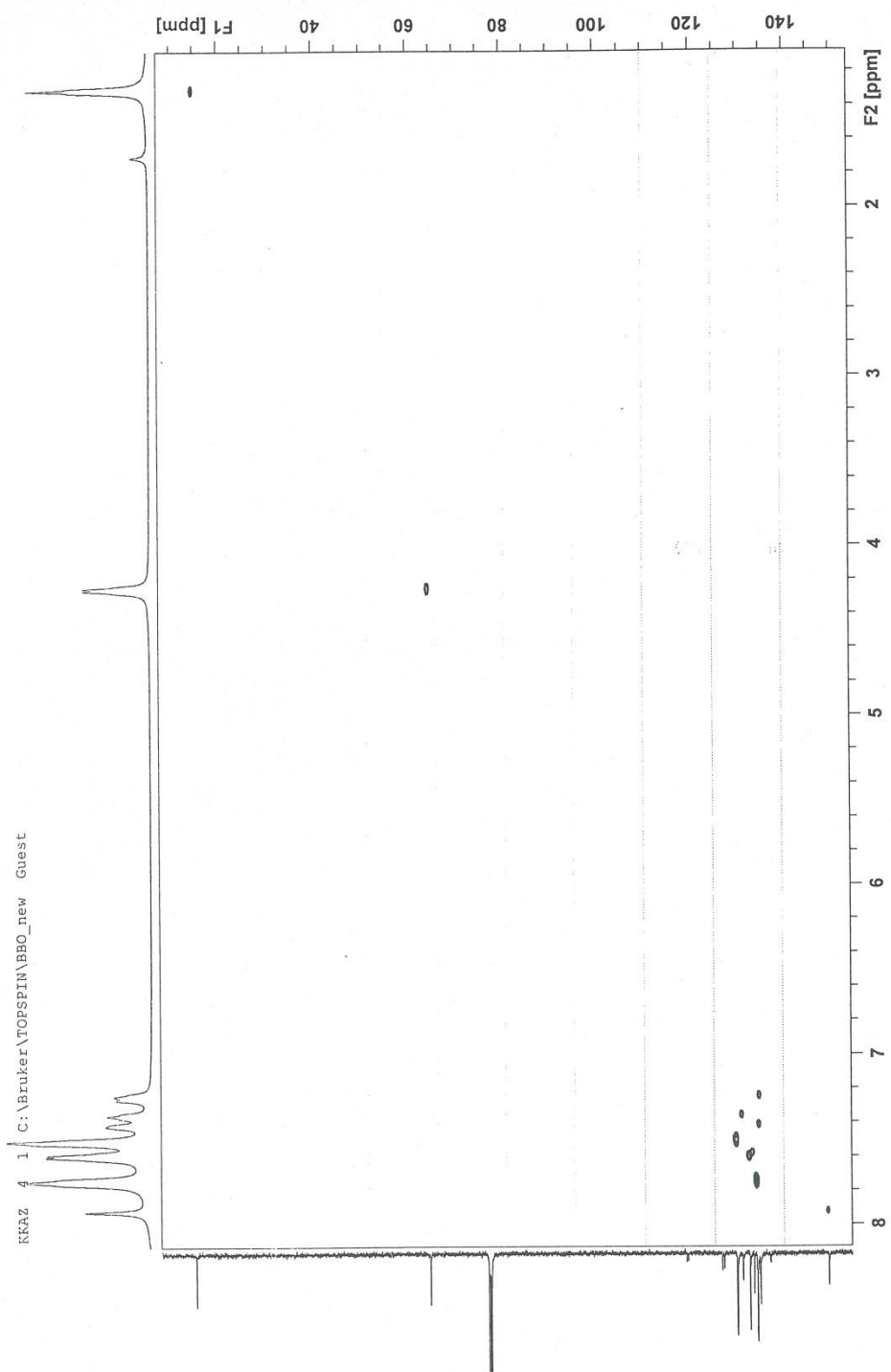




Fig. S17a. HSQC spectrum of complex 3.



**Fig. S17b.** HSQC spectrum of complex **3**.

