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## Supplementary Information

**Xanthosaponins A and B, two unusual steroidal saponins with an unprecedented 16,17-*seco*-cholestane skeleton from *Solanum xanthocarpum* and their cytotoxic activities**

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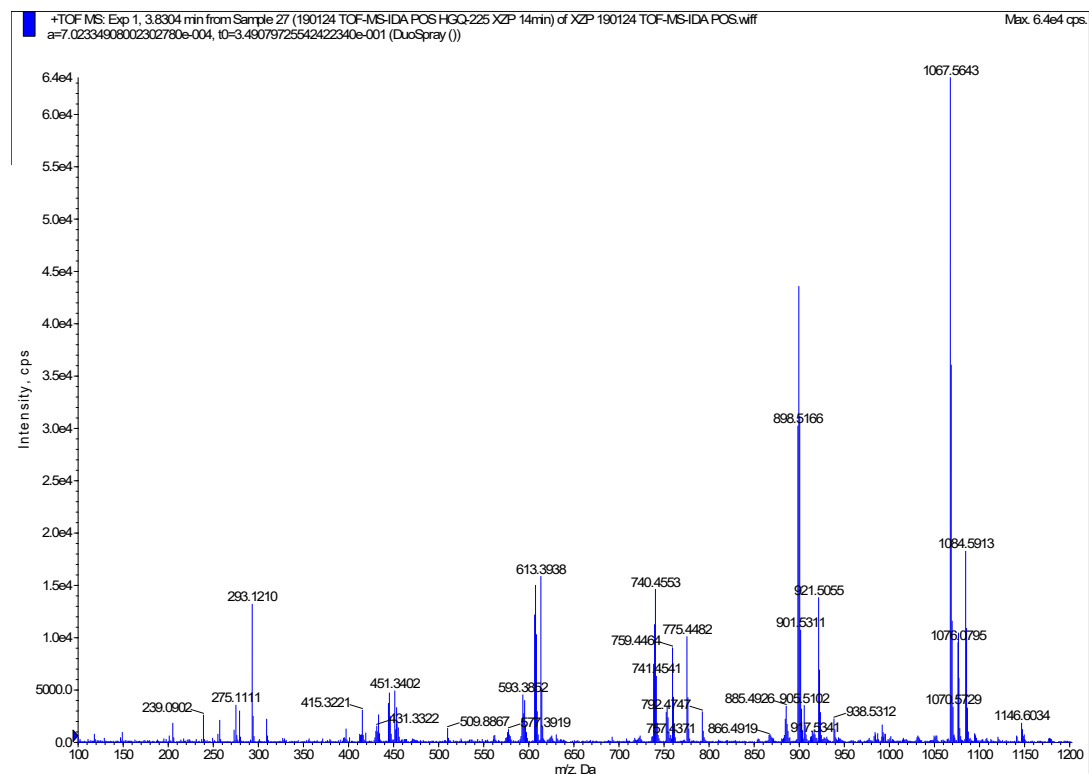
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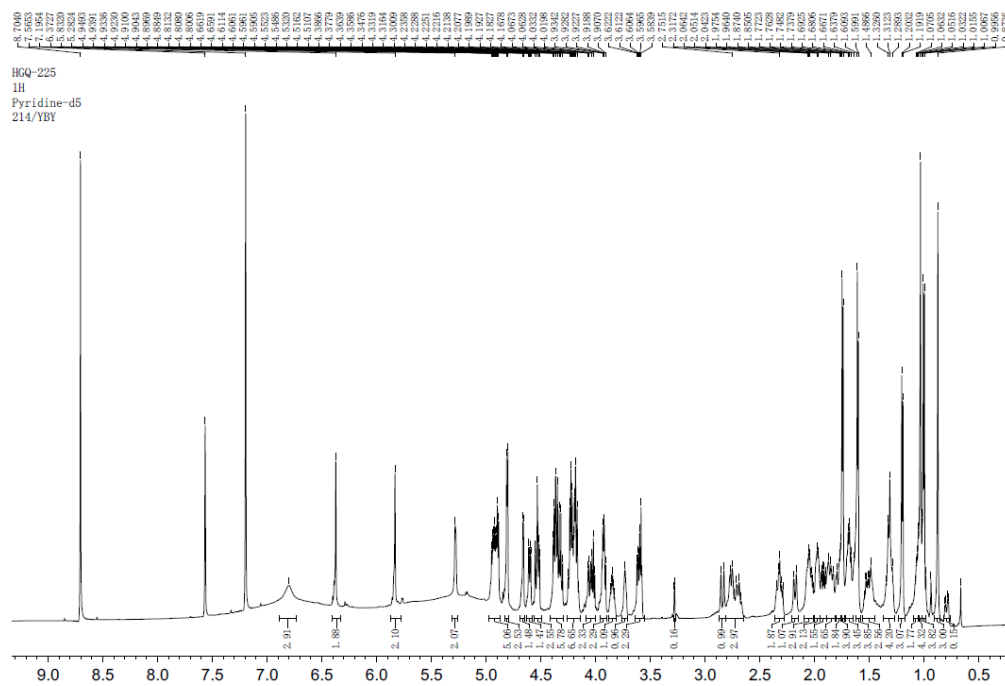
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**Figure S1.** HR-ESI-MS spectrum of **1**.



**Figure S2.** <sup>1</sup>H NMR spectrum of **1** (600 MHz, pyridine-*d*<sub>5</sub>).

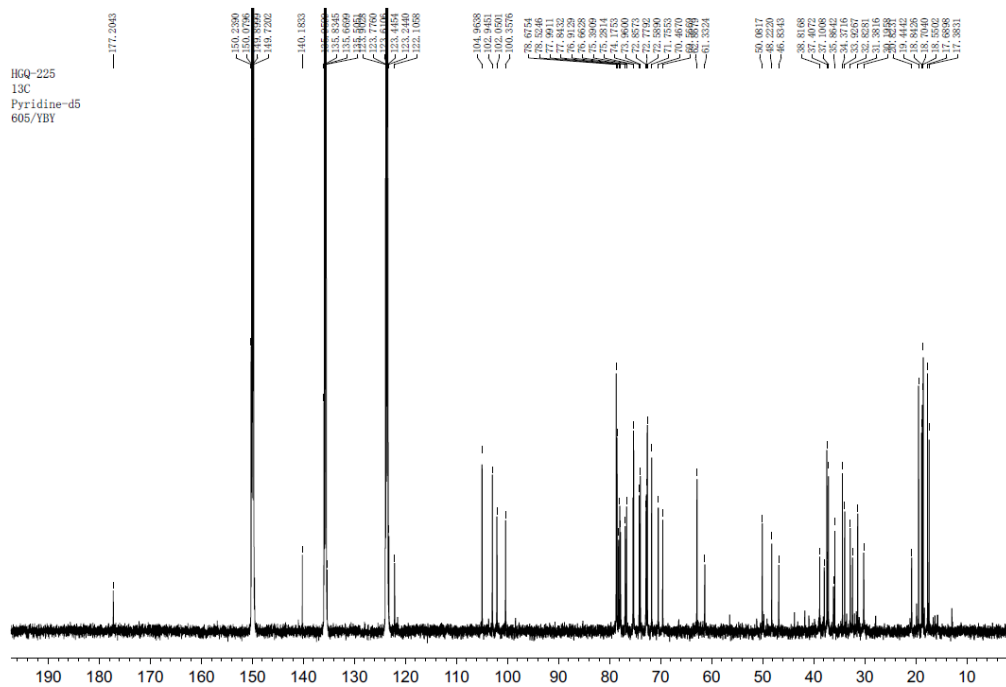


Figure S3.  $^{13}\text{C}$  NMR spectrum of **1** (150 MHz, pyridine- $d_5$ ).

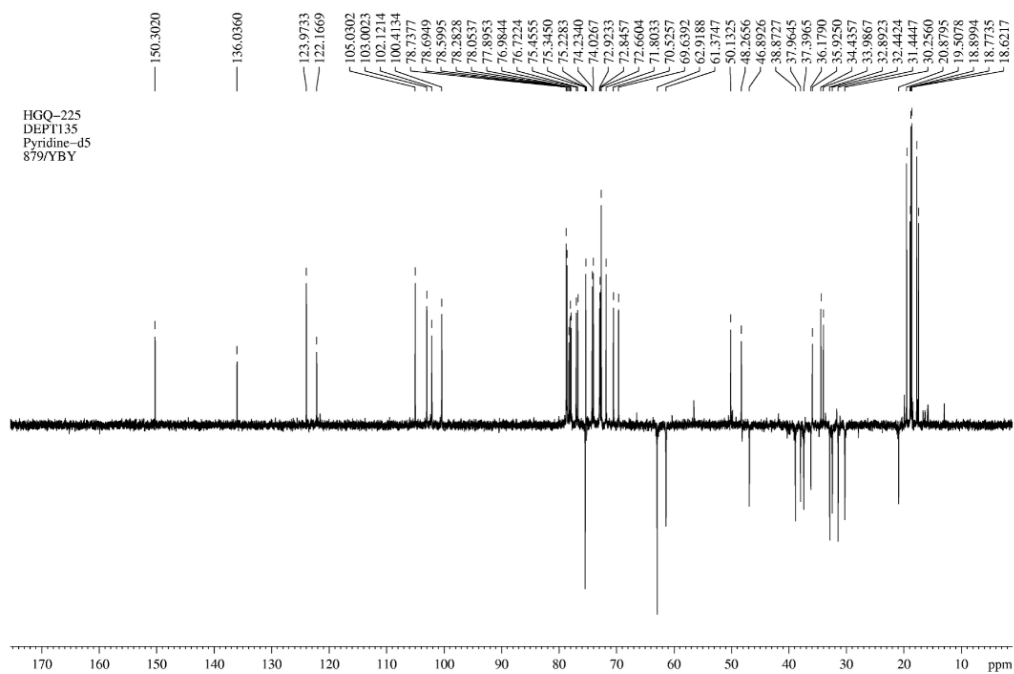
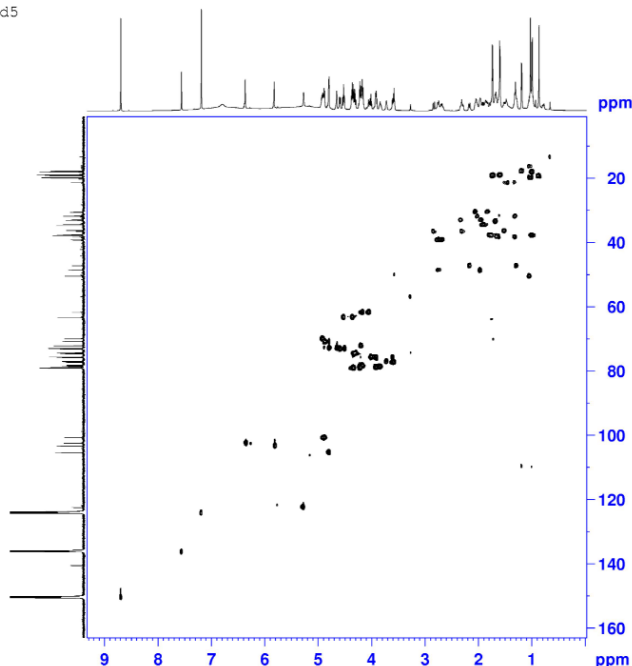


Figure S4. DEPT 135 spectrum of **1**.

HGQ-225  
 HSQC  
 Pyridine-d5  
 882/YBY



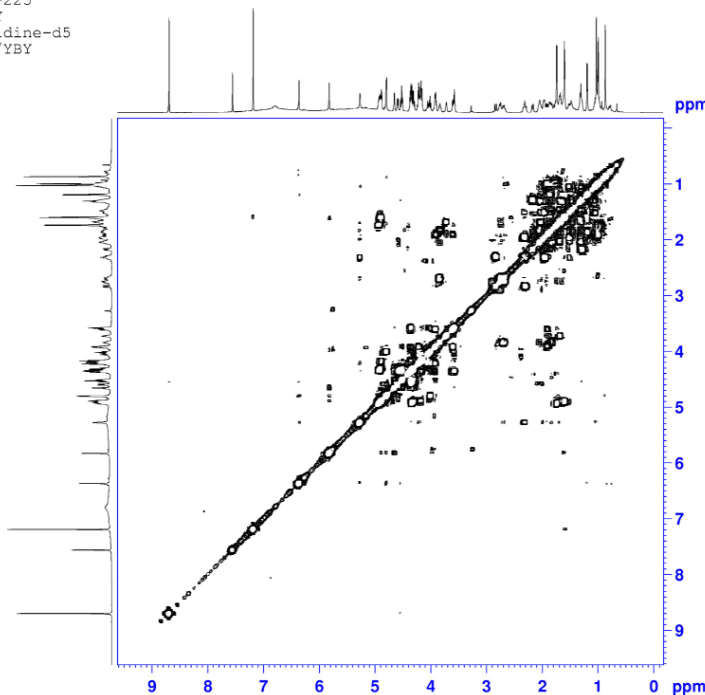
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Figure S5. HSQC spectrum of 1.

HGQ-225  
 COSY  
 Pyridine-d5  
 880/YBY



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FIDRES       3.212577 Hz
AQ           0.1534840 sec
RG           64
SW           16.201
DE           6.200 usec
TE           298.15
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dSFO1CT      0.00000300 sec
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NUC2         1H
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Figure S6. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of 1.

HGQ-225  
HMBC  
Pyridine-d5  
881/YBY

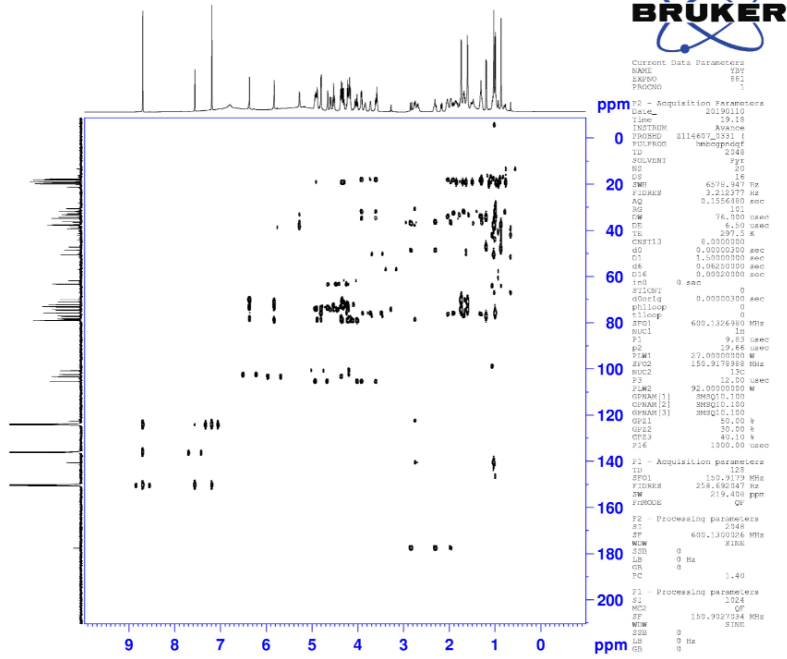


Figure S7. HMBC spectrum of 1.

HGQ-225  
NOESY  
Pyridine-d5  
883/YBY

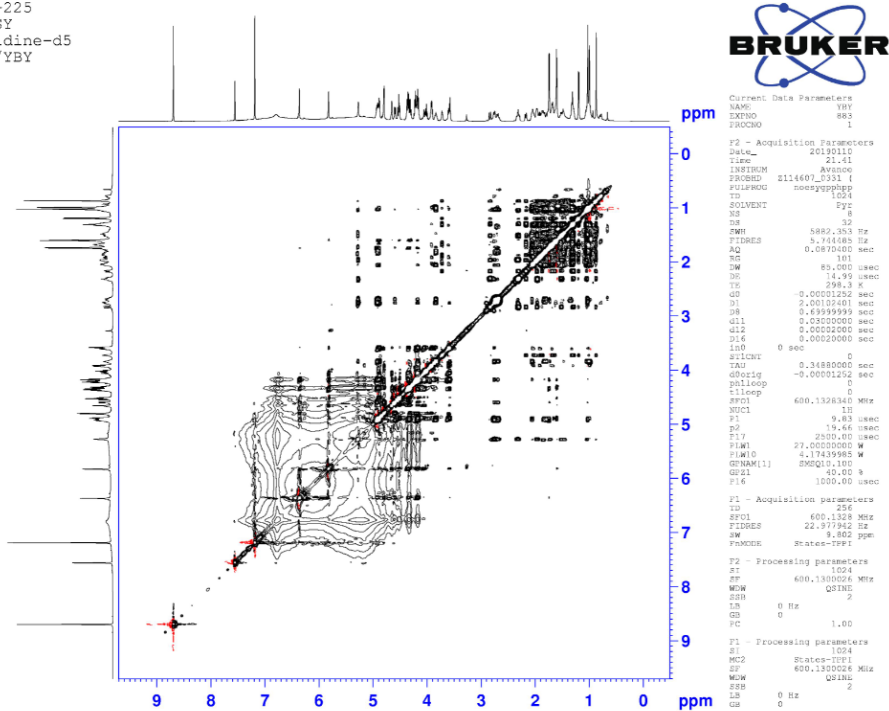


Figure S8. NOESY spectrum of 1.

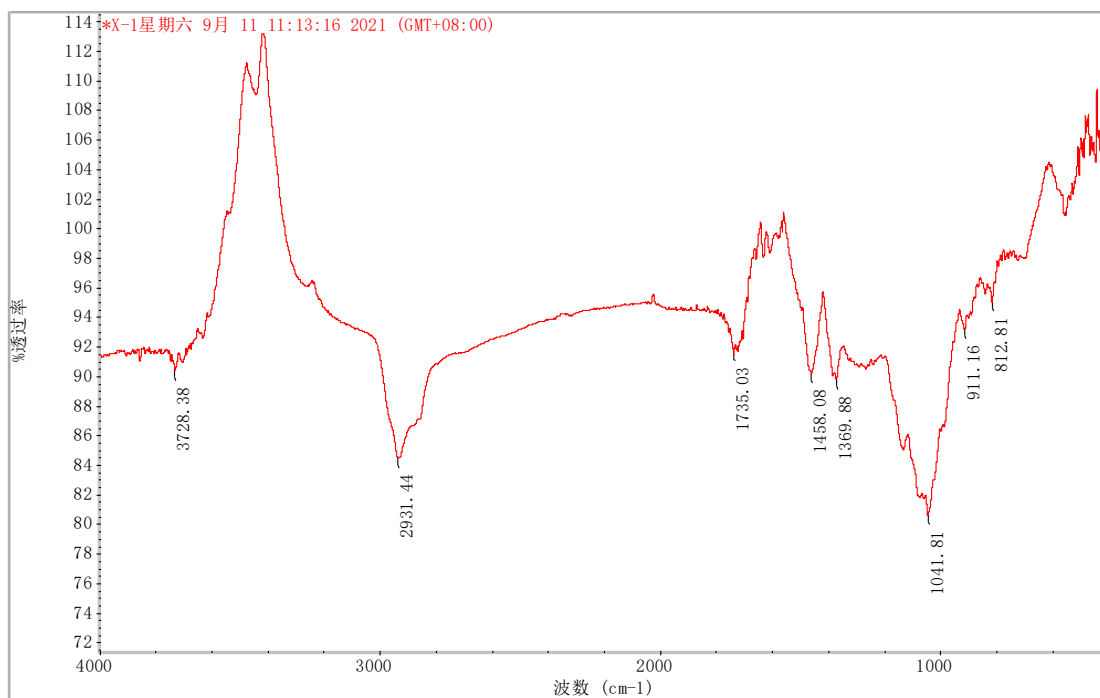


Figure S9. IR spectrum of 1.

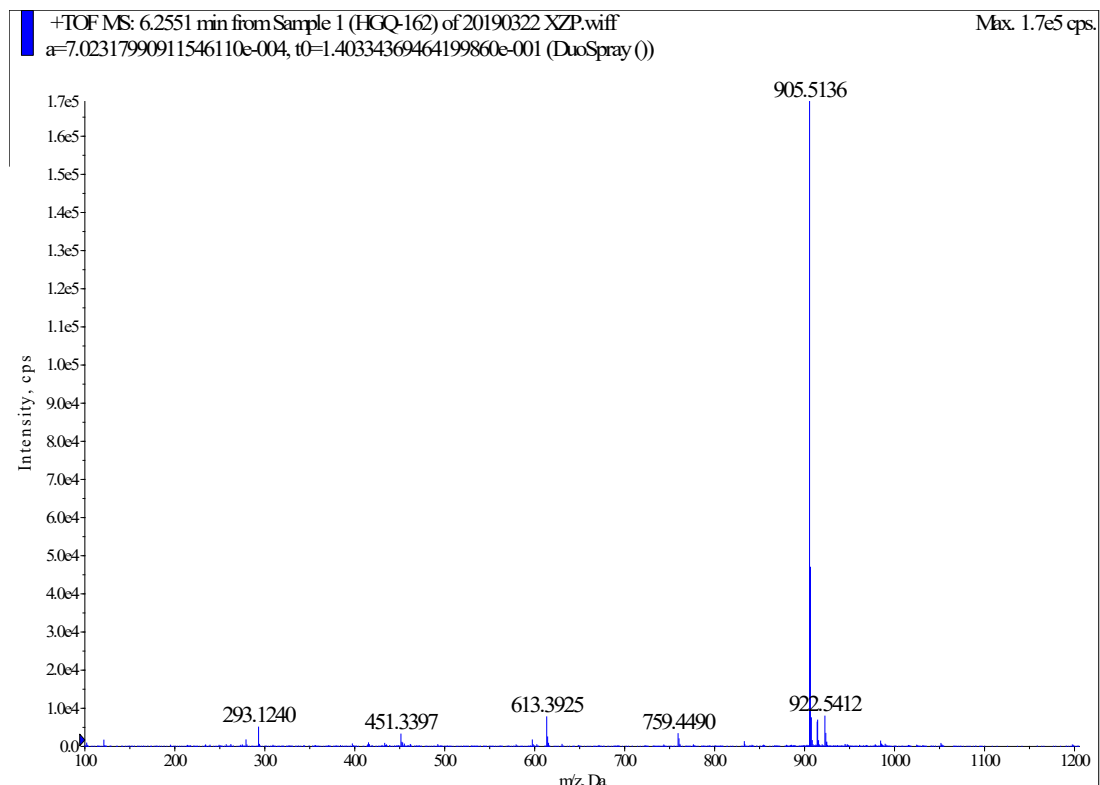


Figure S10. HR-ESI-MS spectrum of 2.





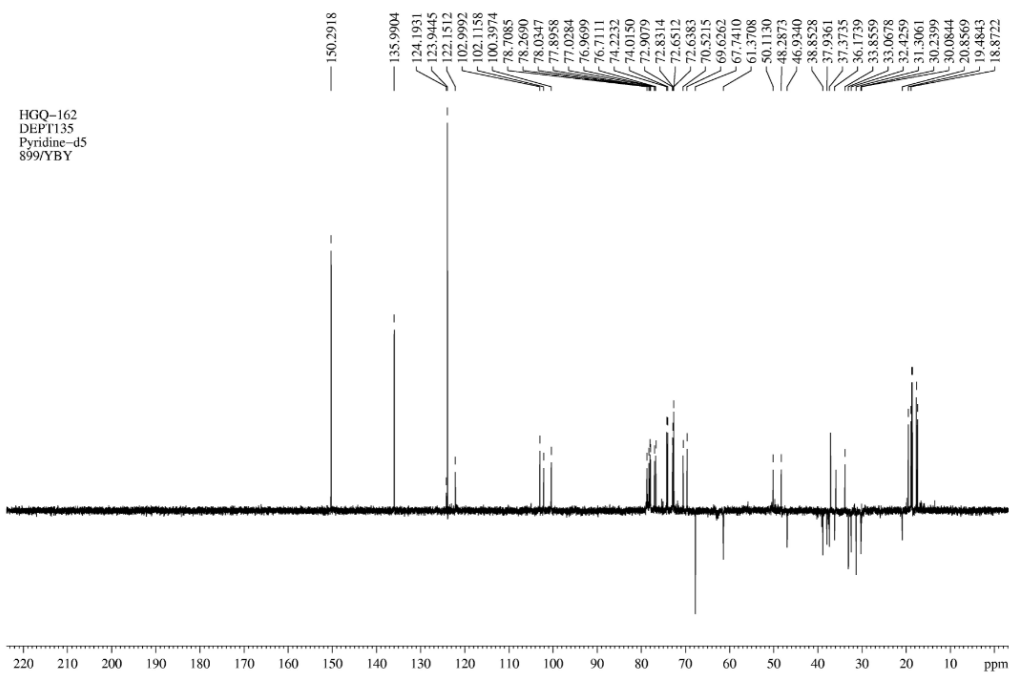


Figure S13. DEPT 135 spectrum of 2.

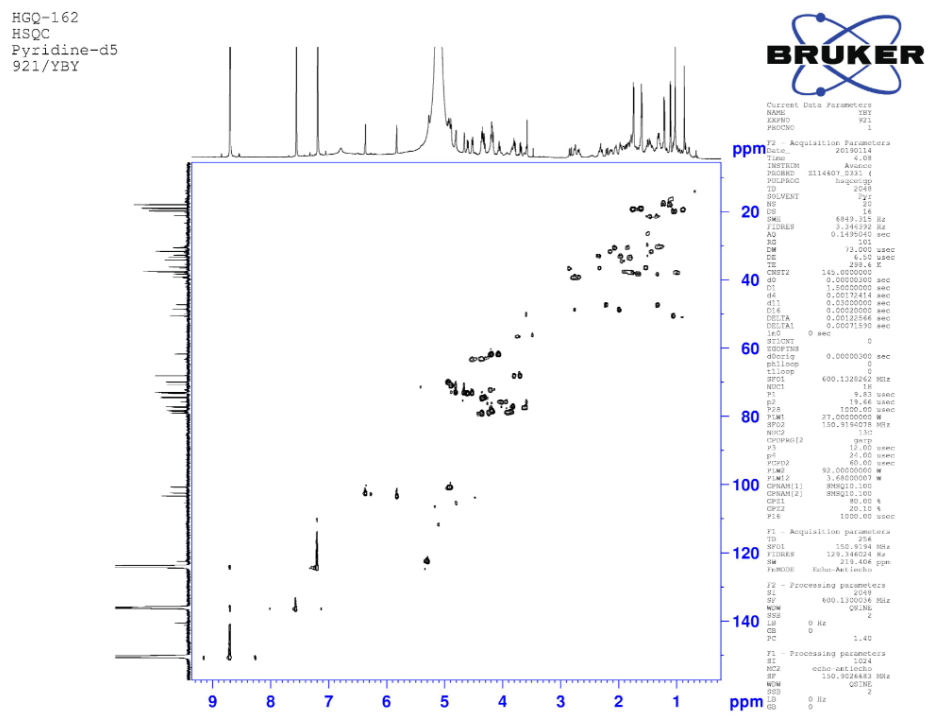


Figure S14. HSQC spectrum of 2.

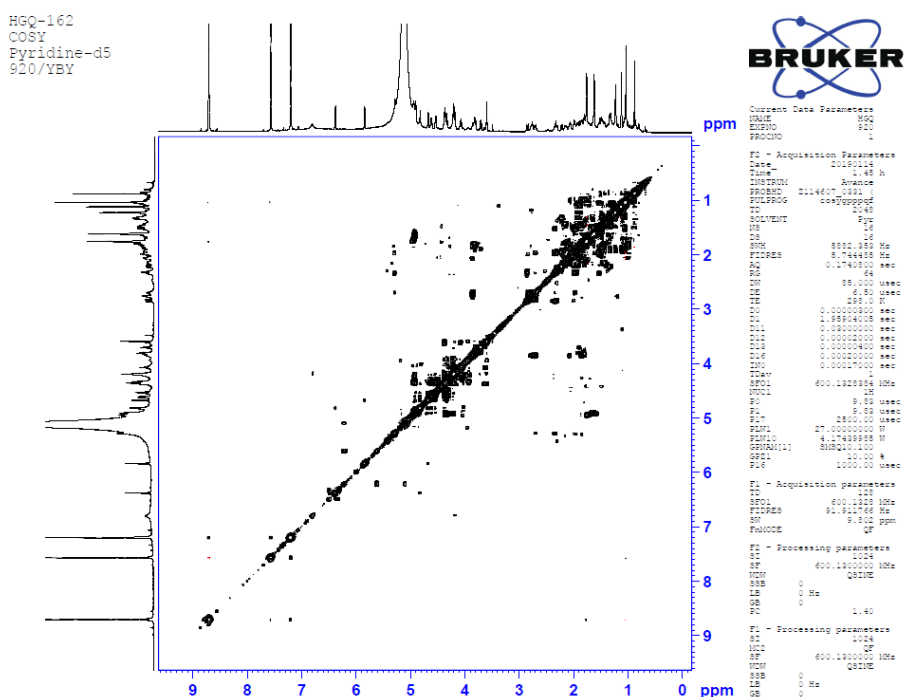


Figure S15.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **2**.

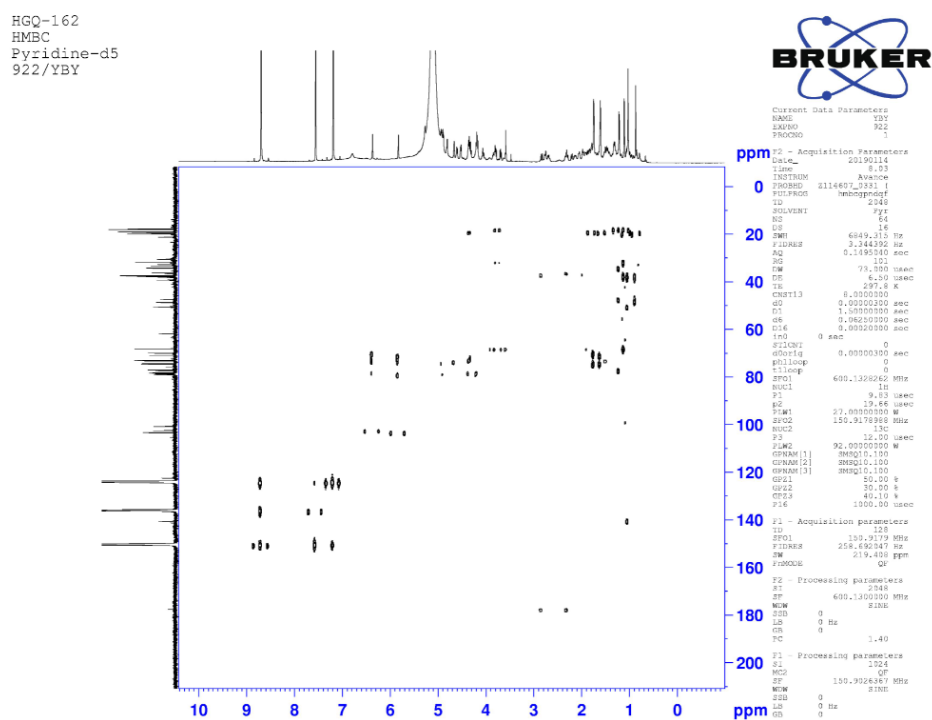


Figure S16. HMBC spectrum of **2**.

HGQ-162  
NOESY  
Pyridine-d5  
923/YBY

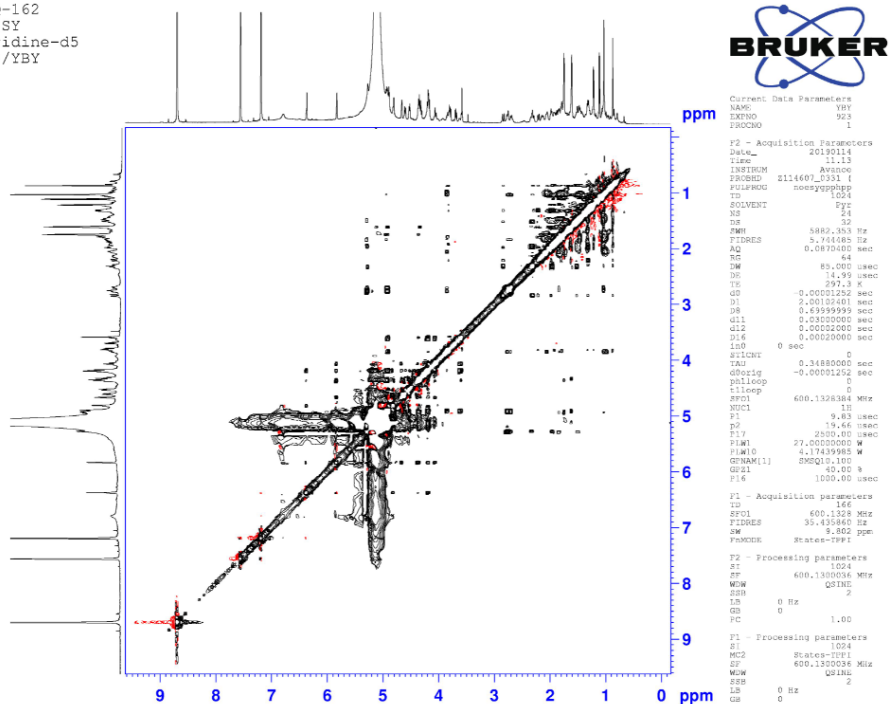


Figure S17. NOESY spectrum of 2.

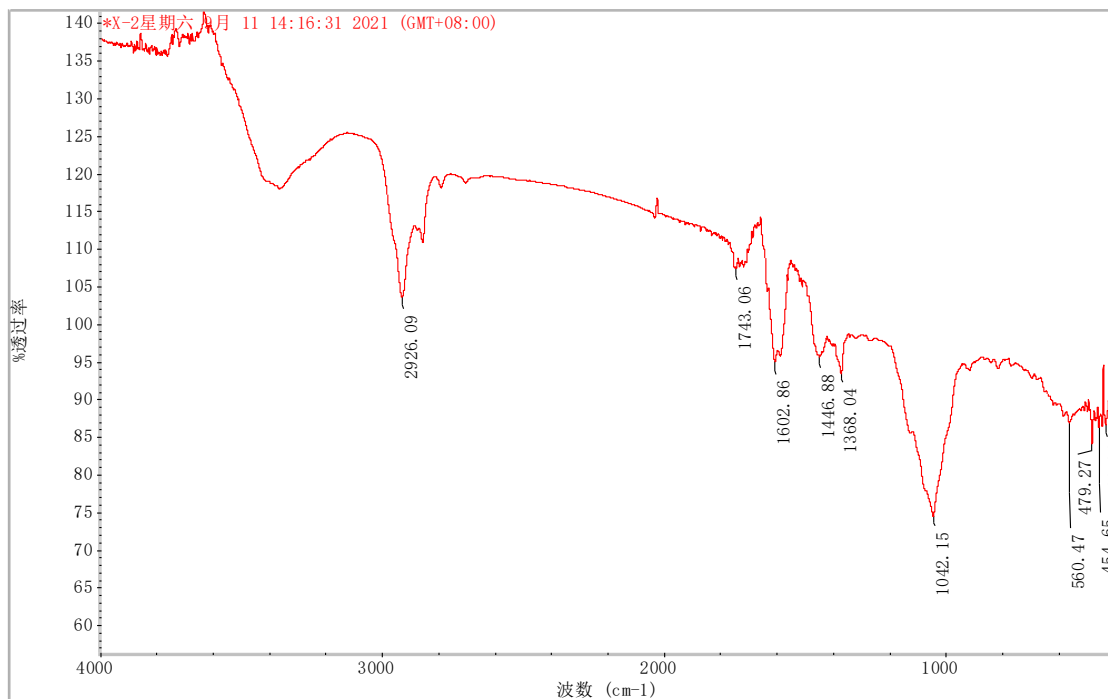
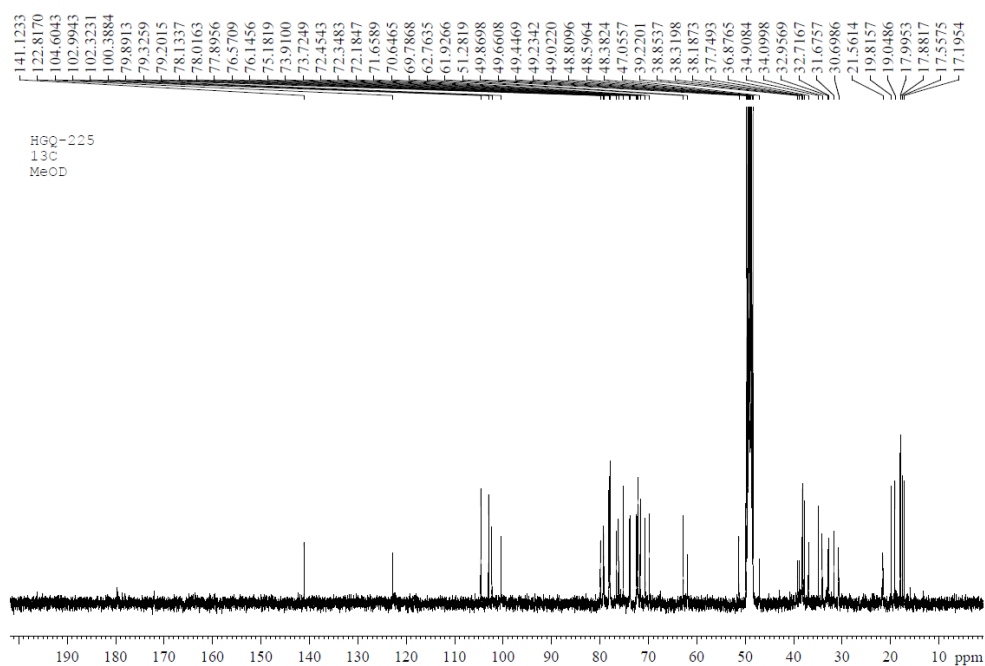
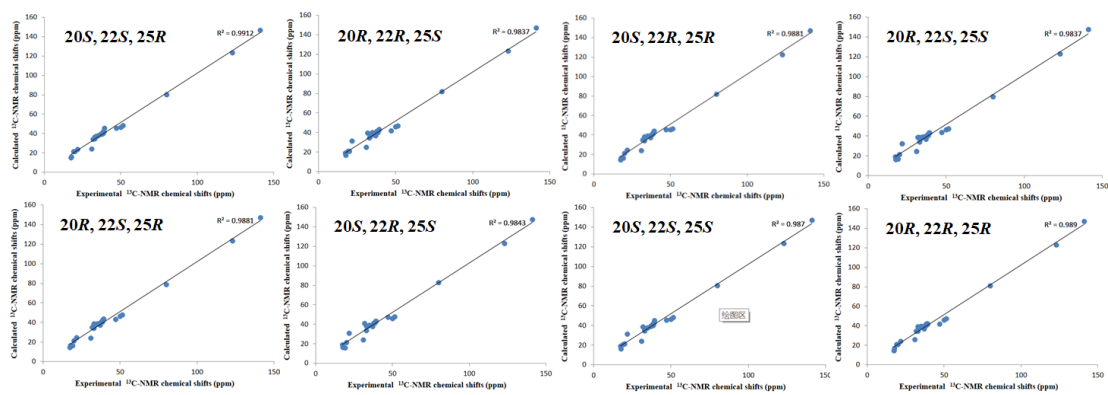


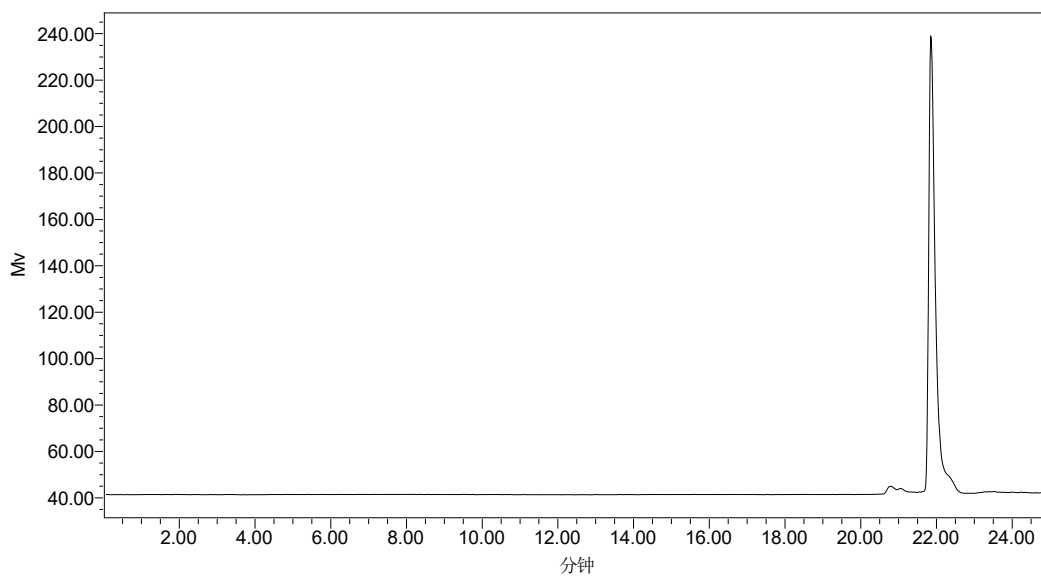
Figure S18. IR spectrum of 2.



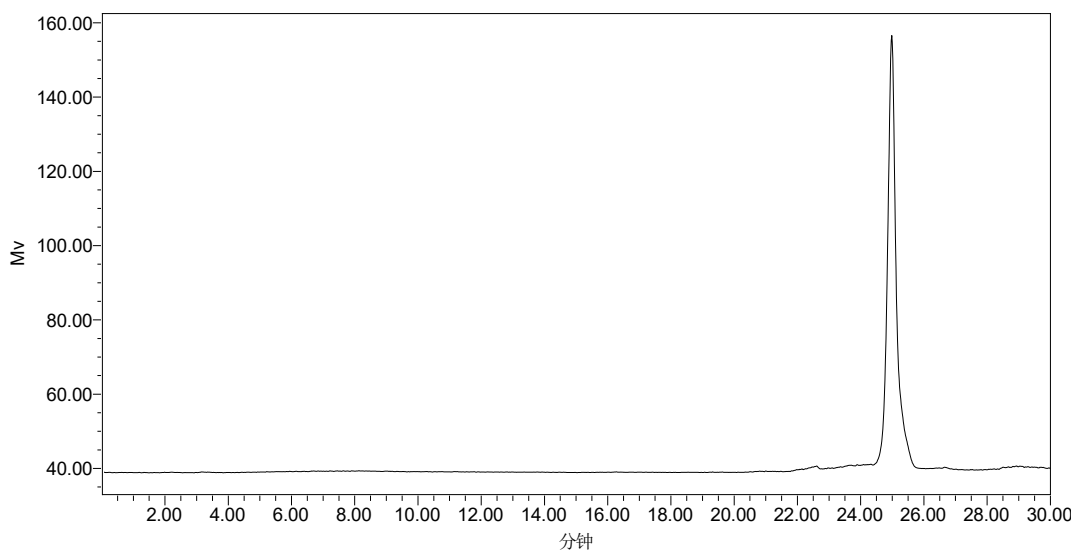
**Figure S19.**  $^{13}\text{C}$  NMR spectrum of **1** (100 MHz, methanol- $d_4$ ).



**Figure S20.** Linear correlations between the calculated of 8 isomers and experimental  $^{13}\text{C}$  NMR chemical shifts for compound **1**.



**Figure S21.** HPLC-ELSD analysis of **1**.



**Figure S22.** HPLC-ELSD analysis of **2**.



HGQ-225  
HSQC  
Pyridine-d5  
882/YBY

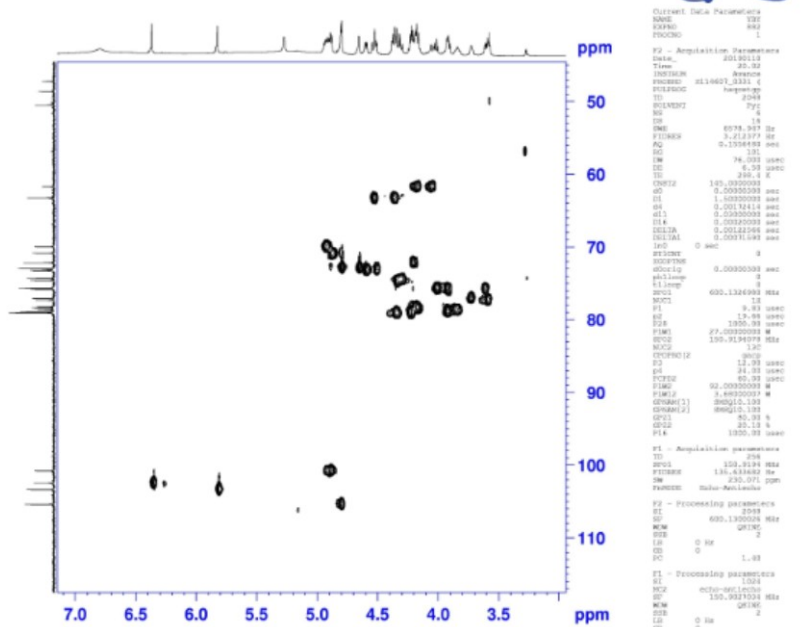


Figure S25. The partial enlargement of the HSQC spectrum of 1 (c).

HGQ-225  
COSY  
Pyridine-d5  
880/YBY

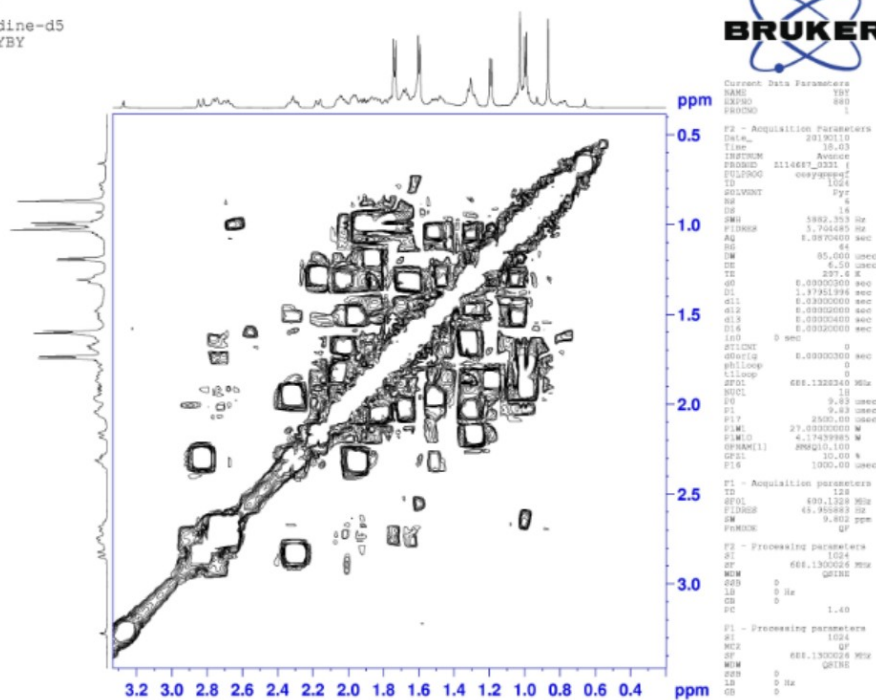


Figure S26. The partial enlargement of the  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of 1 (a).



HQO-225  
COSY  
Pyridine-d5  
880/YBY

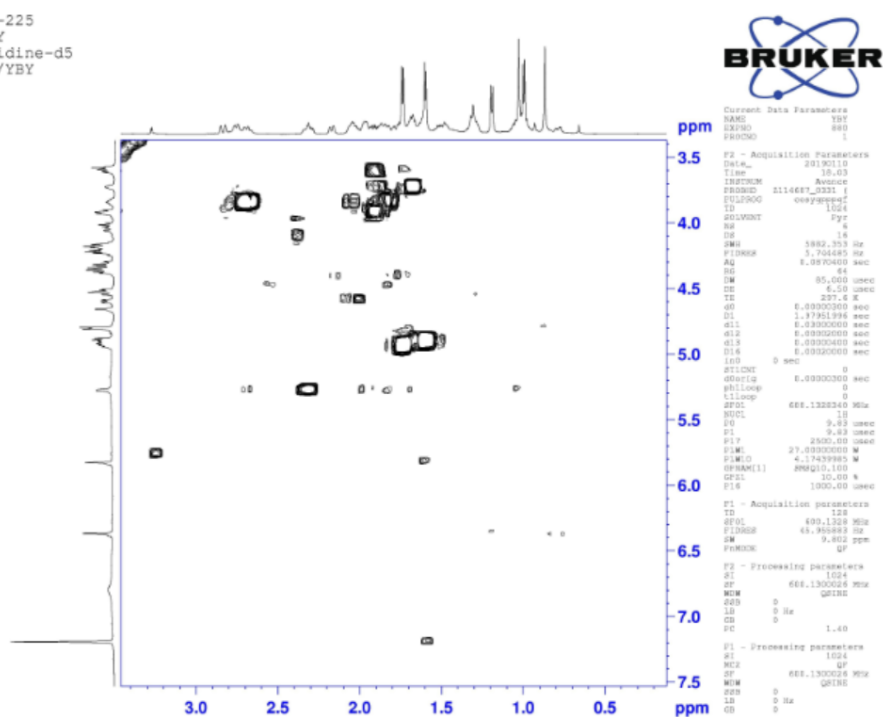


Figure S27. The partial enlargement of the  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1** (b).

HQO-225  
COSY  
Pyridine-d5  
880/YBY

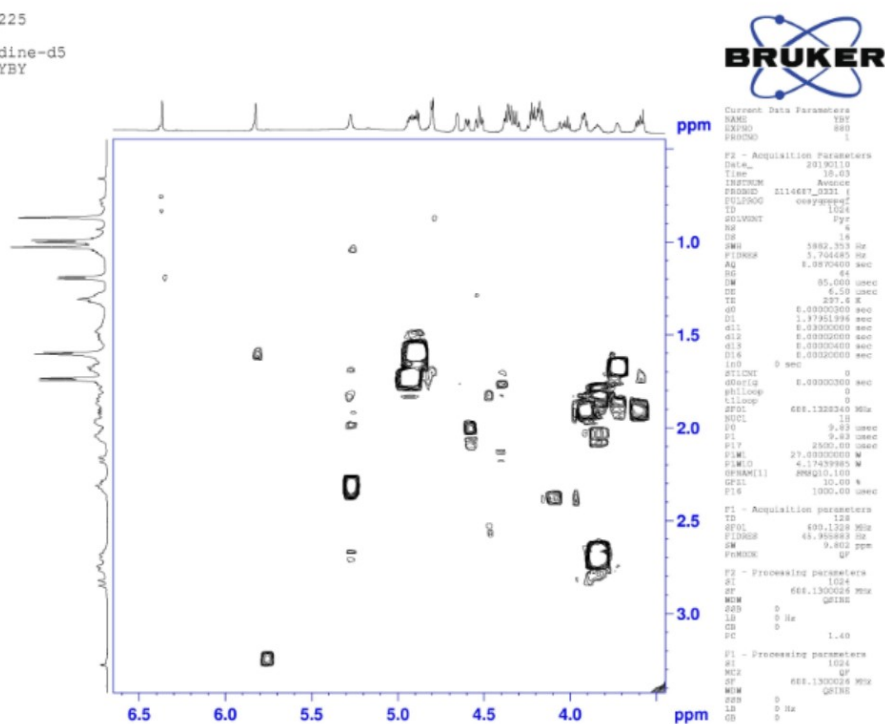


Figure S28. The partial enlargement of the  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1** (c).

HGQ-225  
COSY  
Pyridine-d5  
880/YBY

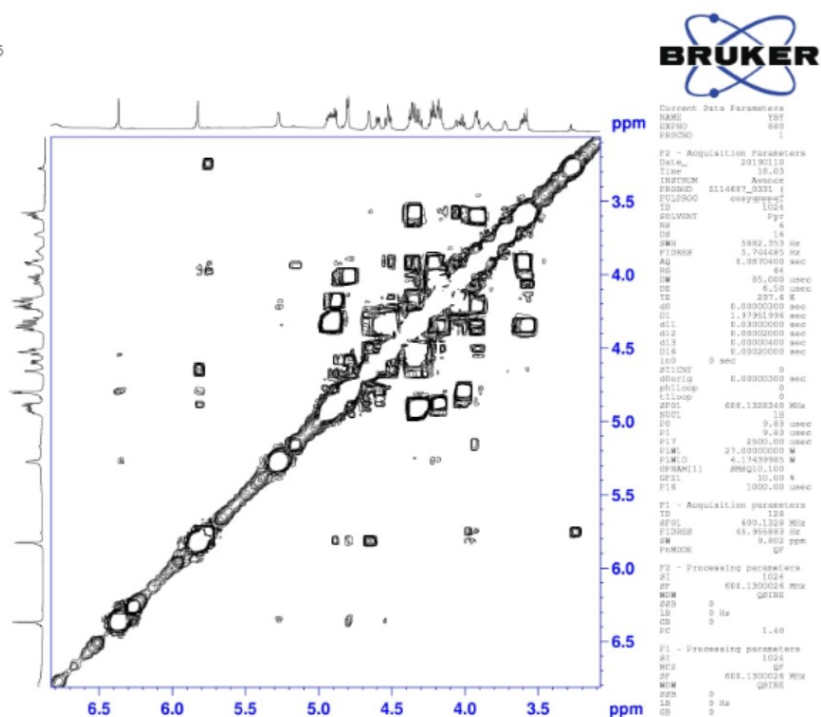


Figure S29. The partial enlargement of the  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1** (e).

HGQ-225  
HMBC  
Pyridine-d5  
881/YBY

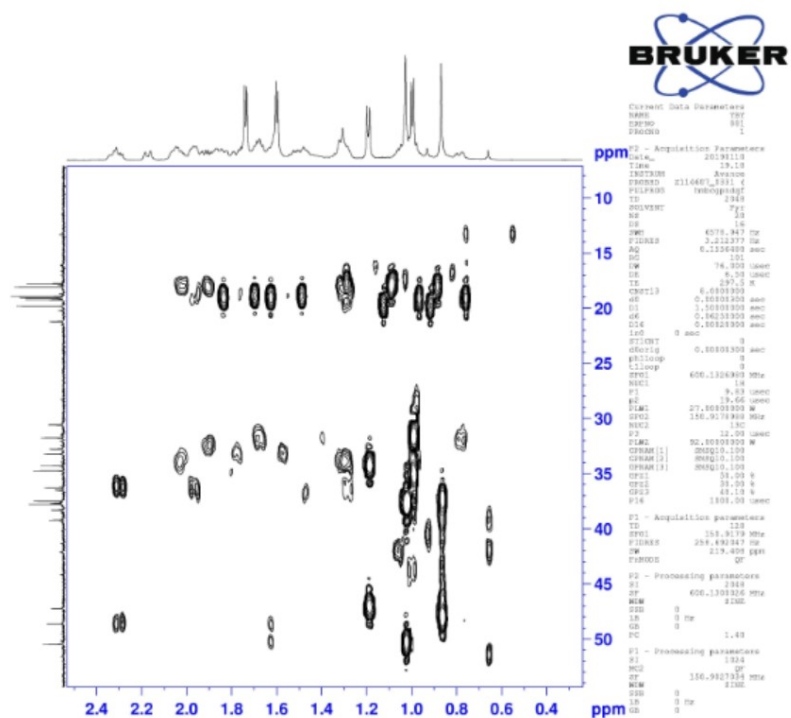


Figure S30. The partial enlargement of the HMBC spectrum of **1** (a).

HQ-225  
HMBC  
Pyridine-d5  
881/YBY

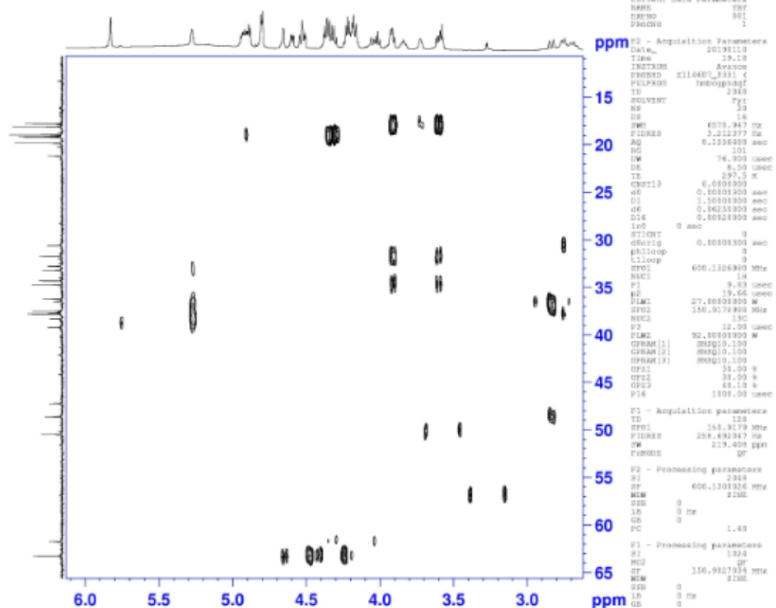


Figure S31. The partial enlargement of the HMBC spectrum of 1 (b).

HQ-225  
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Pyridine-d5  
881/YBY

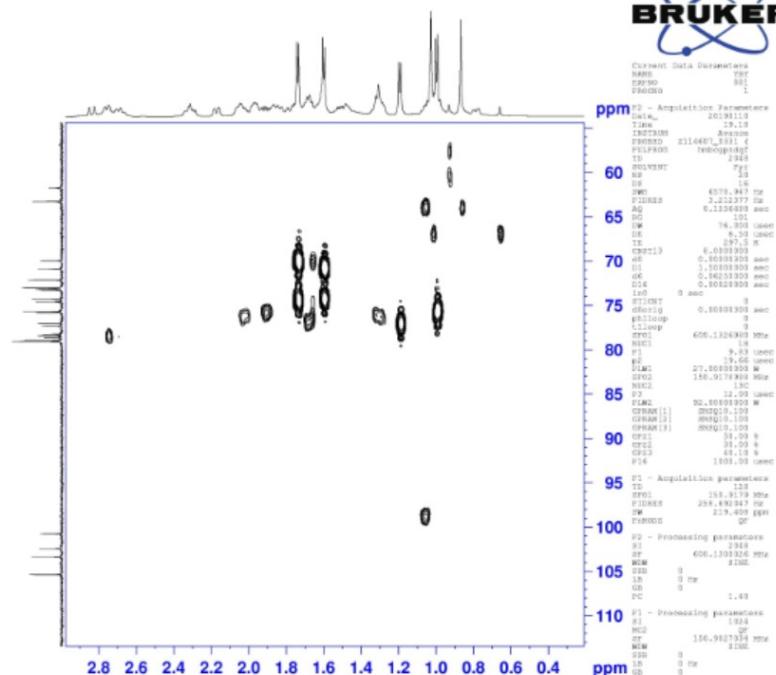


Figure S32. The partial enlargement of the HMBC spectrum of 1 (c).

HGQ-225  
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Pyridine-d5  
881/YBY

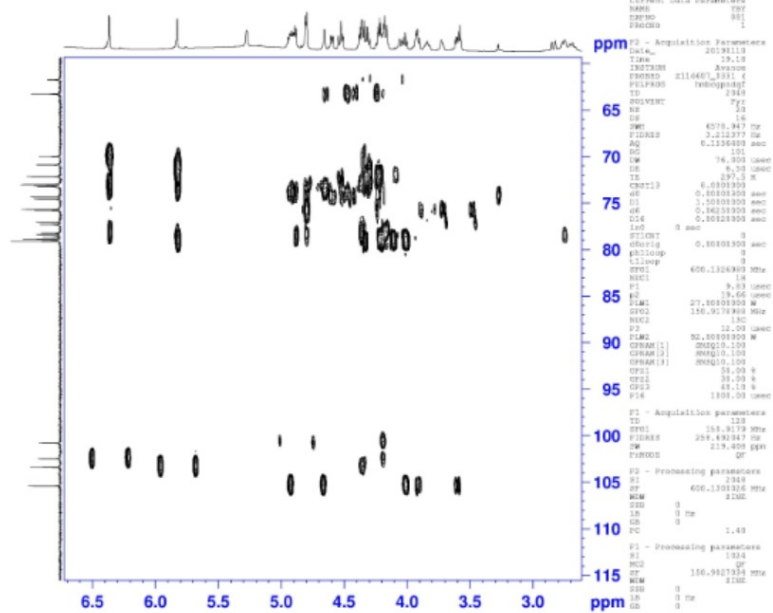


Figure S33. The partial enlargement of the HMBC spectrum of 1 (d).

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Pyridine-d5  
883/YBY

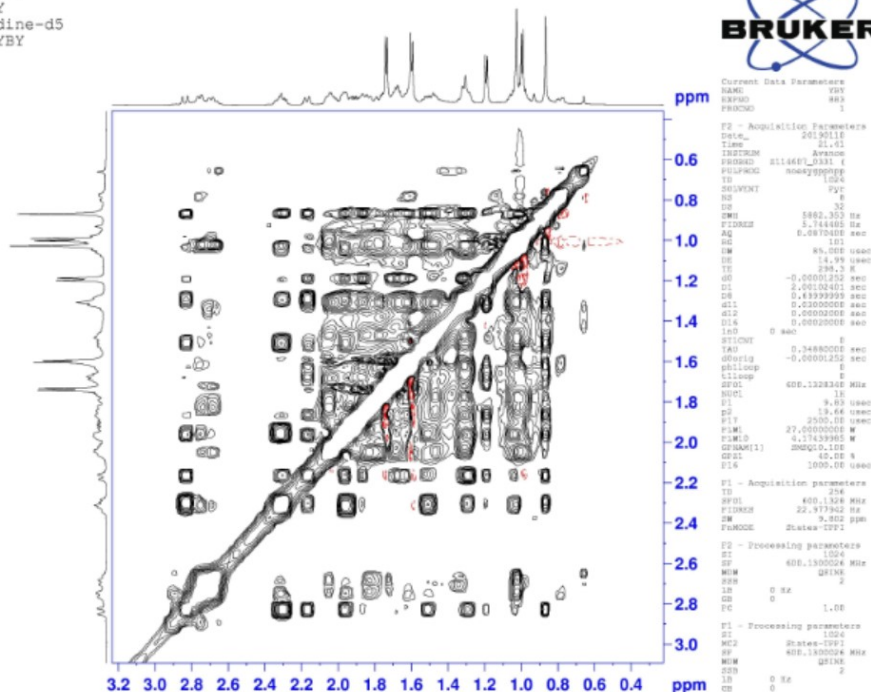


Figure S34. The partial enlargement of the NOESY spectrum of 1 (a).

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Pyridine-d5  
883/YBY

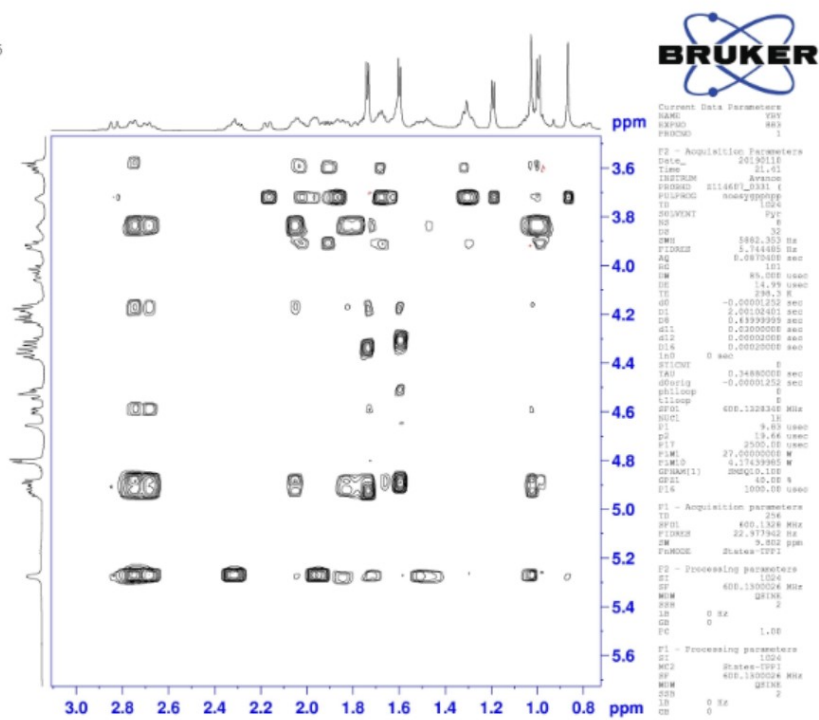


Figure S35. The partial enlargement of the NOESY spectrum of 1 (b).

HGQ-225  
NOESY  
Pyridine-d5  
883/YBY

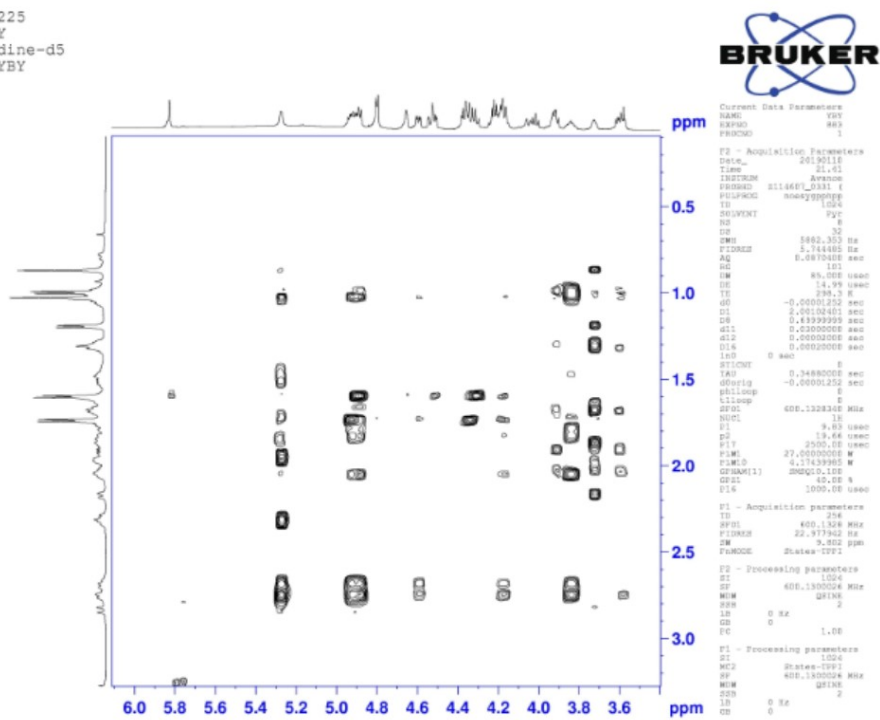
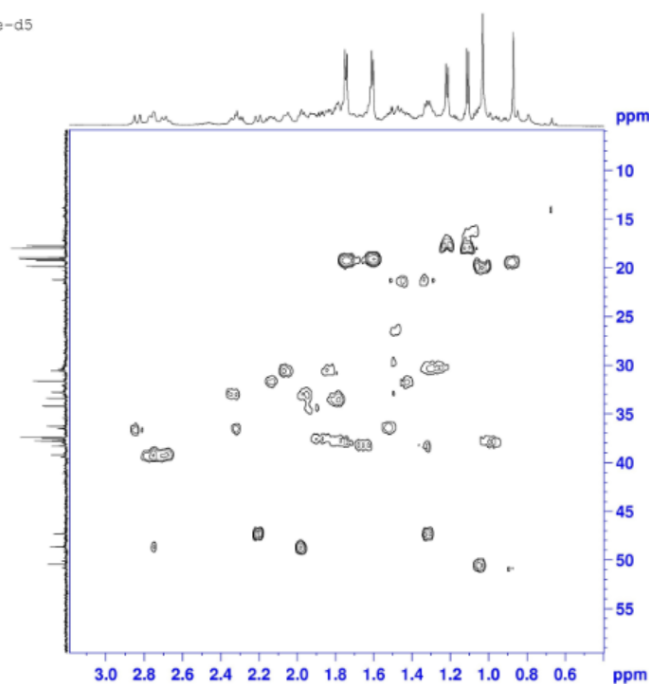


Figure S36. The partial enlargement of the NOESY spectrum of 1 (c).

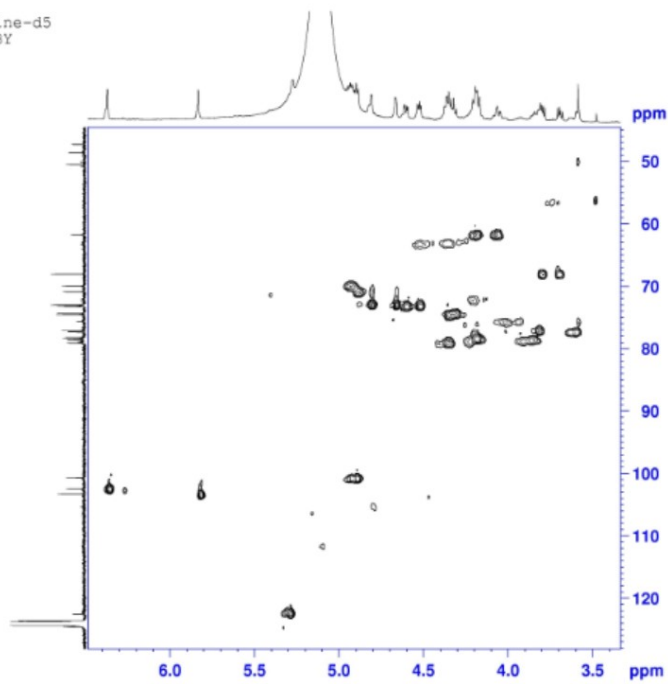
HQ-162  
HSQC  
Pyridine-d5  
921/YBY



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d14: 0.000000 sec
DELTA: 0.000000 sec
DELTA2: 0.0012500 sec
DELTA3: 0.000000 sec
INSTRUM: spect
AQ: 0 sec
d1: 0
d11: 0.000000 sec
d12: 0
d13: 0
d14: 0
P1: 600.132842 MHz
P2: 13
P3: 13 usec
P4: 13.00 usec
P5: 13.00 usec
P6: 1300.00 MHz
P7: 0.0000000 M
P8: 130.918497 MHz
P9: 130
P10: 130
P11: 13.00 usec
P12: 60.00 usec
P13: 60.00 usec
P14: 0.0000000 M
P15: 3.4000000 M
P16: 3.4000000 M
P17: 30.70 usec
P18: 30.70 usec
P19: 1300.00 MHz
P20: 1300.00 MHz
P21 - Acquisition parameters
TD: 65536
SF: 500.132842 MHz
PC: 130.918497 MHz
PULPROG: zgpg30
PC: 0 Hz
DE: 0
PC: 0
P2 - Processing parameters
SI: 32768
SF: 500.132842 MHz
WDW: EM
SSB: 0
LB: 0 Hz
GB: 0
PC: 1.00
P3 - Processing parameters
SI: 32768
SF: 500.132842 MHz
WDW: EM
SSB: 0
LB: 0 Hz
GB: 0
```

Figure S37. The partial enlargement of the HSQC spectrum of 2 (a).

HQ-162  
HSQC  
Pyridine-d5  
921/YBY



```
Current Data Parameters
NAME: 20180114
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20180114
Time: 4.39
INSTRUM: Avance
PROBHD: 514601_3331.c
PULPROG: zgpg30
TD: 65536
SOLVENT: Py
NS: 2048
DS: 4
SWH: 8041.318 Hz
FIDRES: 0.344392 Hz
AQ: 0.197009 sec
RG: 321
AQ2: 79.000 usec
DE: 6.70 usec
TE: 300.2 K
C1P2: 145.000000 sec
d1: 0.000000 sec
d11: 1.000000 sec
d12: 0.0012414 sec
d13: 0.000000 sec
d14: 0.000000 sec
DELTA: 0.000000 sec
DELTA2: 0.0012500 sec
DELTA3: 0.000000 sec
INSTRUM: spect
AQ: 0 sec
d1: 0
d11: 0.000000 sec
d12: 0
d13: 0
d14: 0
P1: 600.132842 MHz
P2: 13
P3: 13 usec
P4: 13.00 usec
P5: 13.00 usec
P6: 1300.00 MHz
P7: 0.0000000 M
P8: 130.918497 MHz
P9: 130
P10: 130
P11: 13.00 usec
P12: 60.00 usec
P13: 60.00 usec
P14: 0.0000000 M
P15: 3.4000000 M
P16: 3.4000000 M
P17: 30.70 usec
P18: 30.70 usec
P19: 1300.00 MHz
P20: 1300.00 MHz
P21 - Acquisition parameters
TD: 65536
SF: 500.132842 MHz
PC: 130.918497 MHz
PULPROG: zgpg30
PC: 0 Hz
DE: 0
PC: 0
P2 - Processing parameters
SI: 32768
SF: 500.132842 MHz
WDW: EM
SSB: 0
LB: 0 Hz
GB: 0
PC: 1.00
P3 - Processing parameters
SI: 32768
SF: 500.132842 MHz
WDW: EM
SSB: 0
LB: 0 Hz
GB: 0
```

Figure S38. The partial enlargement of the HSQC spectrum of 2 (b).

HQO-162  
COSY  
Pyridine-d5  
920/YBY

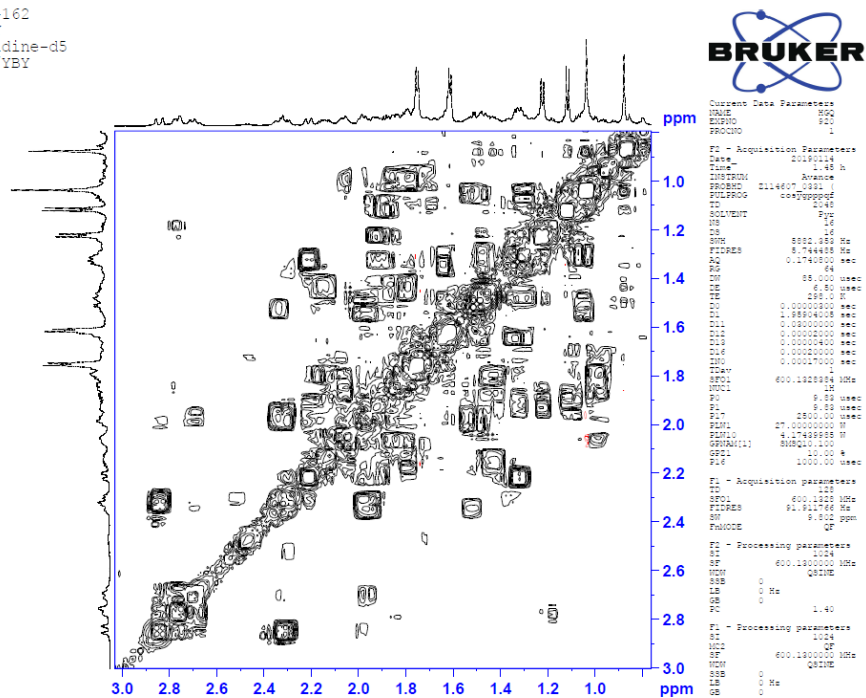


Figure S39. The partial enlargement of the  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of 2 (a).

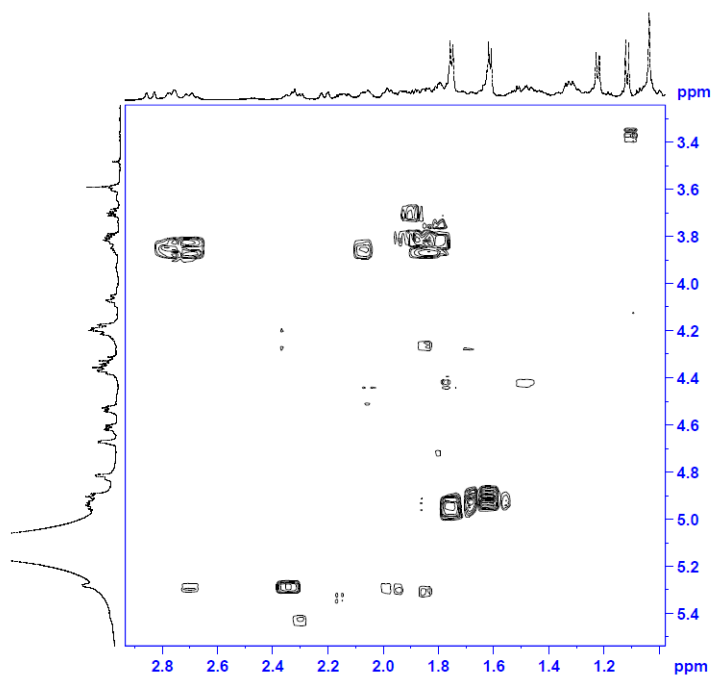


Figure S40. The partial enlargement of the  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of 2 (b).

HQ-162  
HMBC  
Pyridine-d5  
922/YBY

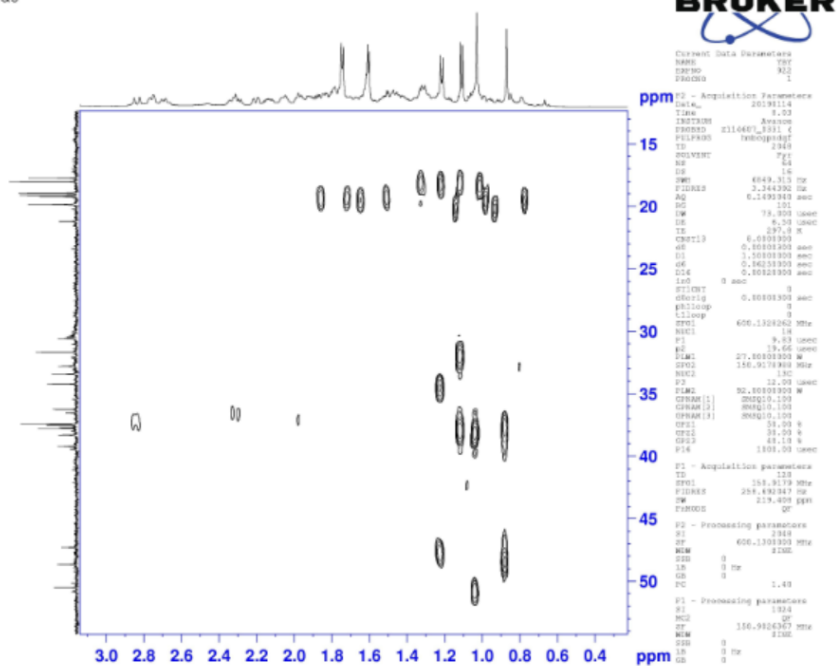


Figure S41. The partial enlargement of the HMBC spectrum of 2 (a).

HQ-162  
HMBC  
Pyridine-d5  
922/YBY

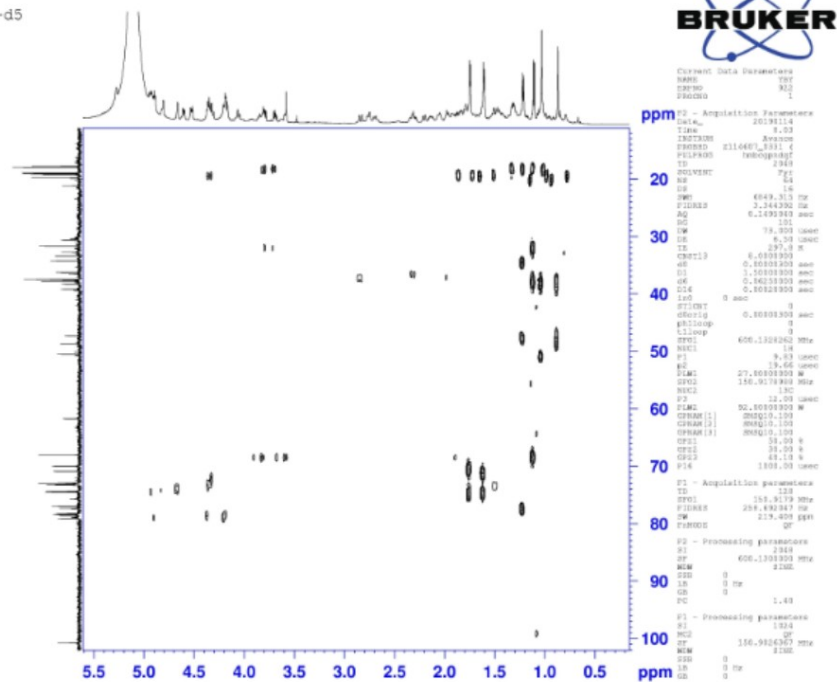


Figure S42. The partial enlargement of the HMBC spectrum of 2 (b).



HGQ-162  
HMBC  
Pyridine-d5  
922/YBY

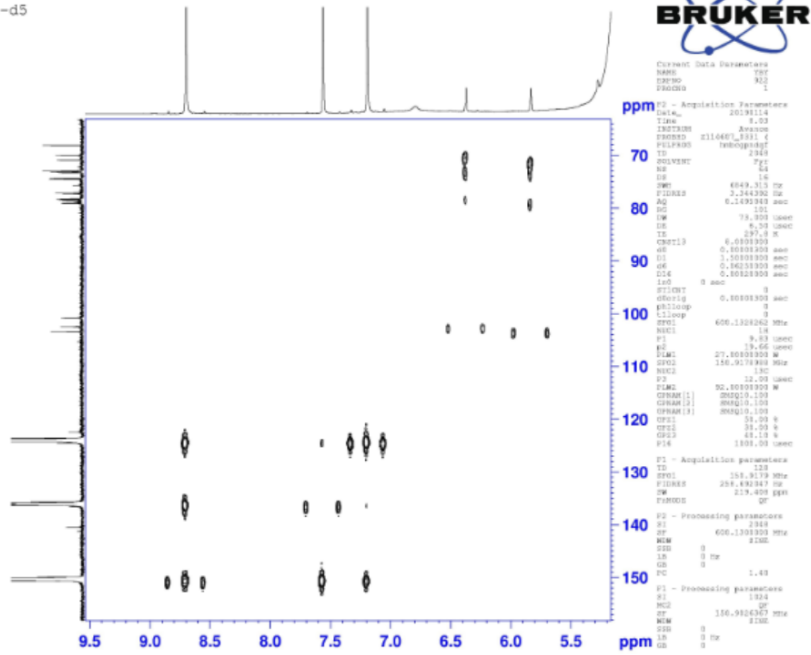


Figure S43. The partial enlargement of the HMBC spectrum of 2 (c).

HGQ-162  
NOESY  
Pyridine-d5  
923/YBY

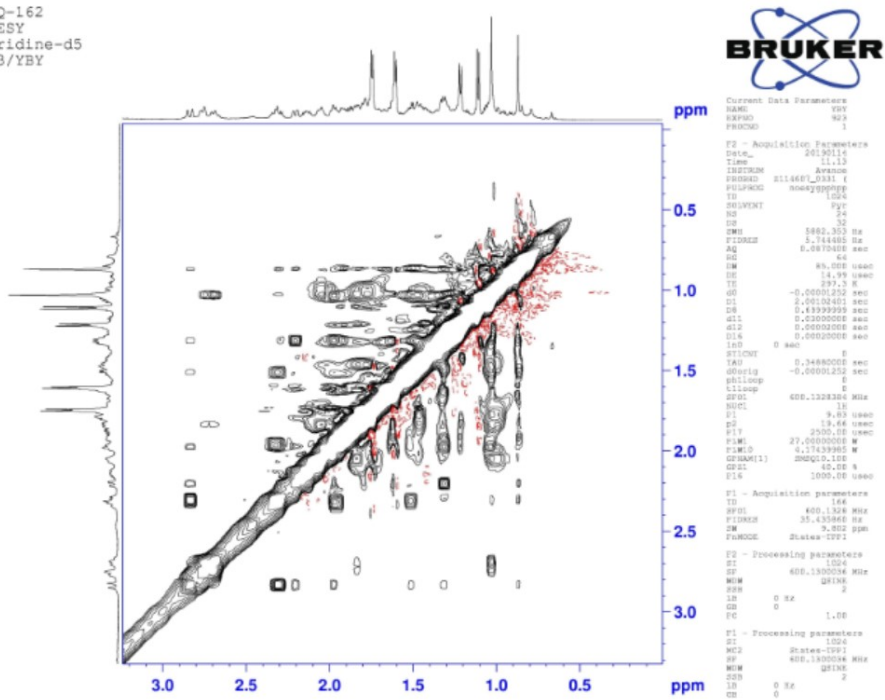


Figure S44. The partial enlargement of the NOESY spectrum of 2 (a).

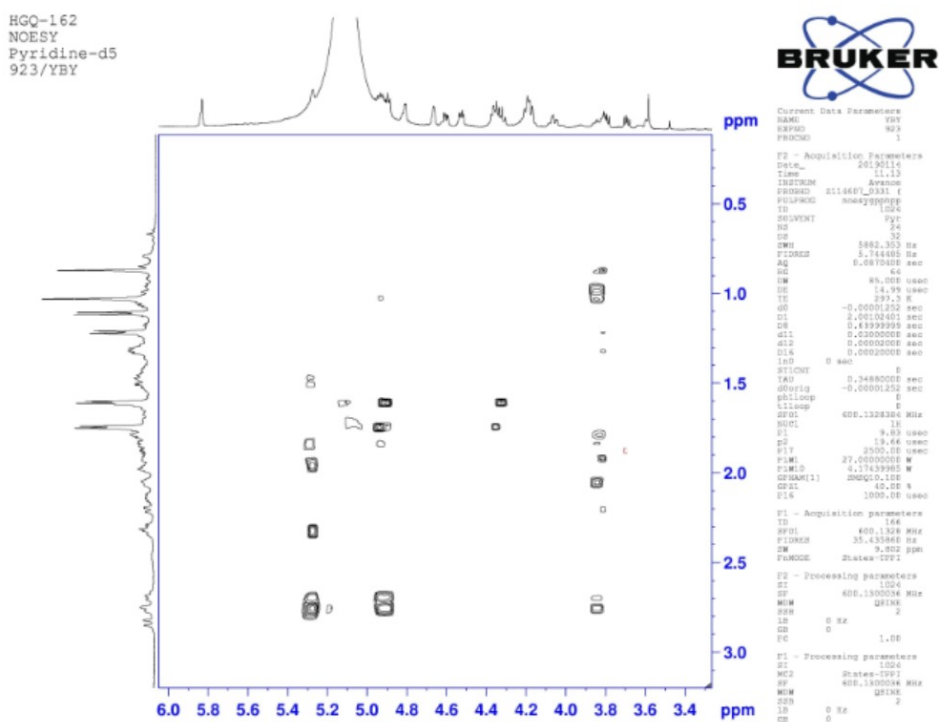


Figure S45. The partial enlargement of the NOESY spectrum of 2 (b).

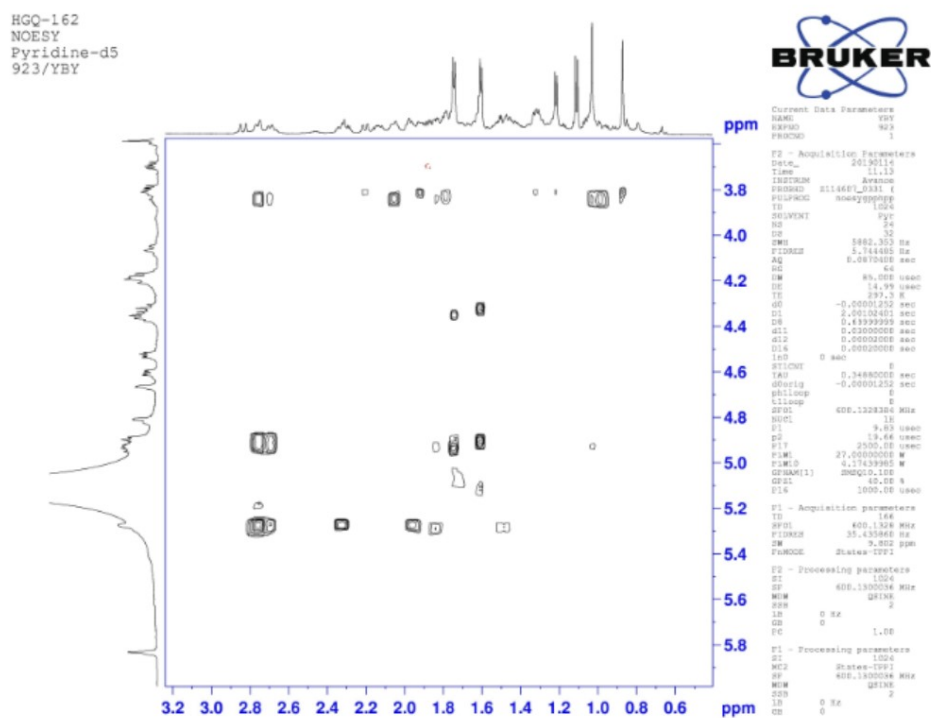


Figure S46. The partial enlargement of the NOESY spectrum of 2 (c).

HGQ-162  
NOESY  
Pyridine-d5  
923/YBY

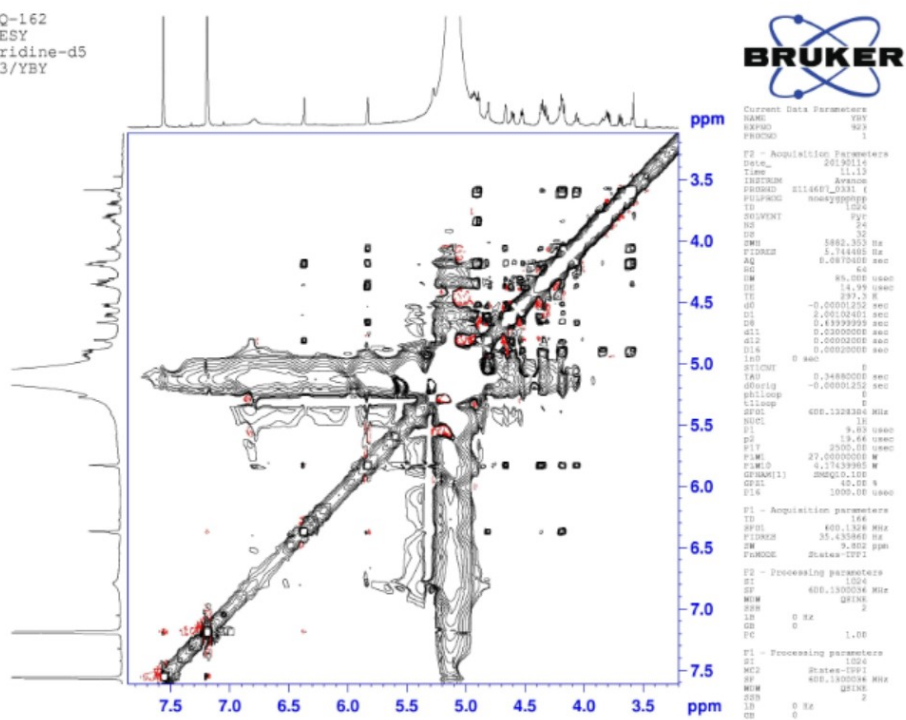


Figure S47. The partial enlargement of the NOESY spectrum of 2 (d).