

Supporting Information for:

Synthesis and Properties of Fluorescence Dyes: Tetracyclic Pyrazolo[3,4-*b*]Pyridine-based Coumarin Chromophores with Intramolecular Charge Transfer Character

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[§] These authors contributed equally to this manuscript.

SI-1 Crystallographic data

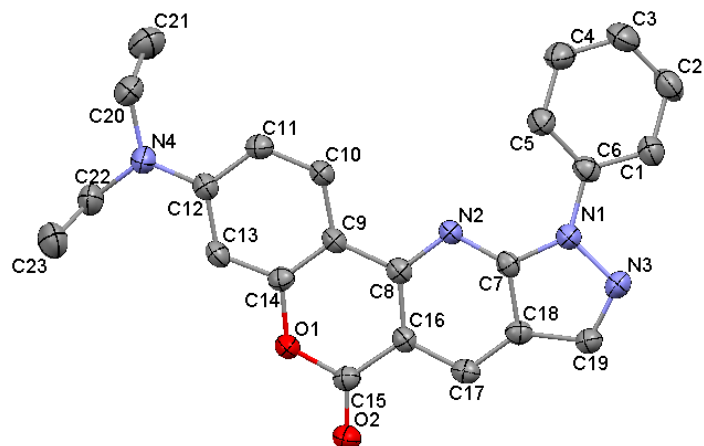


Figure S1. Crystal structures of **1a** with ellipsoids shown at the 50% probability level (hydrogen atoms are omitted for clarity).

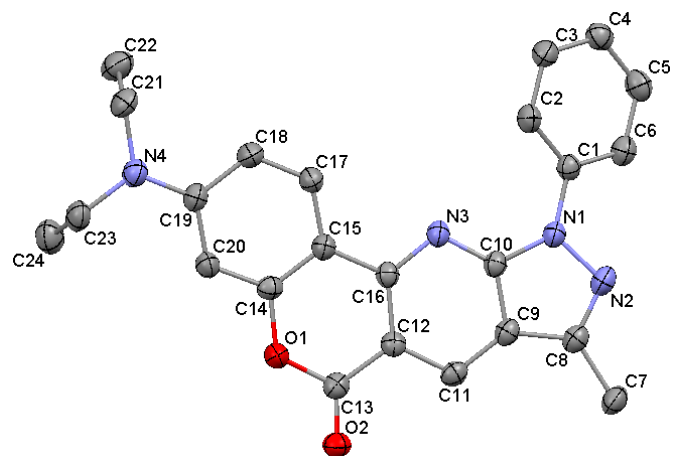


Figure S2. Crystal structures of **1b** with ellipsoids shown at the 50% probability level (hydrogen atoms are omitted for clarity).

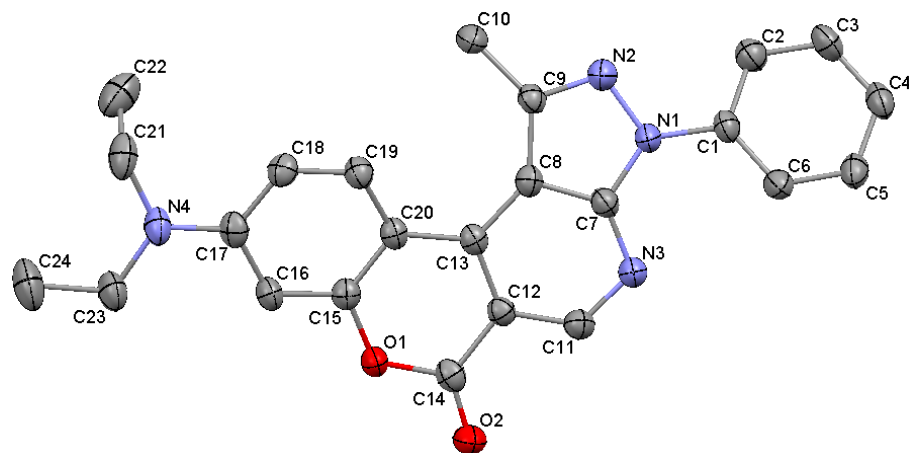


Figure S3. Crystal structures of **2b** with ellipsoids shown at the 50% probability level (hydrogen atoms are omitted for clarity).

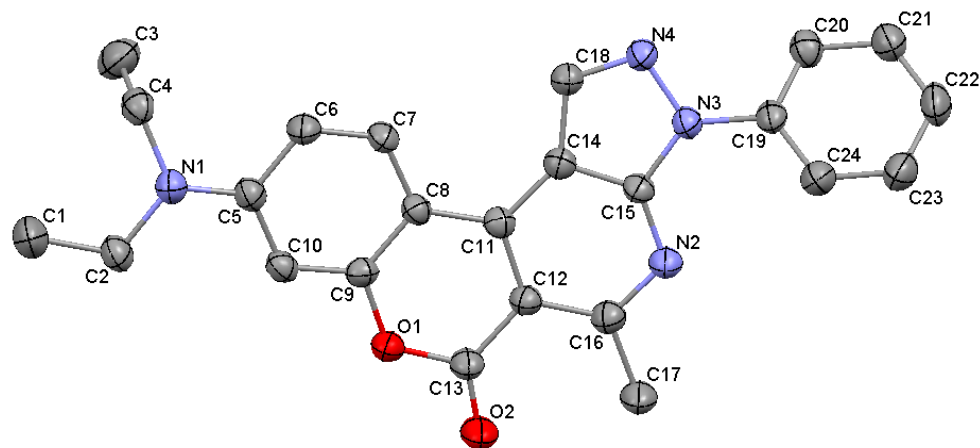


Figure S4. Crystal structures of **4a** with ellipsoids shown at the 50% probability level (hydrogen atoms are omitted for clarity).

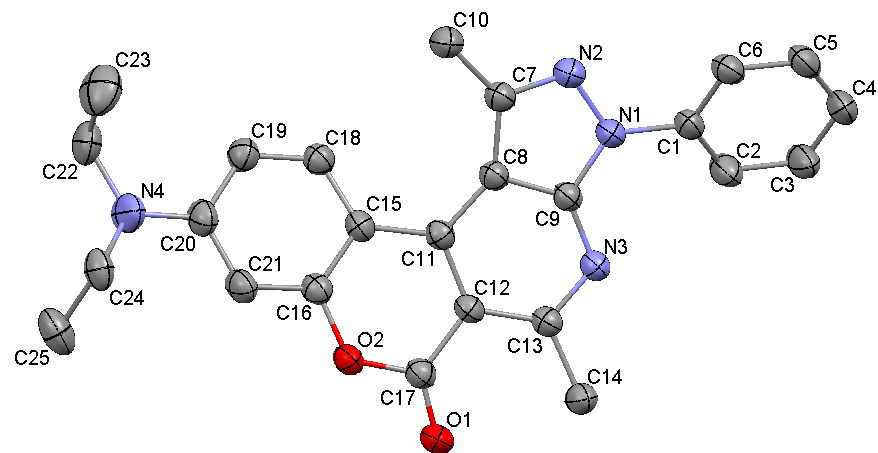


Figure S5. Crystal structures of **4b** with ellipsoids shown at the 50% probability level (hydrogen atoms are omitted for clarity).

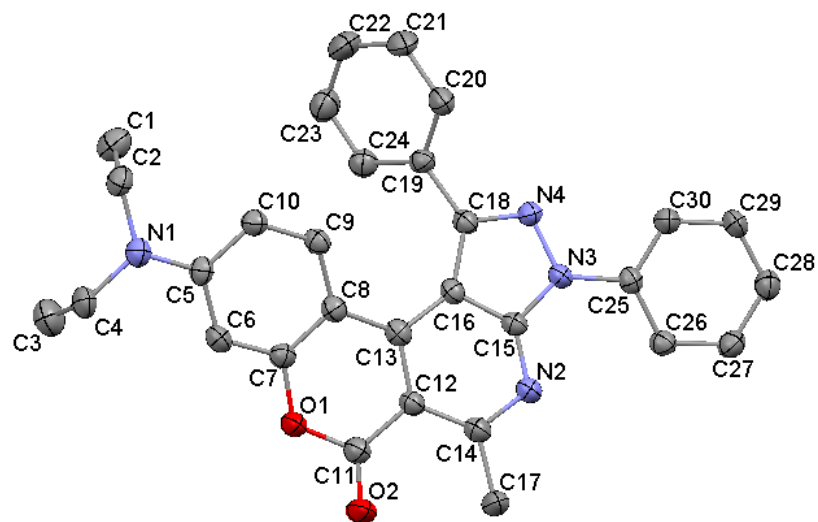


Figure S6. Crystal structures of **4c** with ellipsoids shown at the 50% probability level (hydrogen atoms are omitted for clarity).

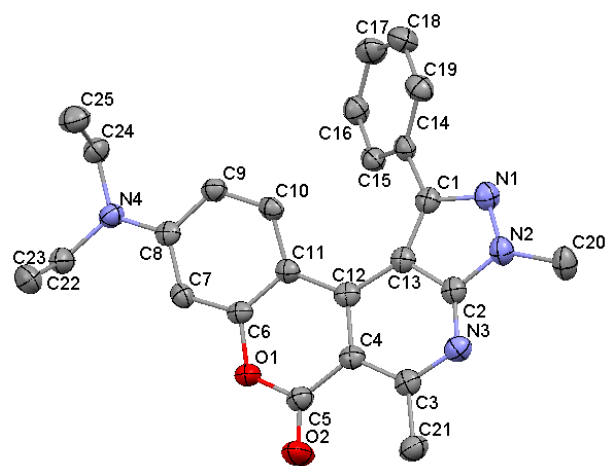


Figure S7. Crystal structures of **4d** with ellipsoids shown at the 50% probability level (hydrogen atoms are omitted for clarity).

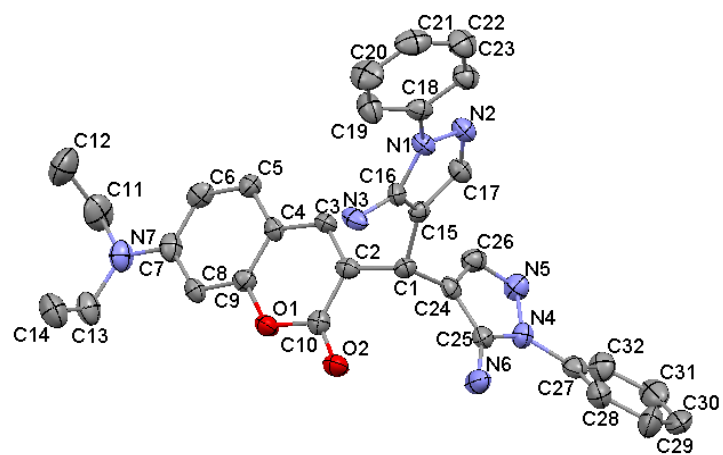


Figure S8. Crystal structures of **9** with ellipsoids shown at the 50% probability level (hydrogen atoms are omitted for clarity).

SI-2 Photophysical data

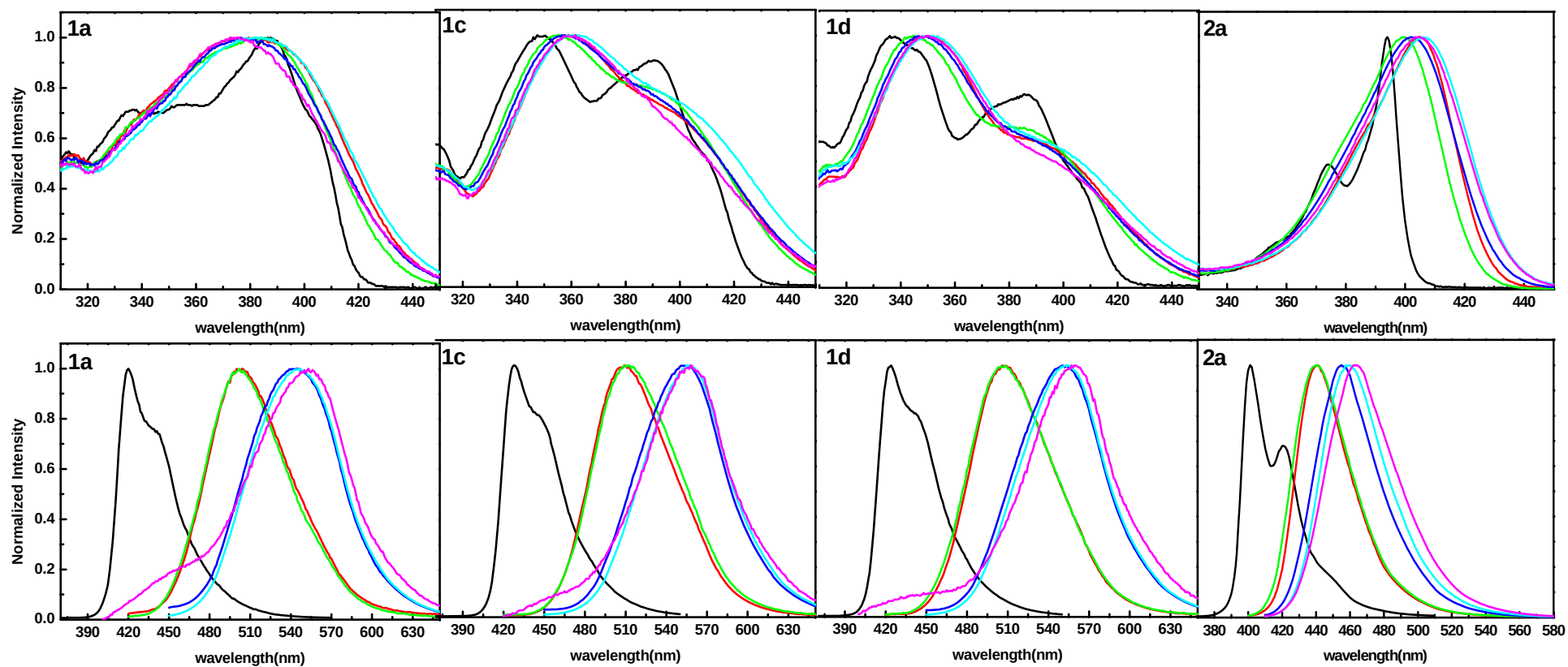


Figure S9. Absorption (top) and fluorescence (bottom) spectra of compounds **1a**, **1c**, **1d** and **2a** in different solvents: black (cyclohexane), red (CH_2Cl_2), green (EA), blue (CH_3CN), cyan (DMF), and magenta (CH_3OH).

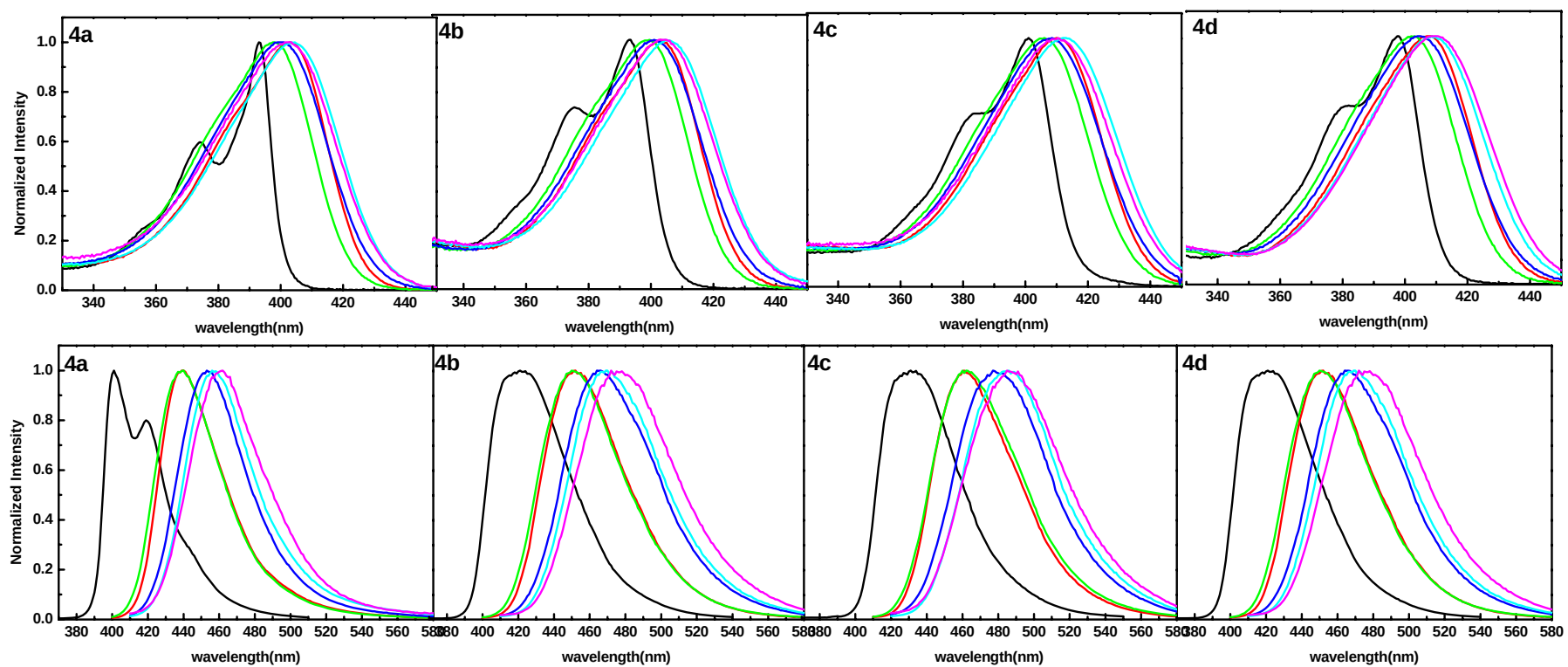


Figure S10. Absorption (top) and fluorescence (bottom) spectra of compounds **4a**, **4b**, **4c** and **4d** in different solvents: black (cyclohexane), red (CH_2Cl_2), green (EA), blue (CH_3CN), cyan (DMF), and magenta (CH_3OH).

SI-3 Electrochemical data

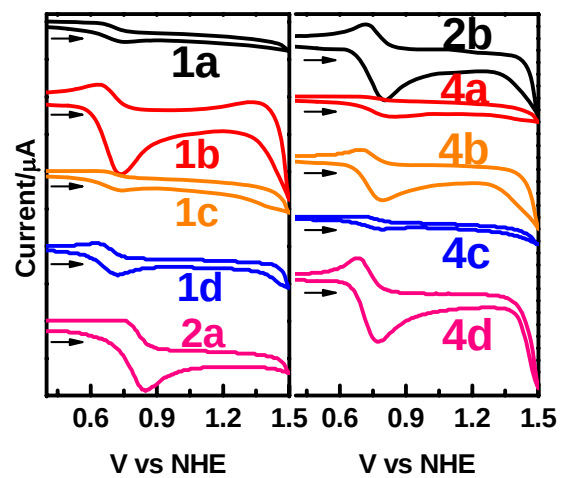


Figure S11. Cyclic voltammograms of compounds **1a-1d**, **2a**, **2b** and **4a-4d** in CH₃CN.

SI-4 Computational data

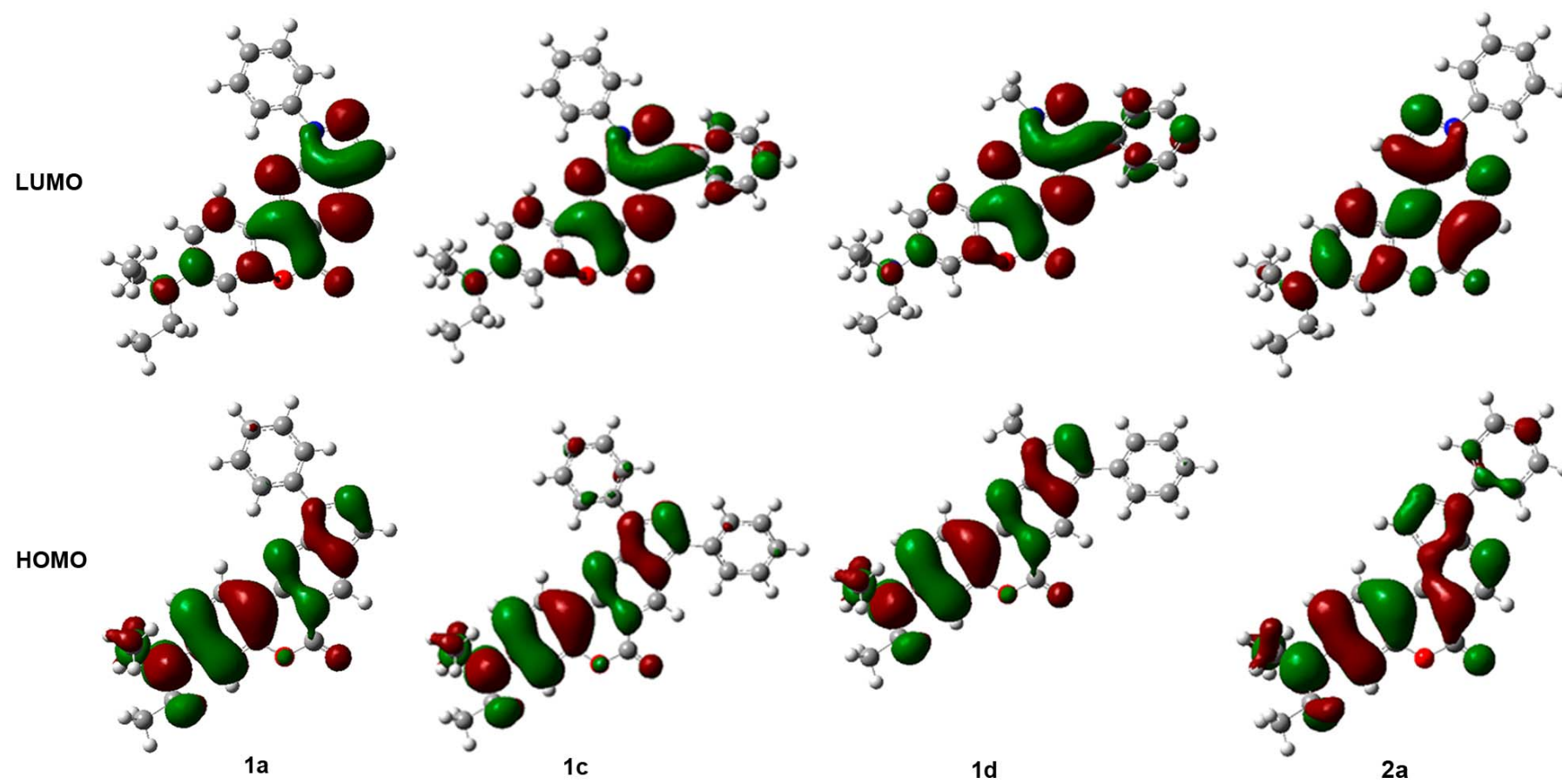


Figure S12. The calculated HOMOs and LUMOs of **1a**, **1c**, **1d** and **2a**.

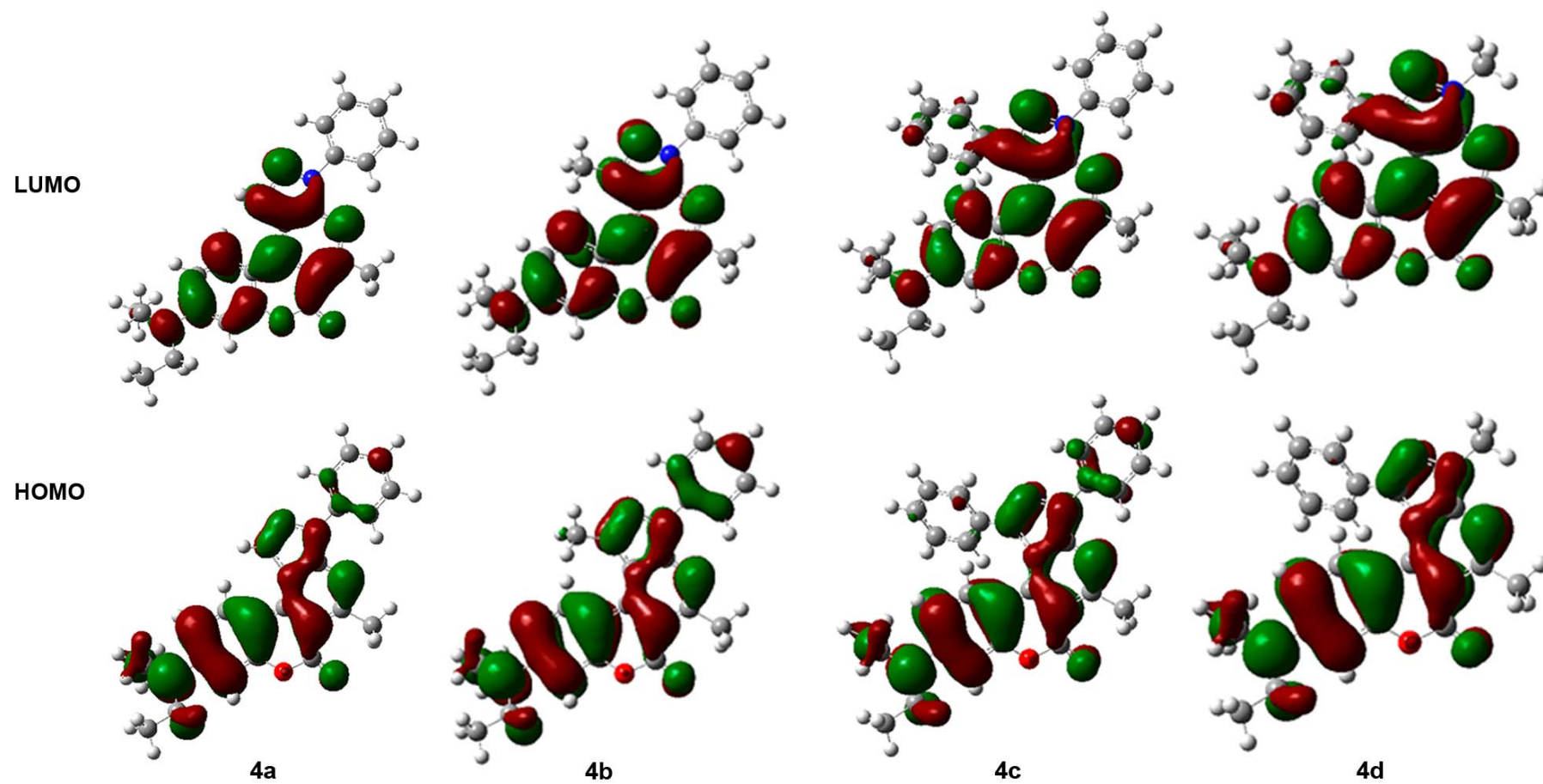


Figure S13. The calculated HOMOs and LUMOs of **4a-4d**.

SI-5 Spectrum of 1a with different proportion of water

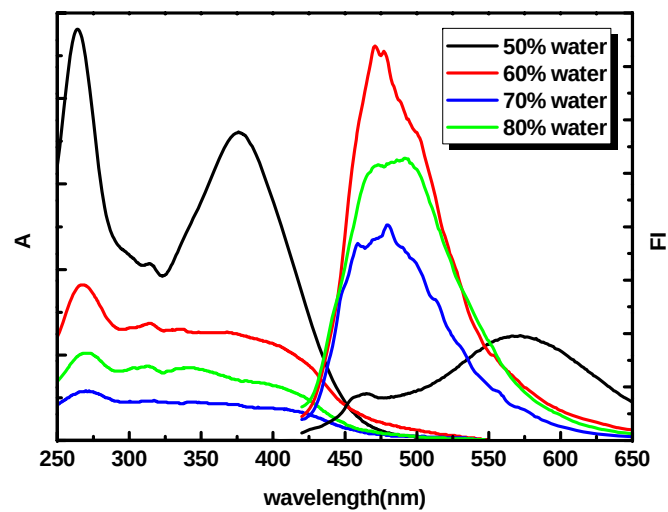
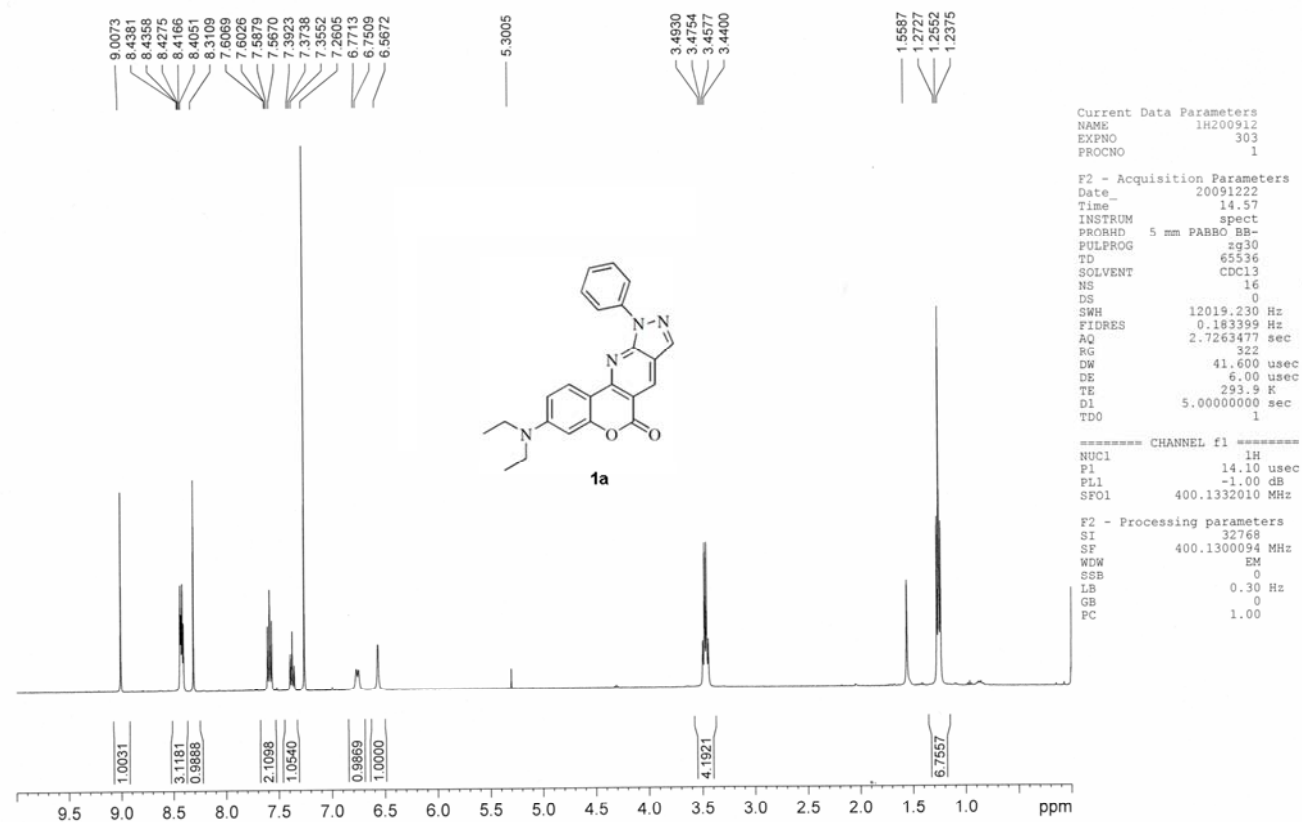
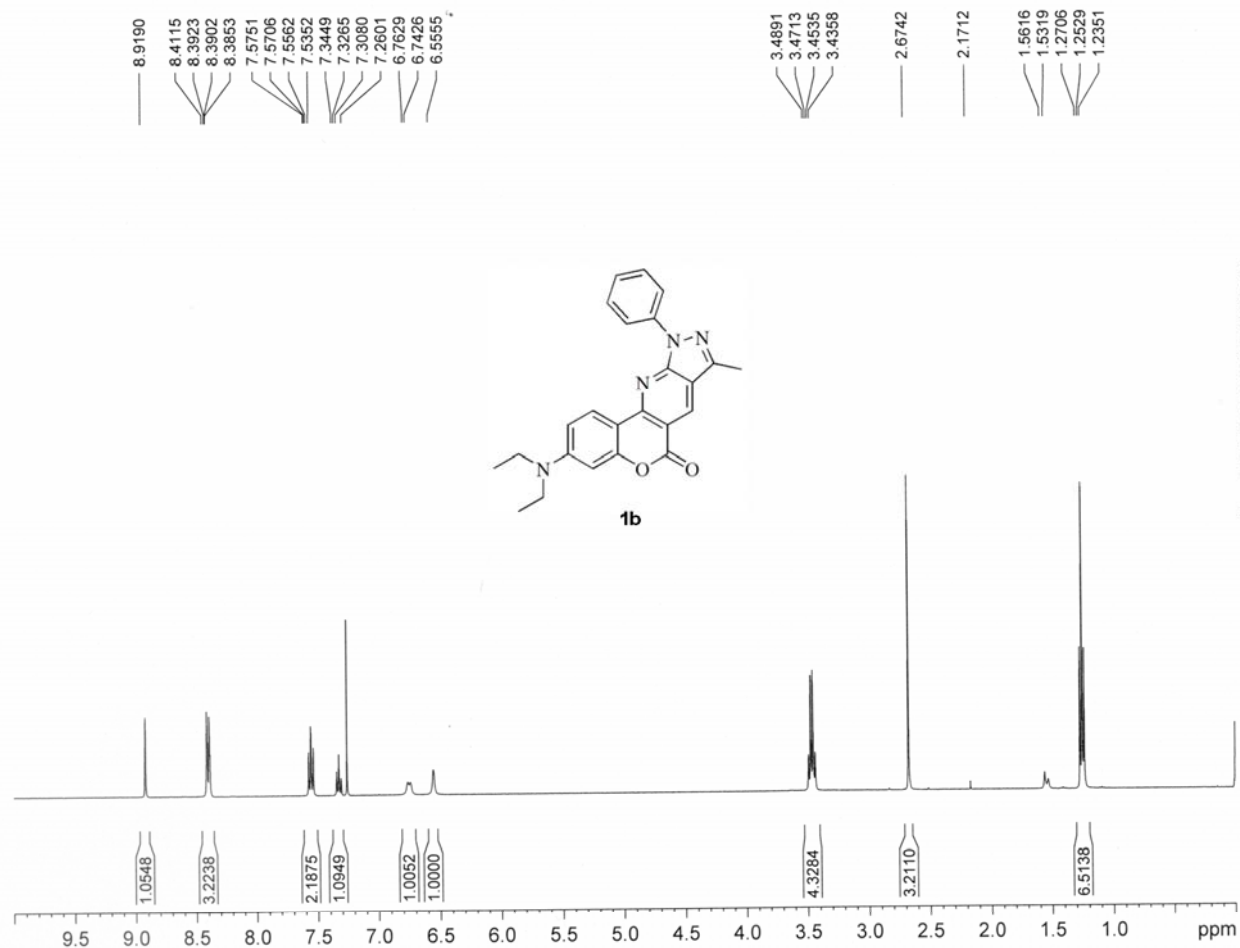


Figure S14. Absorption and fluorescence spectra of compound **1a** (10 μM) in different proportion of water and C₂H₅OH.

SI-6 NMR spectra

¹H NMR spectra of new compounds.



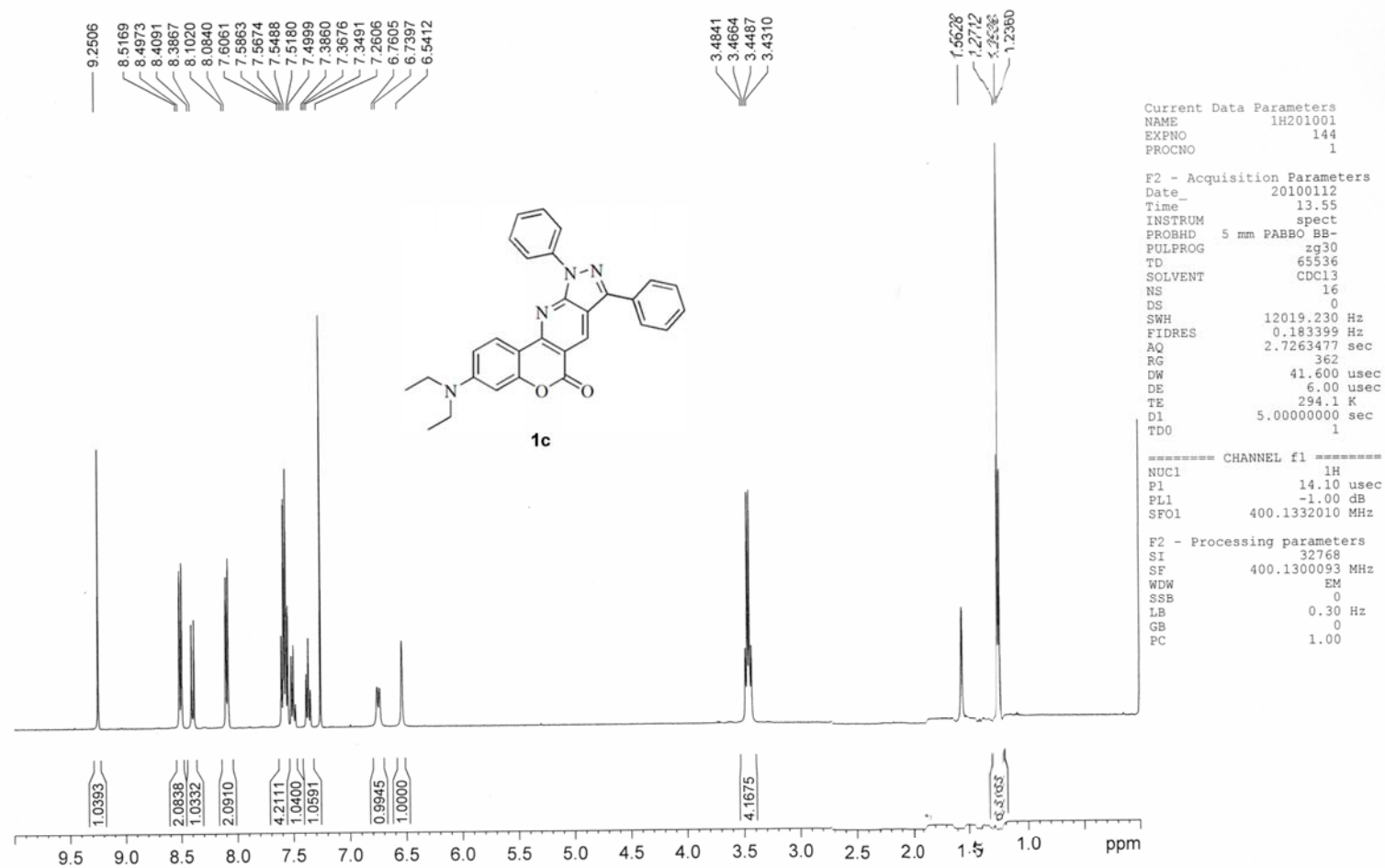


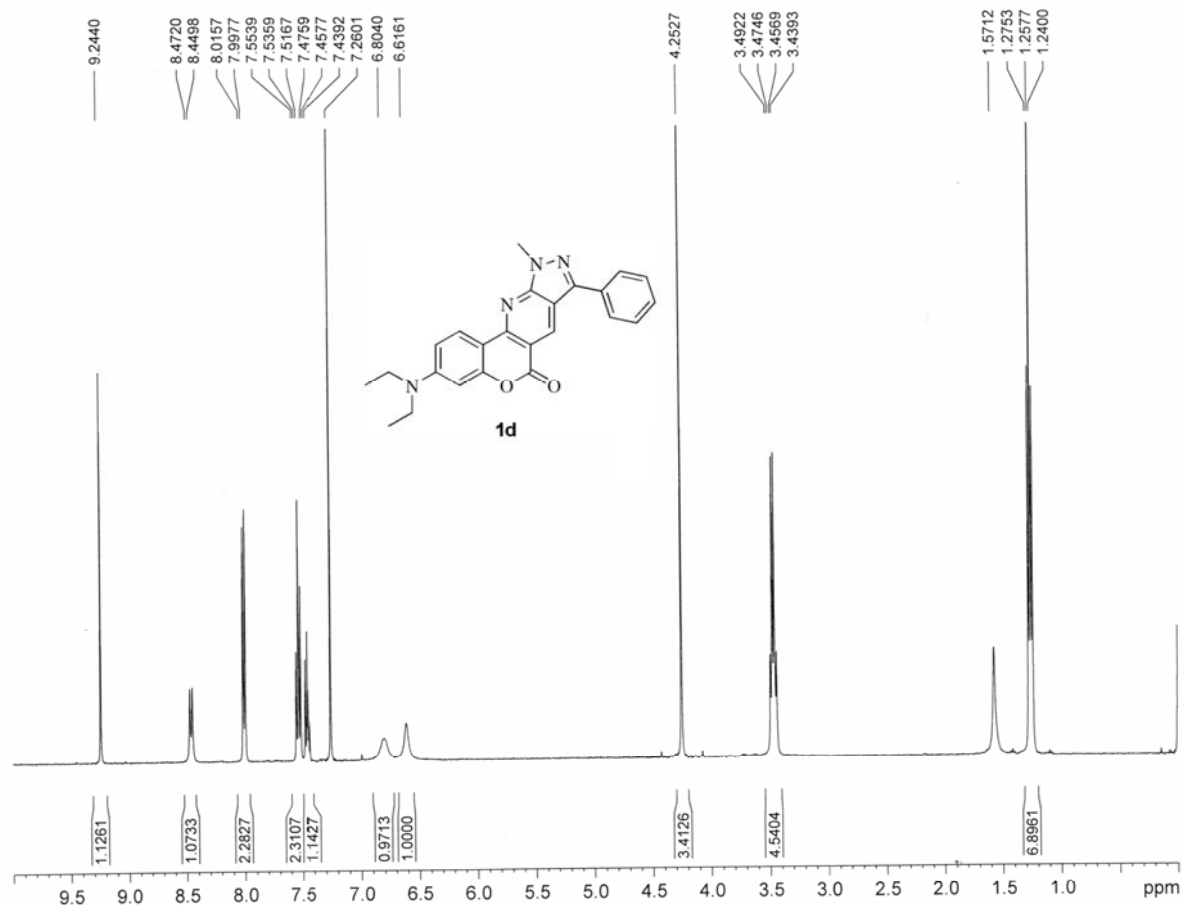
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FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 362
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DE 6.00 usec
TE 296.1 K
D1 5.00000000 sec
TD0 1

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PL1 -1.00 dB
SFO1 400.1332010 MHz

F2 - Processing parameters
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SF 400.1300094 MHz
WDW EM
SSB 0
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GB 0
PC 1.00



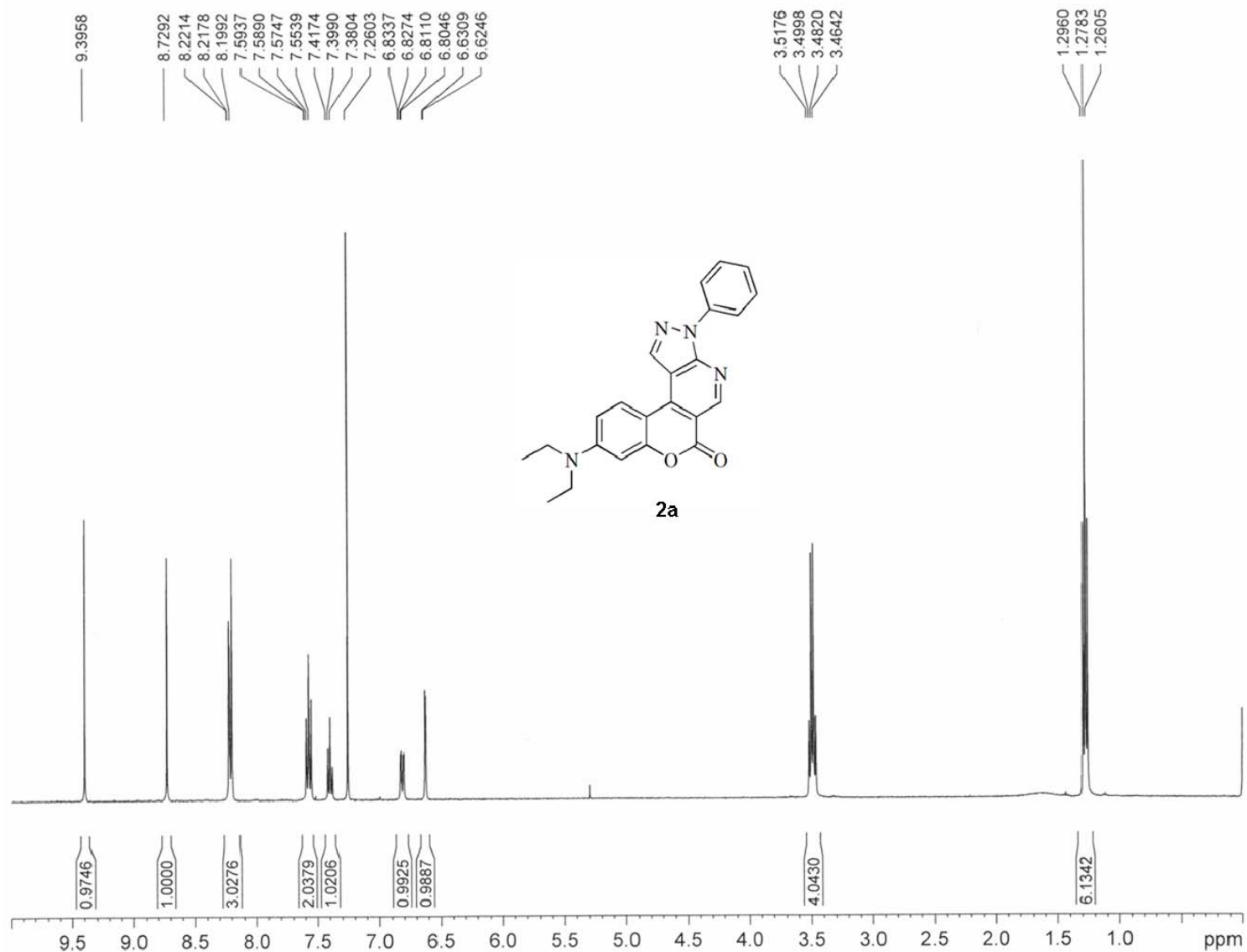


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FIDRES 0.183399 Hz
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RG 406
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DE 6.00 usec
TE 292.1 K
D1 5.00000000 sec
TD0 1

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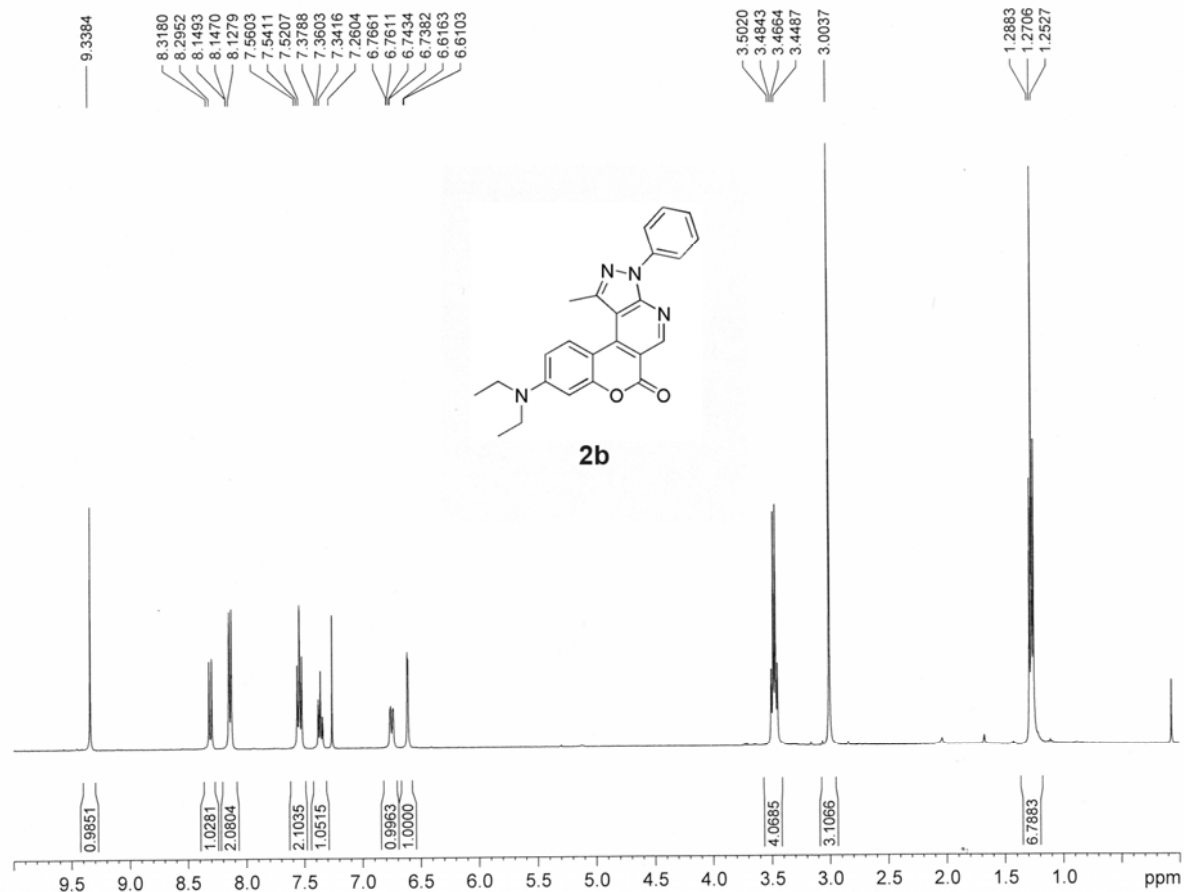
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RG        362
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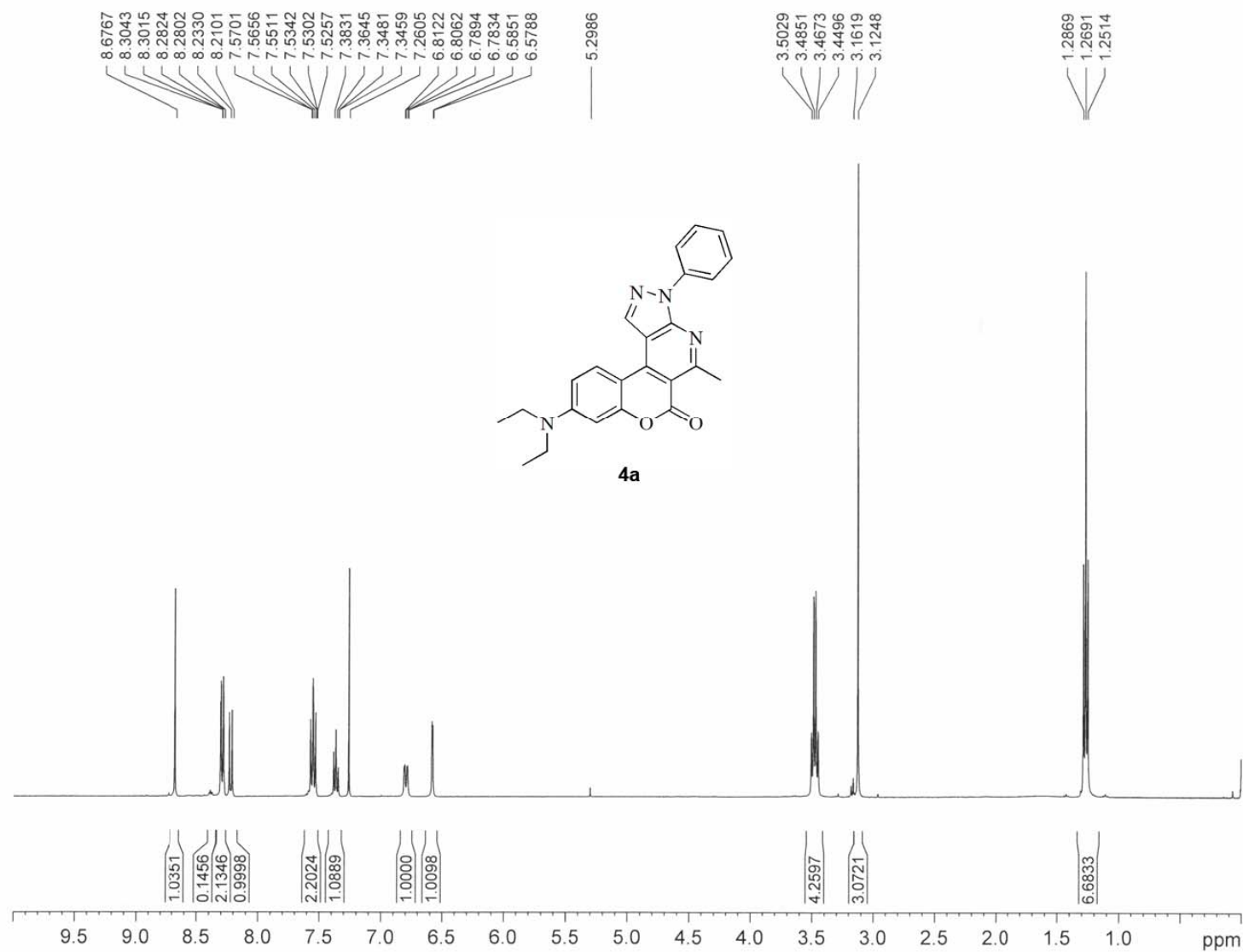



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 FIDRES 0.183399 Hz
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 RG 512
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 D1 5.00000000 sec
 TDO 1

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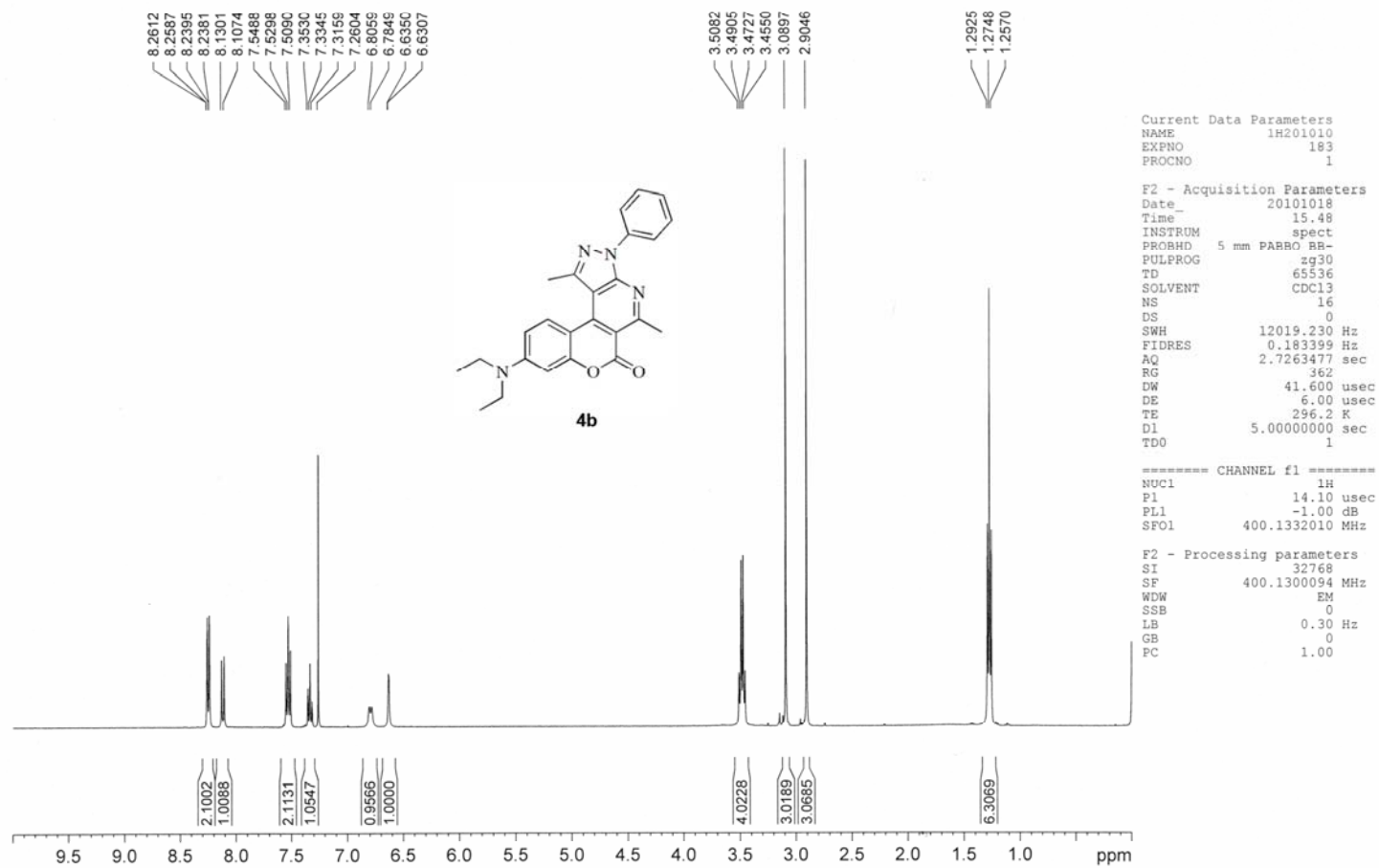


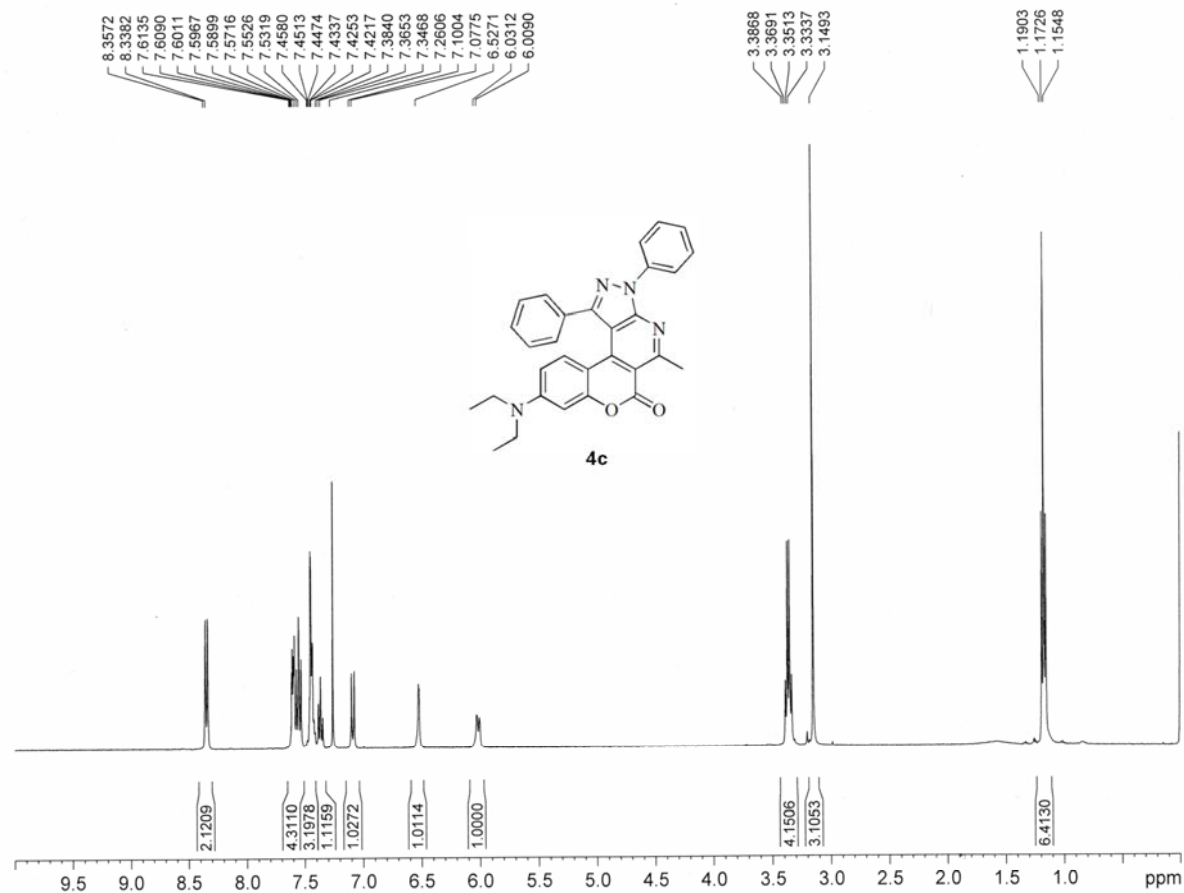
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 RG 228
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 DE 6.00 usec
 TE 295.5 K
 D1 5.00000000 sec
 TD0 1

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F2 - Processing parameters
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 PC 1.00



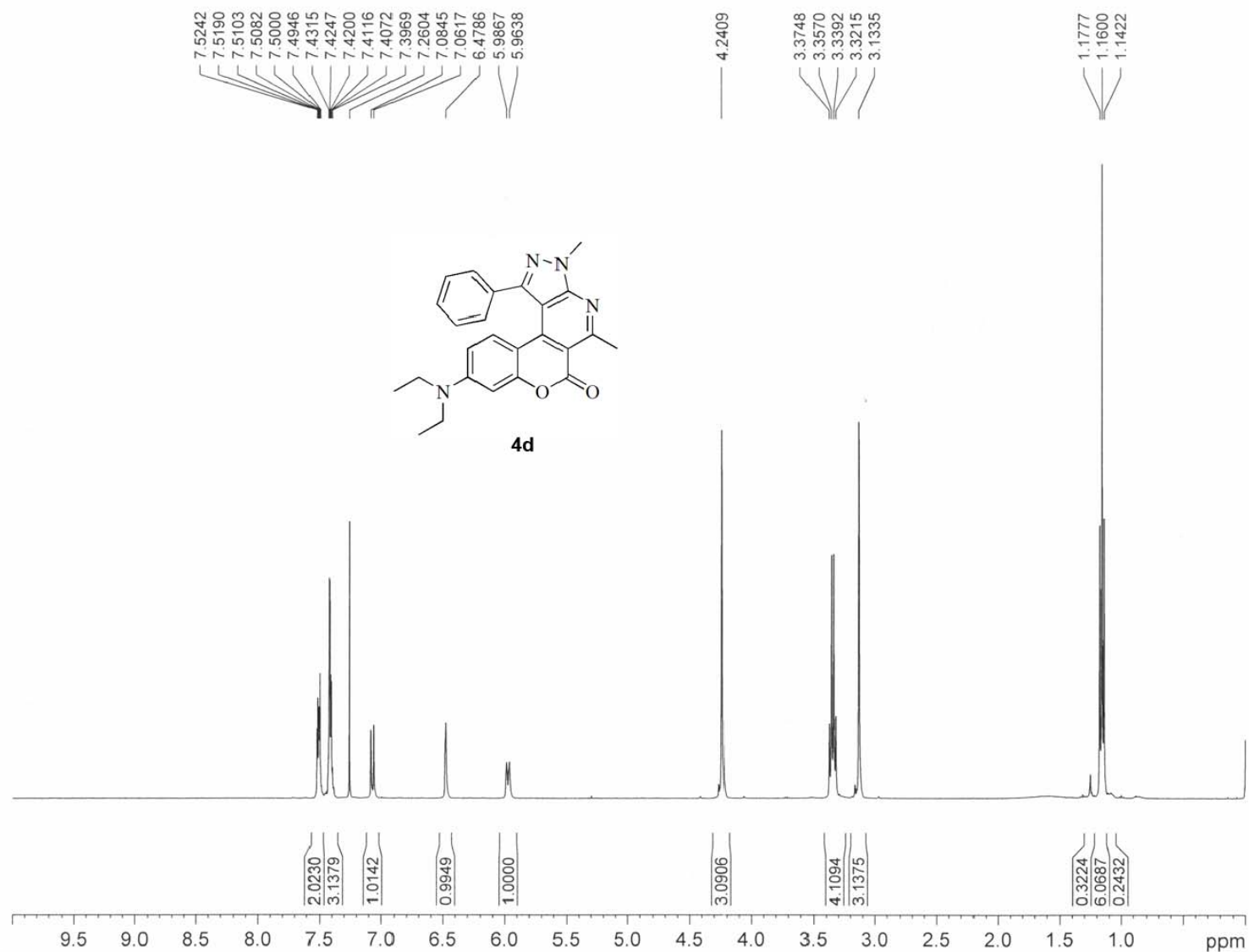


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SOLVENT CDCl3
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FIDRES 0.183399 Hz
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RG 1150
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DE 6.00 usec
TE 298.2 K
D1 5.00000000 sec
TD0 1

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F2 - Processing parameters
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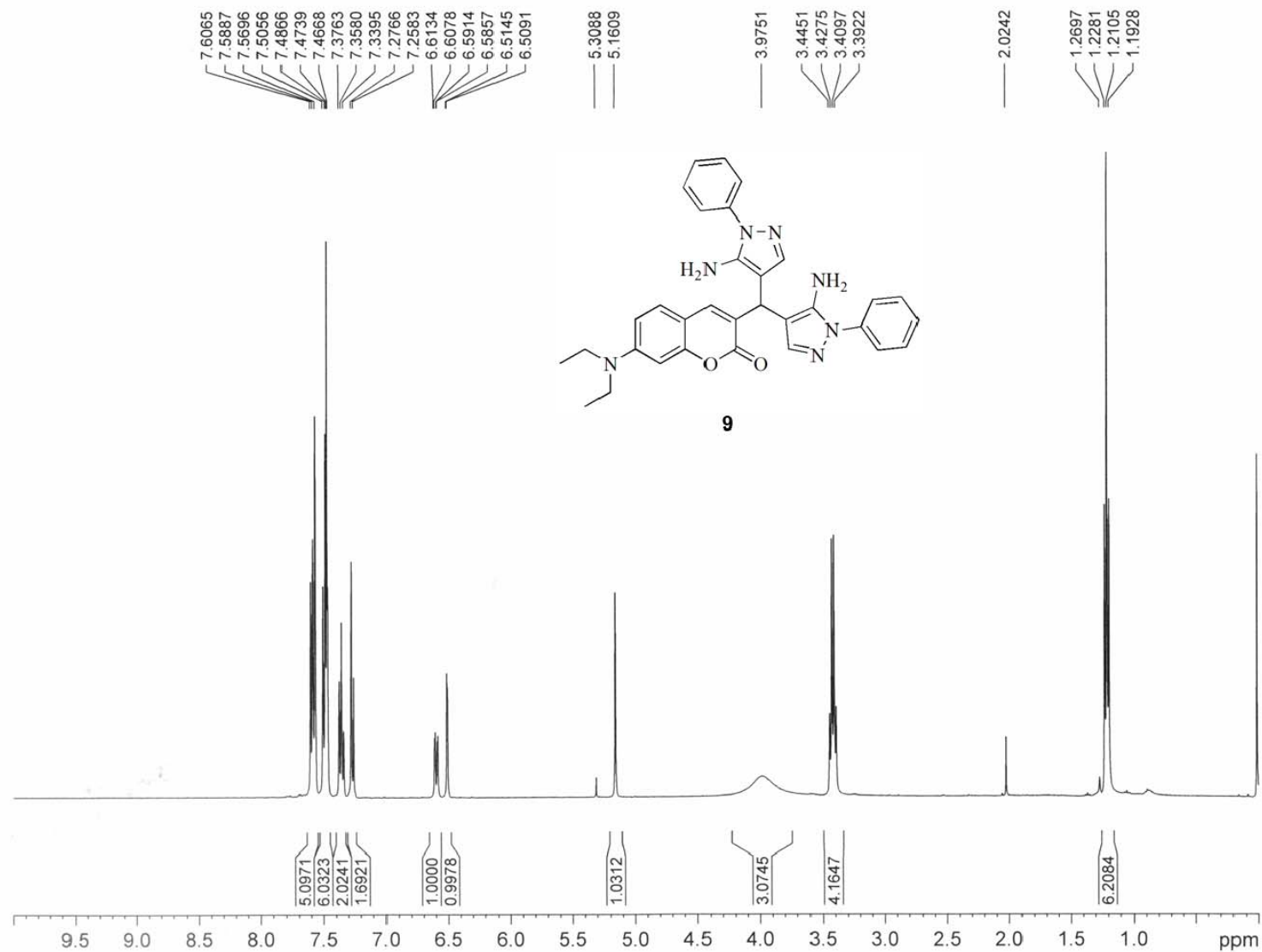


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 NS 16
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 FIDRES 0.183399 Hz
 AQ 2.7263477 sec
 RG 362
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 DE 6.00 usec
 TE 298.5 K
 D1 5.00000000 sec
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===== CHANNEL f1 =====
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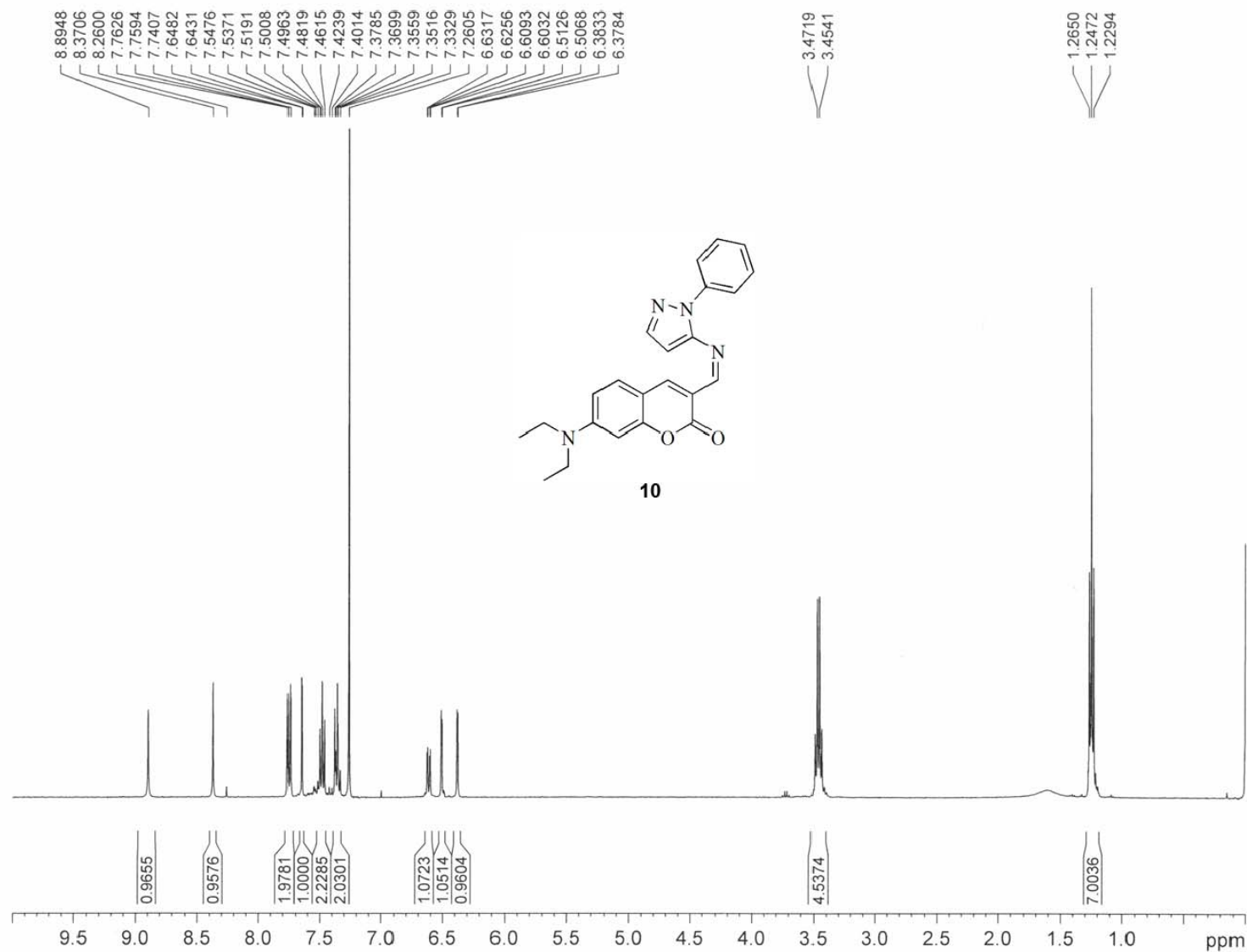


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 NS 16
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 FIDRES 0.183399 Hz
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 RG 228
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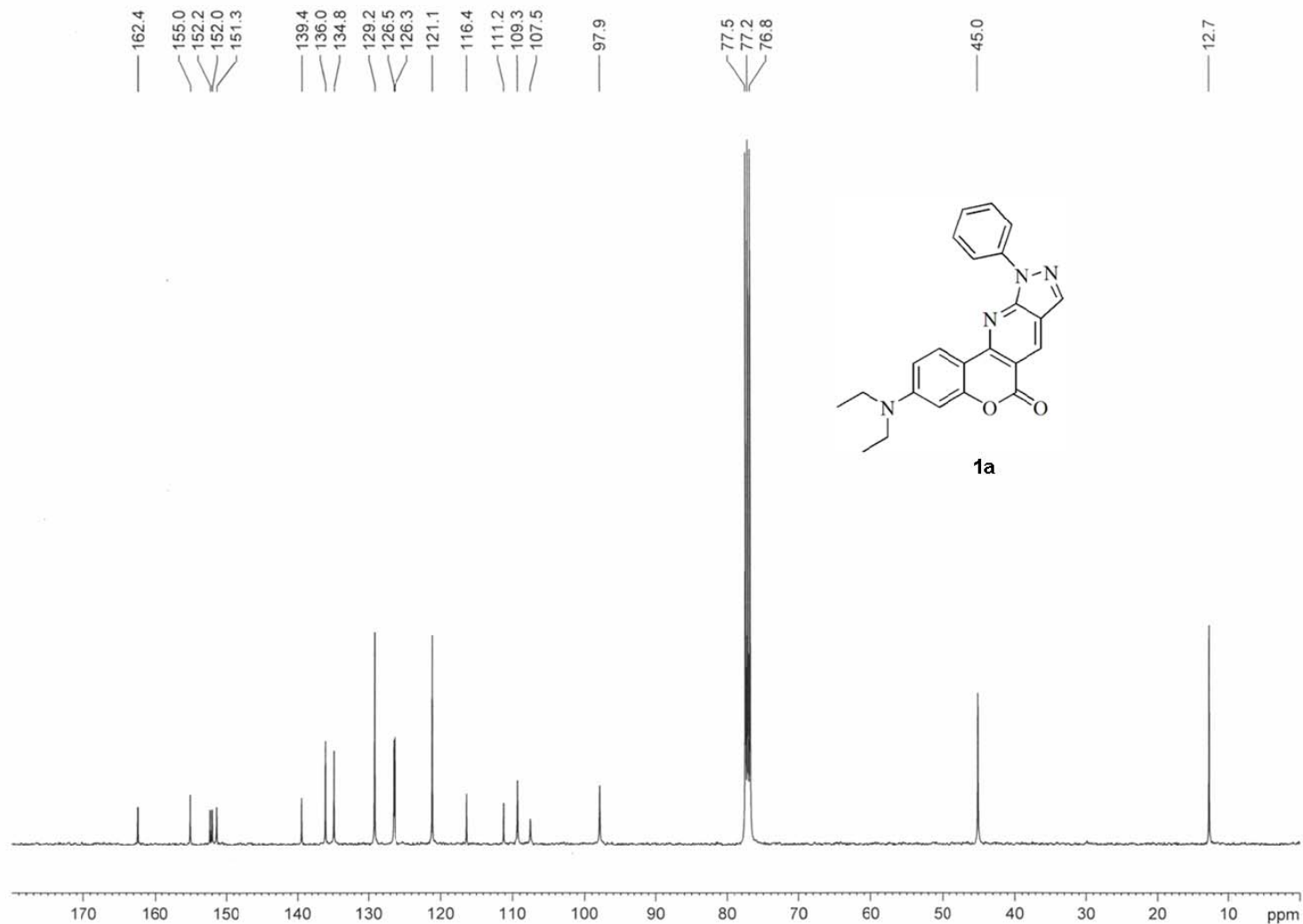
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FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 322
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DE 6.00 usec
TE 295.2 K
D1 5.00000000 sec
TD0 1

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SFO1 400.1332010 MHz

F2 - Processing parameters
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¹³C NMR spectra of new compounds.



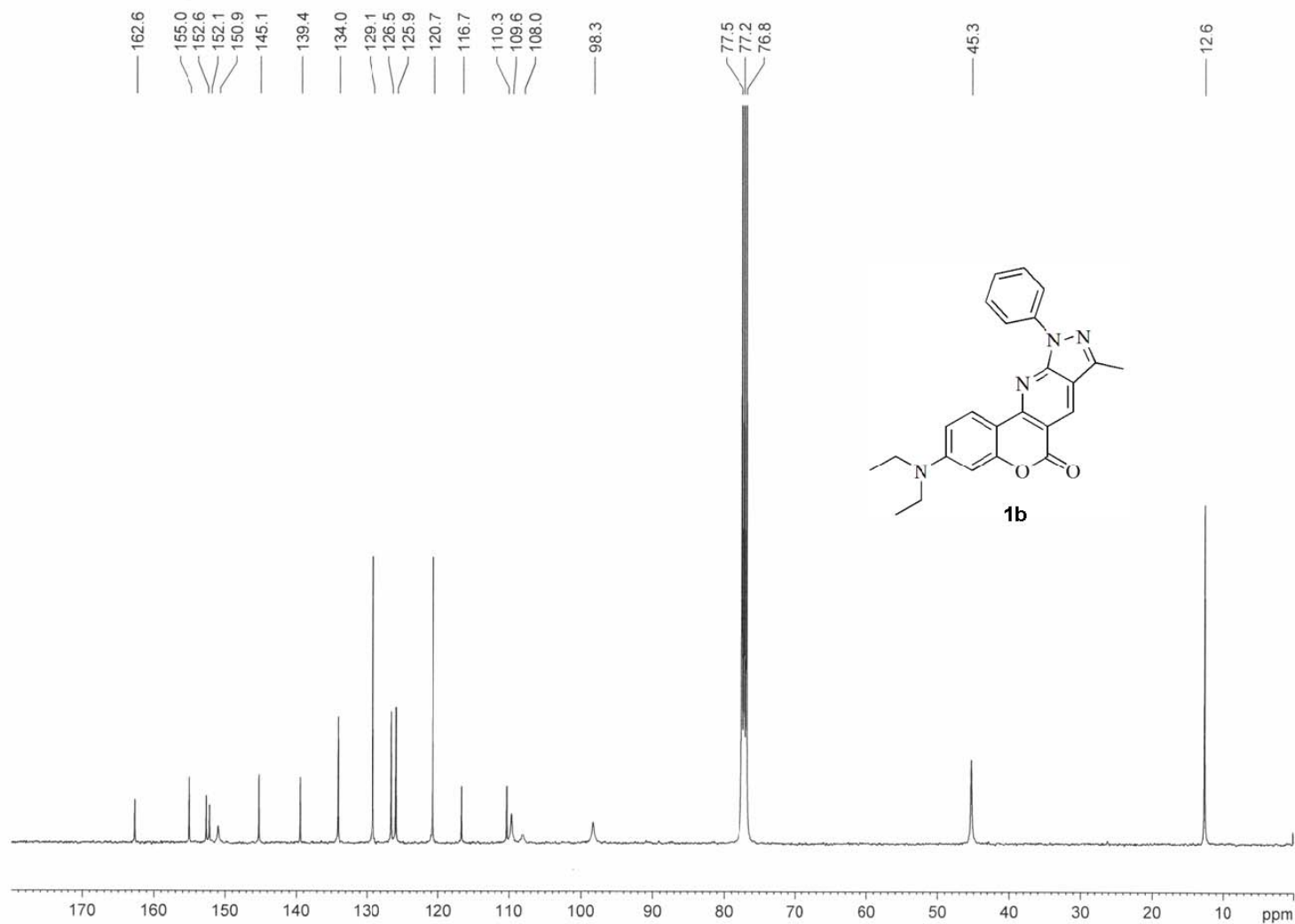
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FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 114
DW 19.800 usec
DE 6.00 usec
TE 298.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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PCPD2 80.00 usec
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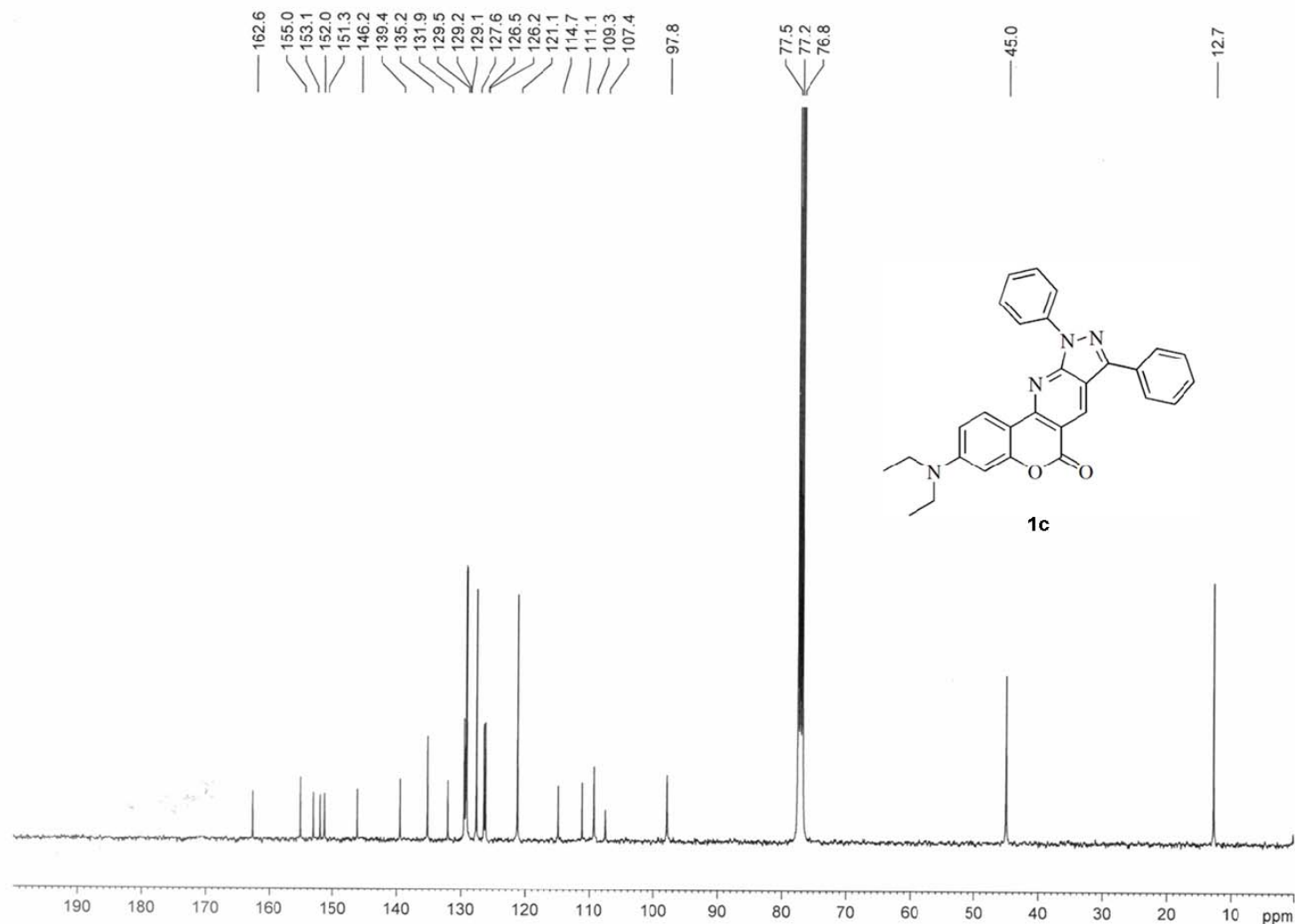
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FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 406
DW 19.800 usec
DE 6.00 usec
TE 296.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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SFO1 100.6228303 MHz

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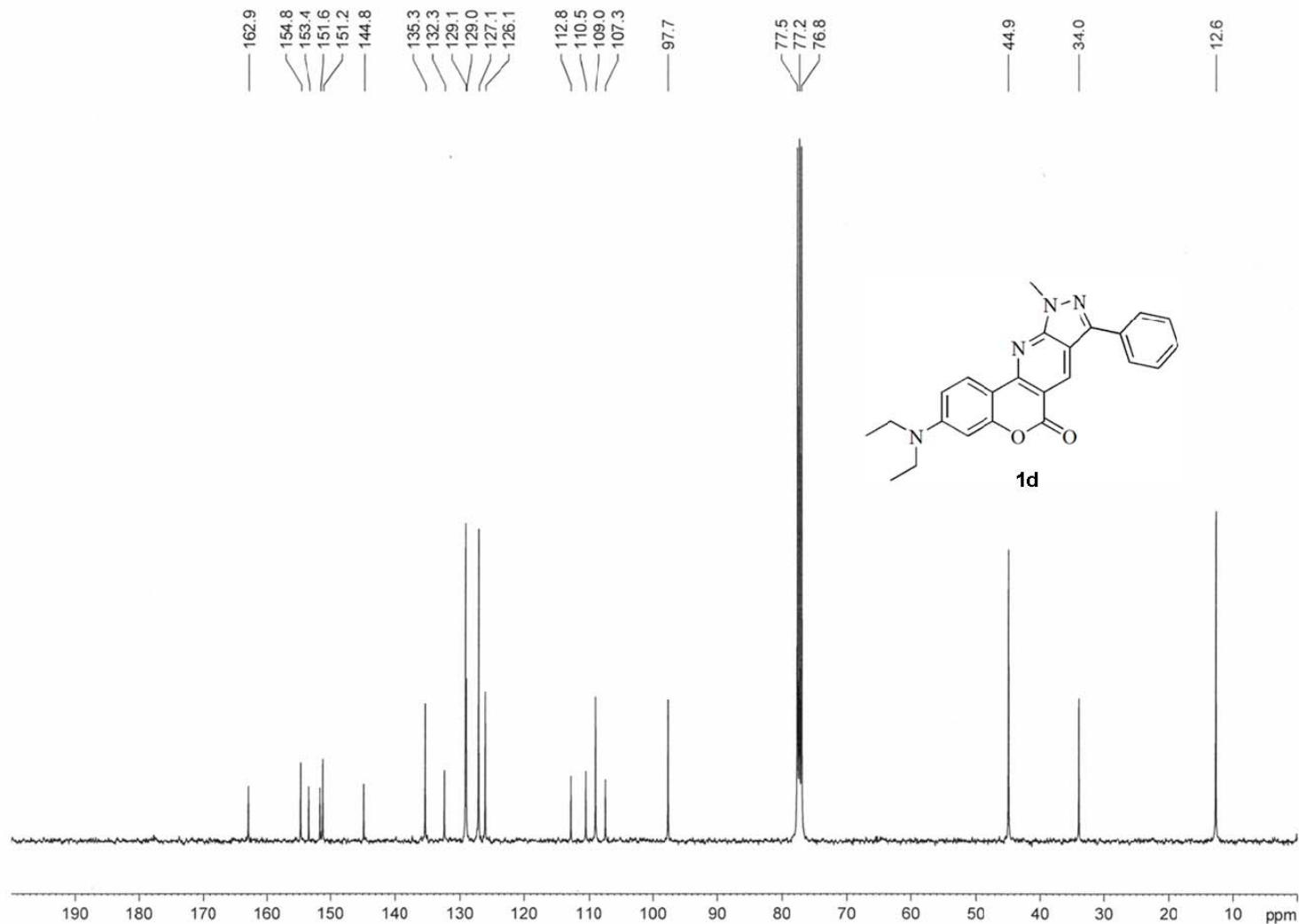
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FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 406
DW 19.800 usec
DE 6.00 usec
TE 295.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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PL1 -1.00 dB
SFO1 100.6228303 MHz

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PL13 14.50 dB
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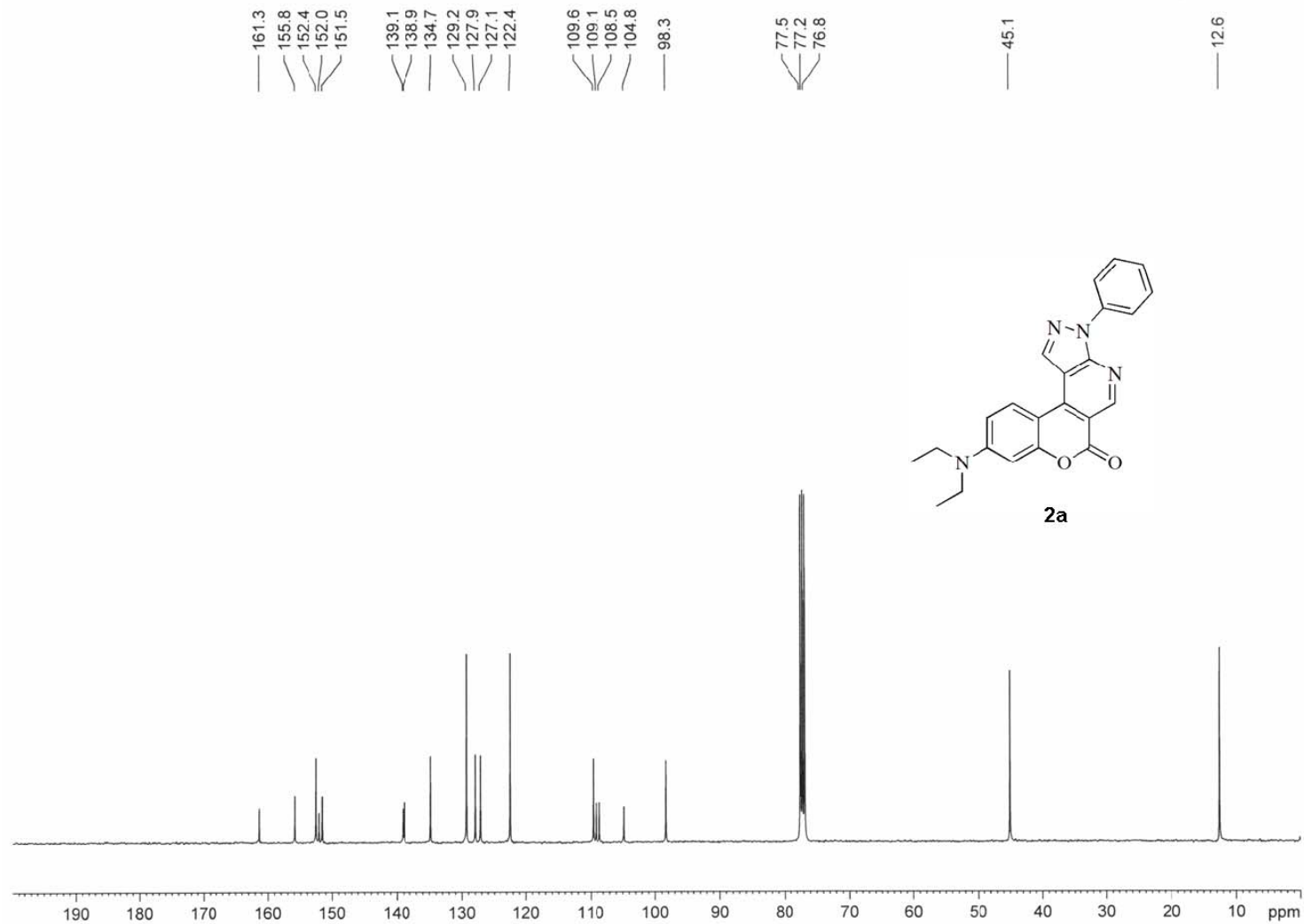
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 FIDRES 0.385323 Hz
 AQ 1.2976629 sec
 RG 128
 DW 19.800 usec
 DE 6.00 usec
 TE 297.4 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
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 PL1 -1.00 dB
 SFO1 100.6228303 MHz

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 PL12 14.50 dB
 PL13 14.50 dB
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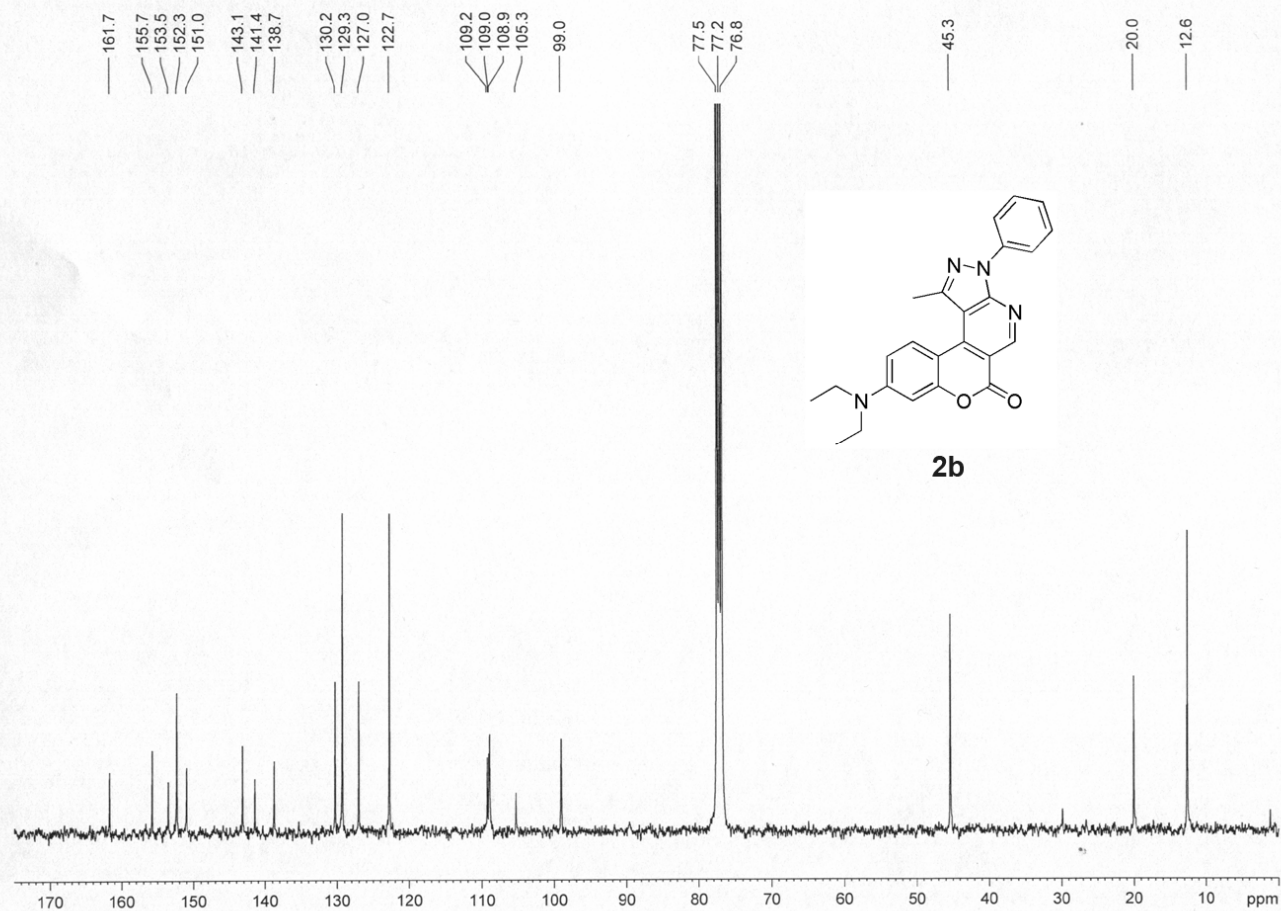
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 NS 2696
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 FIDRES 0.385323 Hz
 AQ 1.2976629 sec
 RG 114
 DW 19.800 usec
 DE 6.00 usec
 TE 297.1 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

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 P1 9.40 usec
 PL1 -1.00 dB
 SFO1 100.6228303 MHz

===== CHANNEL f2 =====
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 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 14.50 dB
 PL13 14.50 dB
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 SF 100.6127586 MHz
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 LB 5.00 Hz
 GB 0
 PC 1.40



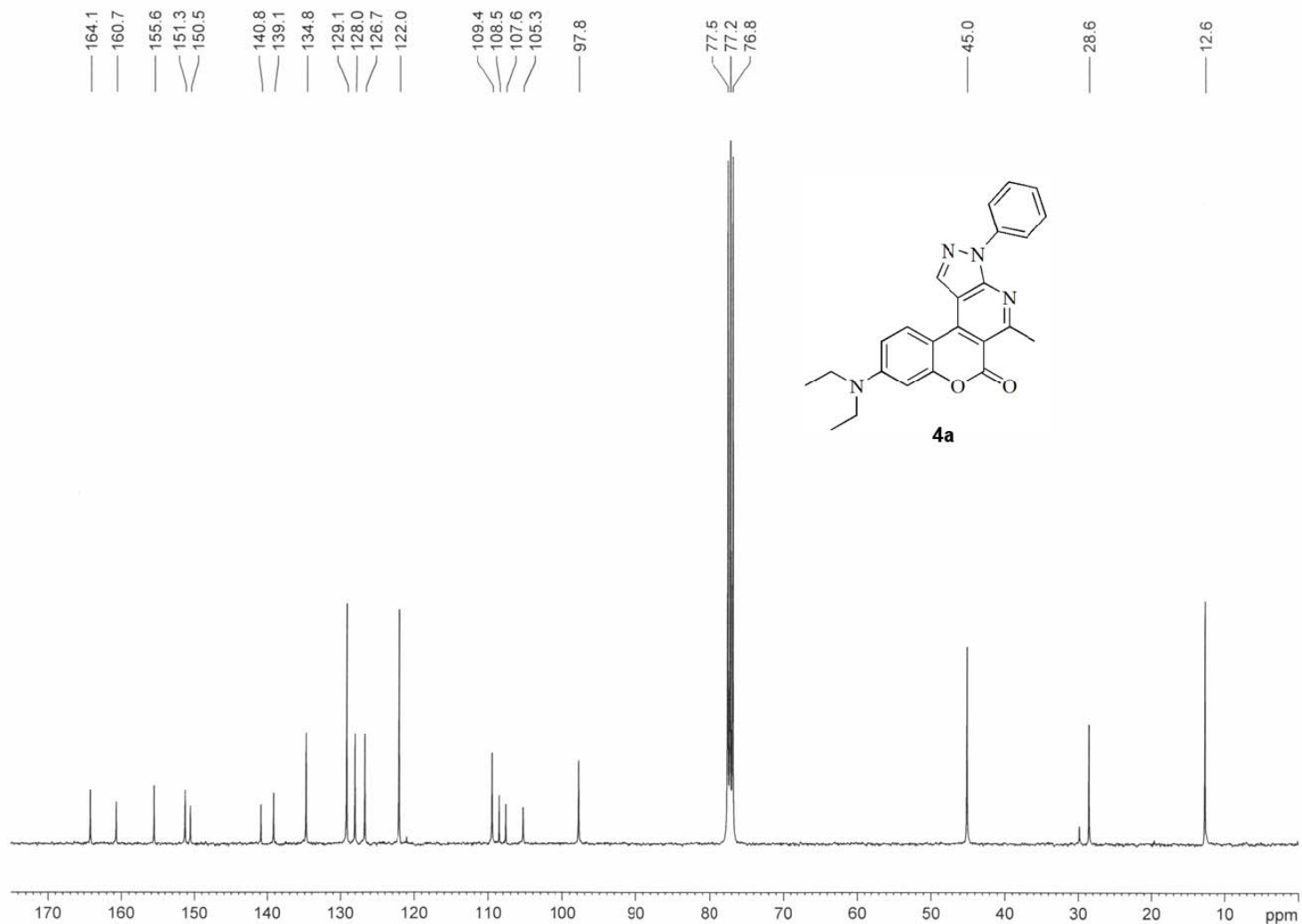
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SOLVENT CDCl3
NS 3064
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SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 322
DW 19.800 usec
DE 6.00 usec
TE 298.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.40 usec
PL1 -1.00 dB
SFO1 100.6228303 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 14.50 dB
PL13 14.50 dB
SFO2 400.1324710 MHz

F2 - Processing parameters
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SSB 0
LB 5.00 Hz
GB 0
PC 1.40



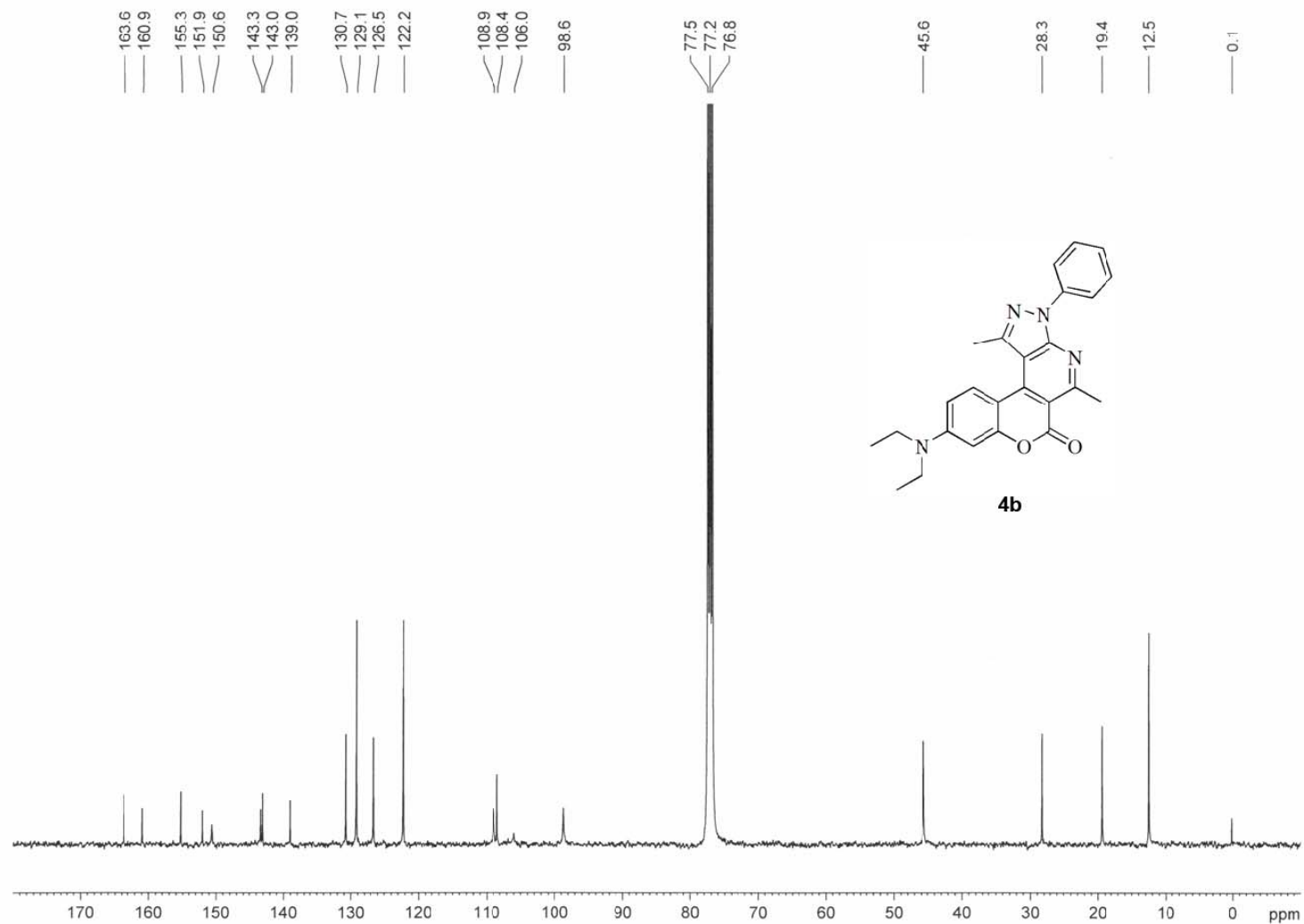
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PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3408
DS 2
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 362
DW 19.800 usec
DE 6.00 usec
TE 296.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.40 usec
PL1 -1.00 dB
SFO1 100.6228303 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 14.50 dB
PL13 14.50 dB
SFO2 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 100.6127571 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40



```

Current Data Parameters
NAME          13c
EXPNO         797
PROCNO        1

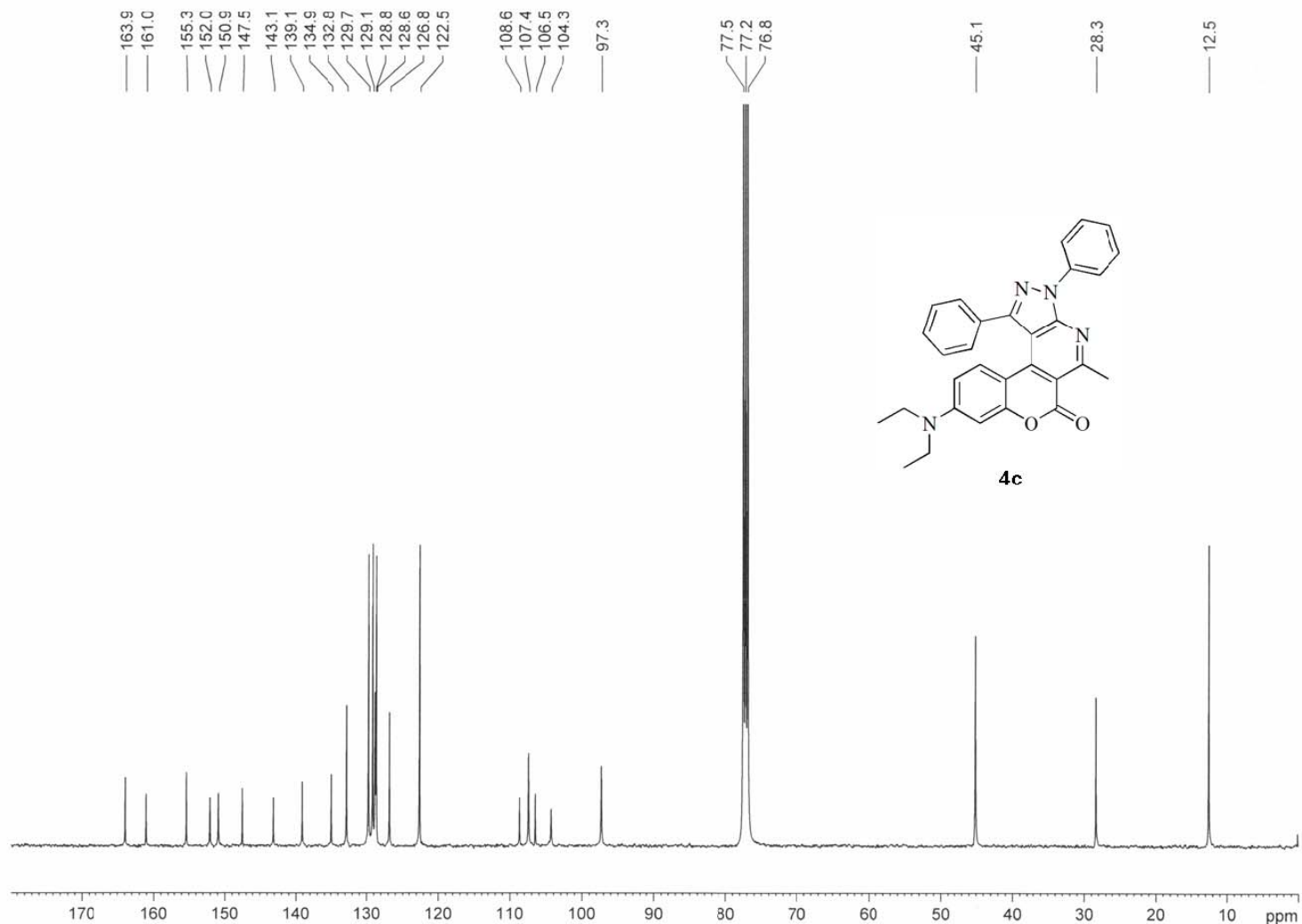
F2 - Acquisition Parameters
Date_         20101018
Time          15.56
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDC13
NS            17856
DS            2
SWH           25252.525 Hz
FIDRES        0.385323 Hz
AQ            1.2976629 sec
RG            362
DW            19.800 usec
DE            6.00 usec
TE            296.9 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0           1

===== CHANNEL f1 =====
NUC1          13C
P1            9.40 usec
PL1           -1.00 dB
SFO1          100.6228303 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -1.00 dB
PL12          14.50 dB
PL13          14.50 dB
SFO2          400.1324710 MHz

F2 - Processing parameters
SI            32768
SF            100.6127542 MHz
WDW           EM
SSB           0
LB            5.00 Hz
GB            0
PC            1.40

```



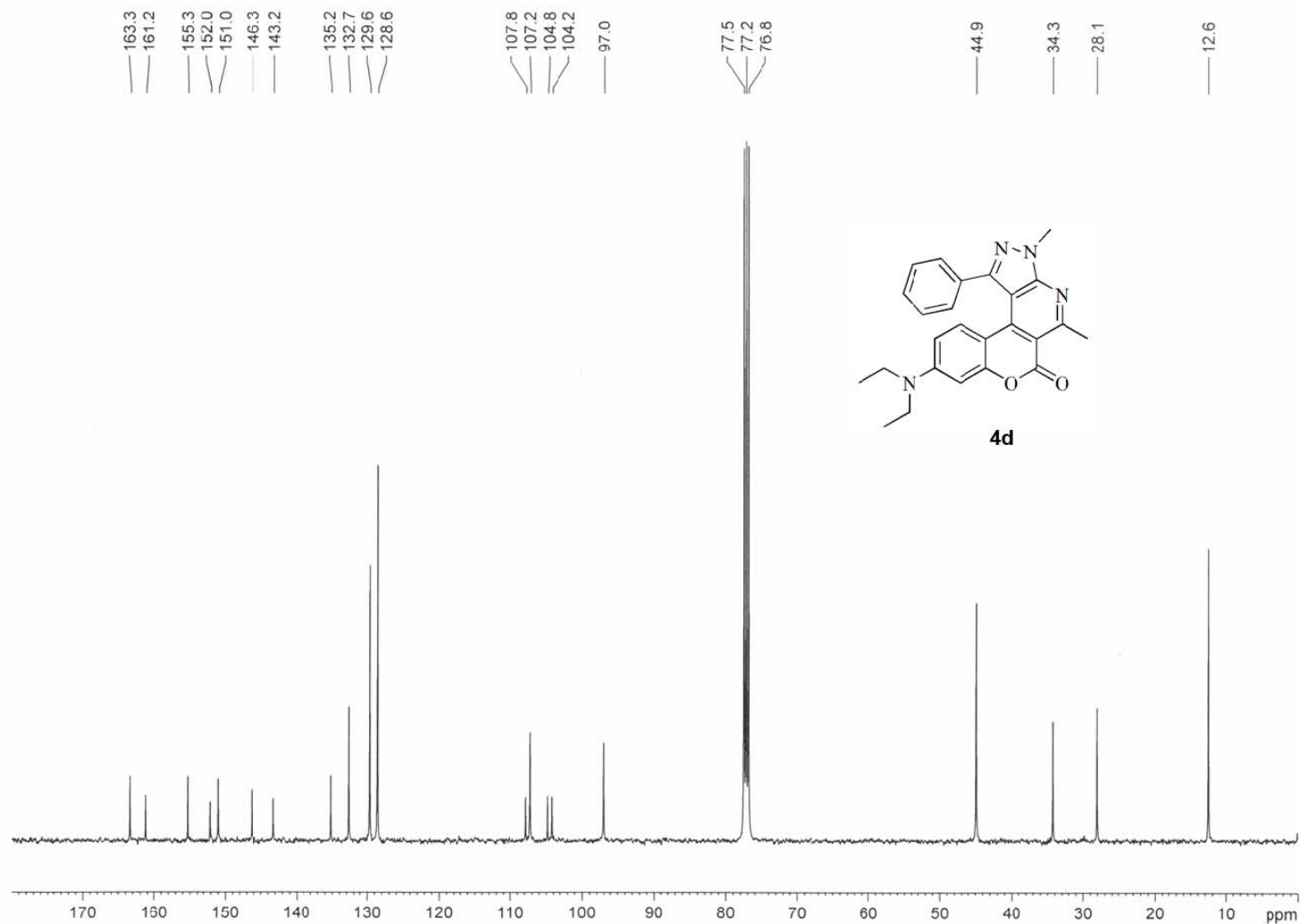
Current Data Parameters
NAME 13c
EXPNO 785
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101011
Time 17.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16576
DS 2
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 362
DW 19.800 usec
DE 6.00 usec
TE 296.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.40 usec
PL1 -1.00 dB
SFO1 100.6220303 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 14.50 dB
PL13 14.50 dB
SFO2 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 100.6127557 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40



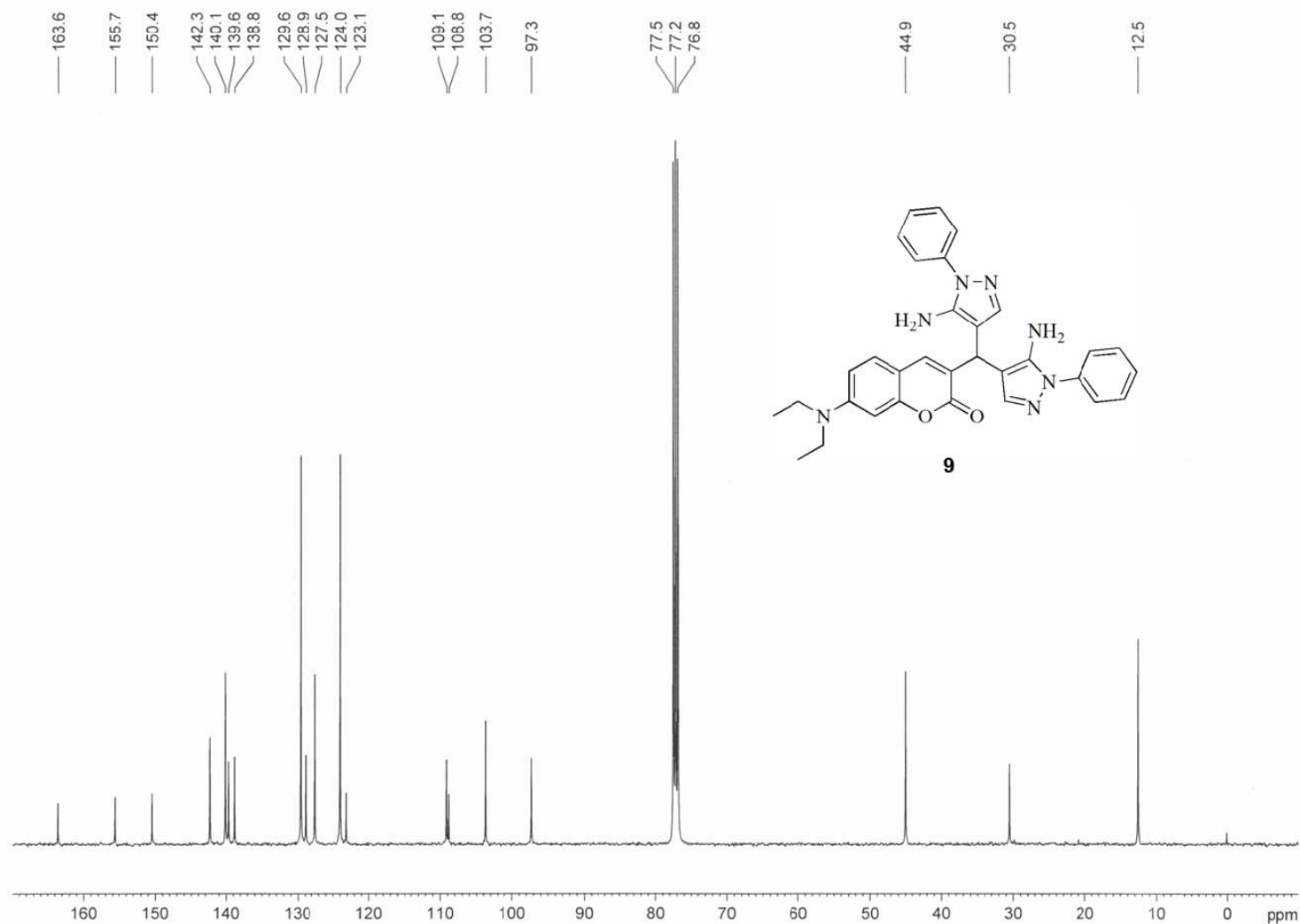
Current Data Parameters
NAME 13c
EXPNO 784
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101011
Time_ 14.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1272
DS 2
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 406
DW 19.800 usec
DE 6.00 usec
TE 297.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.40 usec
PL1 -1.00 dB
SFO1 100.6228303 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 14.50 dB
PL13 14.50 dB
SFO2 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 100.6127574 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40



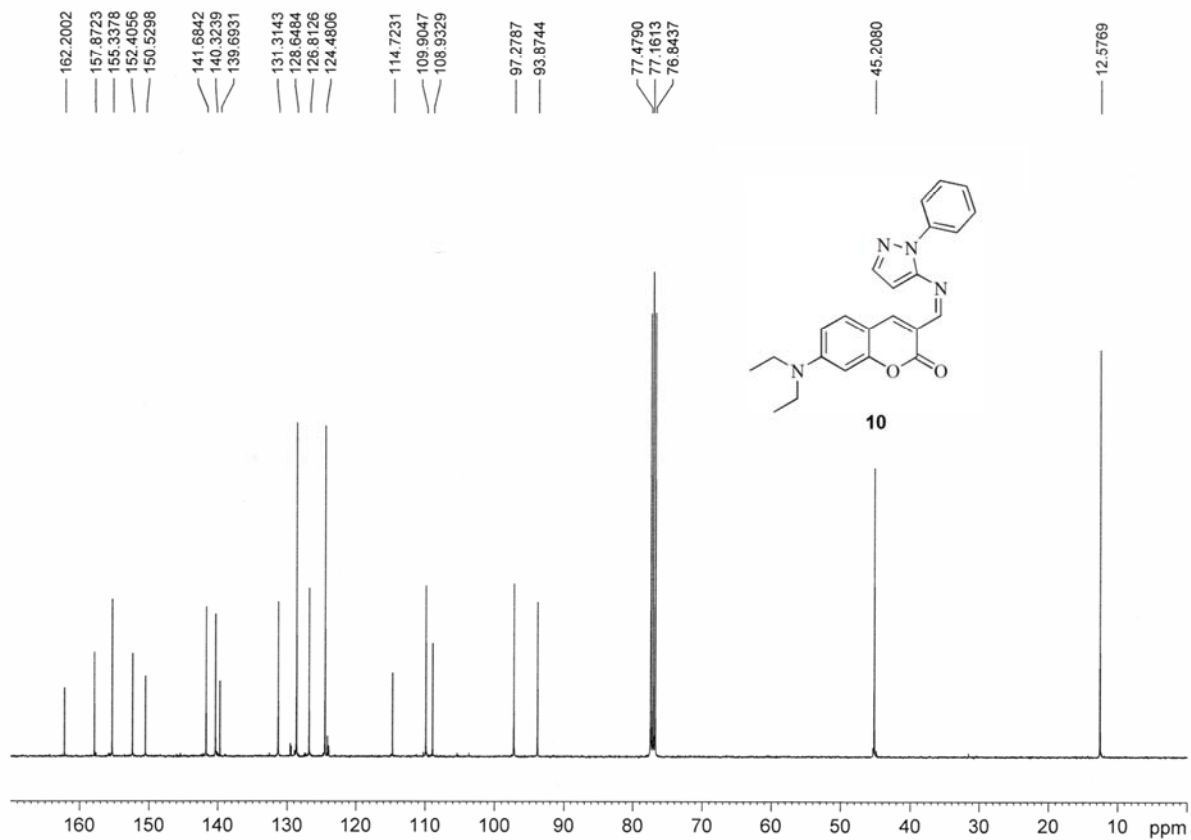
Current Data Parameters
NAME 13c
EXPNO 594
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100325
Time 11.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2472
DS 2
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 203
DW 19.800 usec
DE 6.00 usec
TE 295.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.39999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.40 usec
PL1 -1.00 dB
SFO1 100.6228303 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 14.50 dB
PL13 14.50 dB
SFO2 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 100.6127599 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 13C
EXPNO 11
PROCNO 1

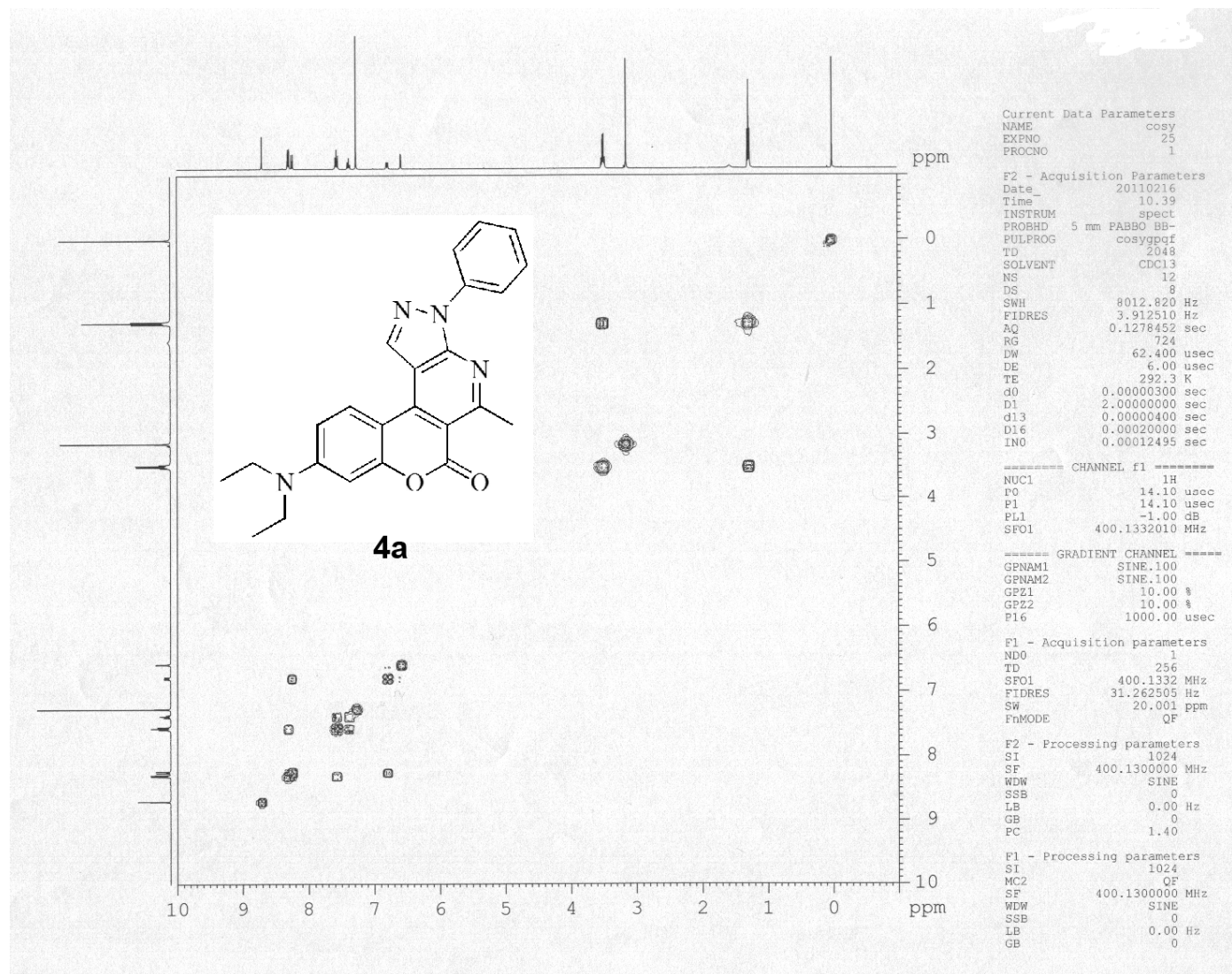
F2 - Acquisition Parameters
Date_ 20120313
Time 11.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3528
DS 4
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 205.5
DW 19.800 usec
DE 6.50 usec
TE 297.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

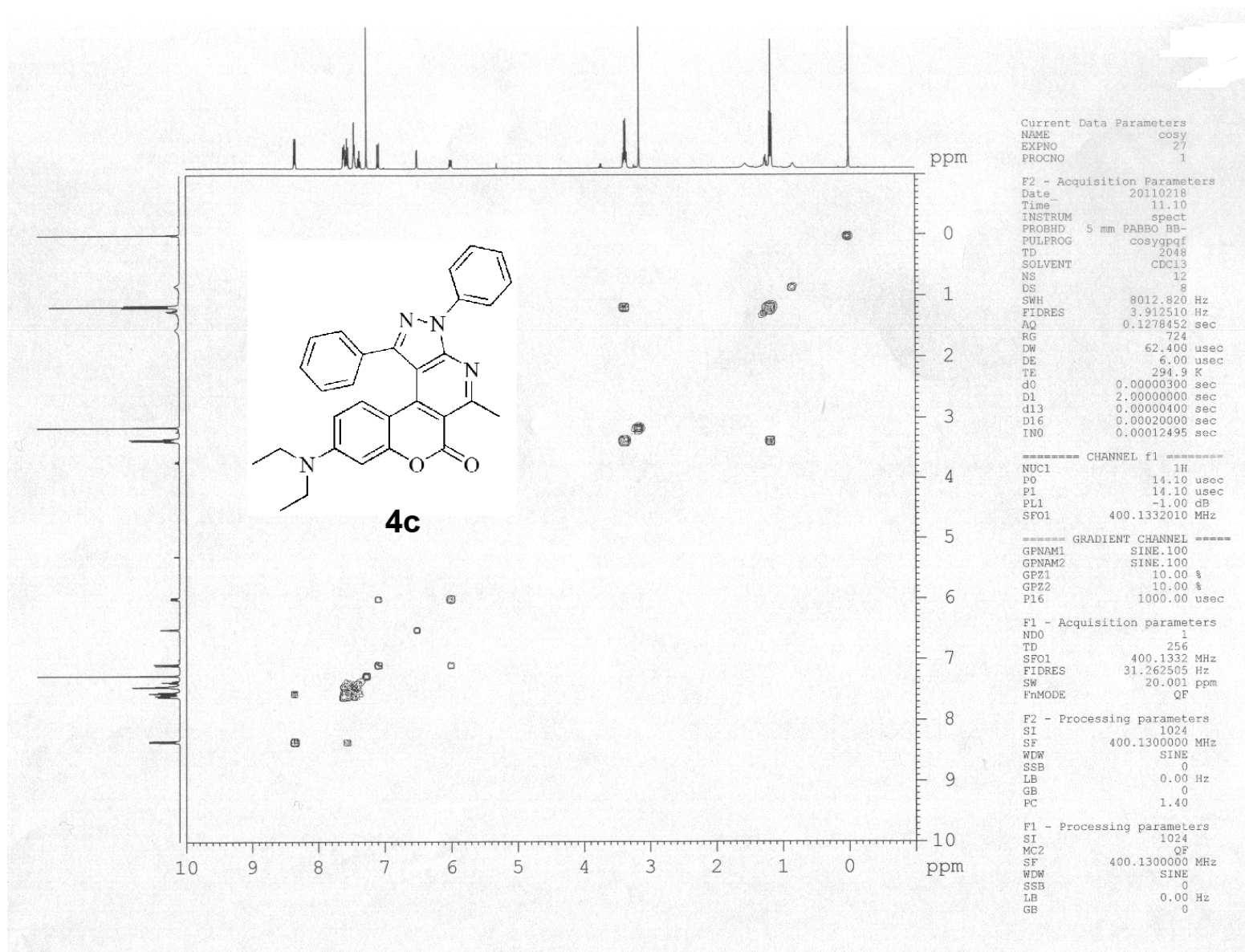
===== CHANNEL f1 =====
NUC1 13C
P1 8.70 usec
PLW1 100.00000000 W
SFO1 100.6479778 MHz

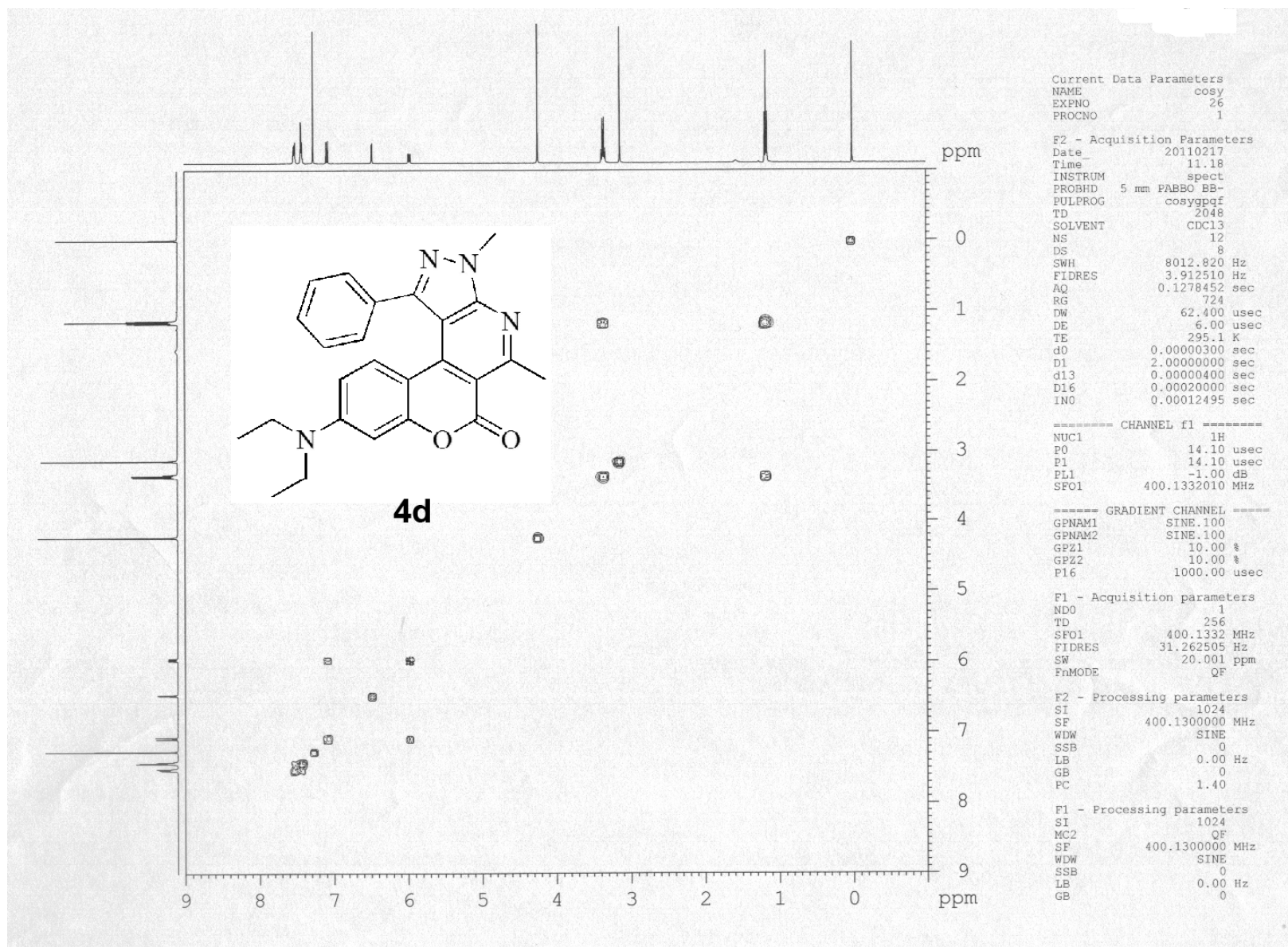
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 9.39999962 W
PLW12 0.24822000 W
PLW13 0.24822000 W
SFO2 400.2316009 MHz

F2 - Processing parameters
SI 32768

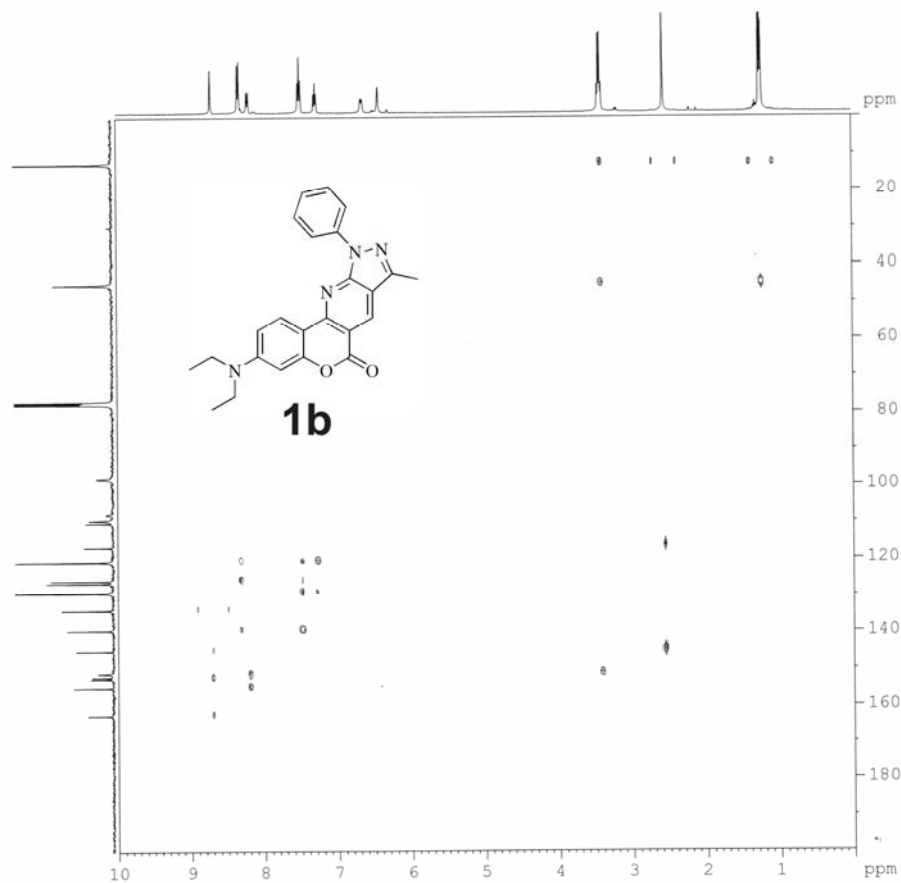
2D H-H COSY of compounds 4a, 4c and 4d







2D C-H COSY of compounds 1b



```

Current Data Parameters
NAME      hmbc
EXPNO     8
PROCNO    1

F2 - Acquisition Parameters
Date_     20111130
Time      11.43
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   hmbcgp1pdqf
TD        4096
SOLVENT   CDCl3
NS        16
DS        16
SWH       4854.369 Hz
FIDRES    1.185149 Hz
AQ        0.4219380 sec
RG        2050
DW        103.000 usec
DE        8.00 usec
TE        296.8 K
CNST2     145.0000000
CNST13    10.0000000
d0         0.00000300 sec
d1         1.47132802 sec
d2         0.00344828 sec
d6         0.05000000 sec
d16        0.00020000 sec
IN0        0.00002240 sec

===== CHANNEL f1 =====
NUC1       1H
P1         13.50 usec
p2         27.00 usec
PL1        0.00 dB
SFO1       400.1319247 MHz

===== CHANNEL f2 =====
NUC2       13C
P3         10.00 usec
PL2        -3.00 dB
SFO2       100.6228138 MHz

===== GRADIENT CHANNEL =====
GPNAM1     SINE.100
GPNAM2     SINE.100
GPNAM3     SINE.100
GPZ1       50.00 %
GPZ2       30.00 %
GPZ3       40.10 %
P16        1000.00 usec

F1 - Acquisition parameters
ND0        2
TD         128
SFO1       100.6228 MHz
FIDRES     174.386154 Hz
SW         221.833 ppm
FnMODE     QF

F2 - Processing parameters
SI         2048
SF         400.1300074 MHz
WDW        SINE
  
```