Electronic Supplementary Material (ESI) for RSC Advances.

Bifurcated hydrogen bonding mediated planar 9,10-anthraquinone dyes: synthesis, structure and property

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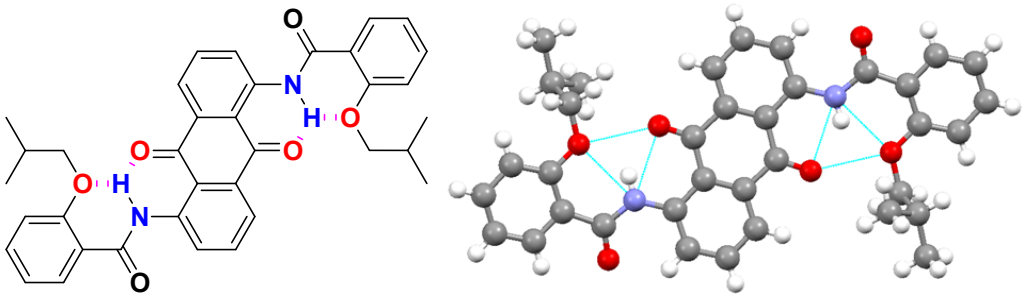
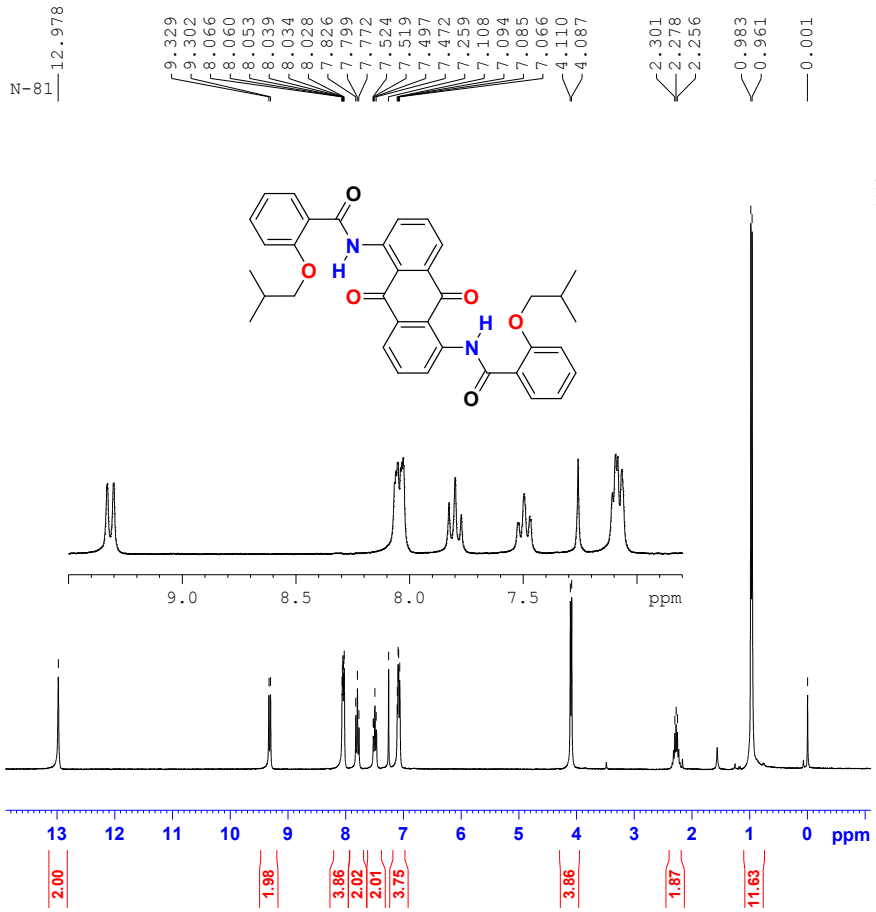
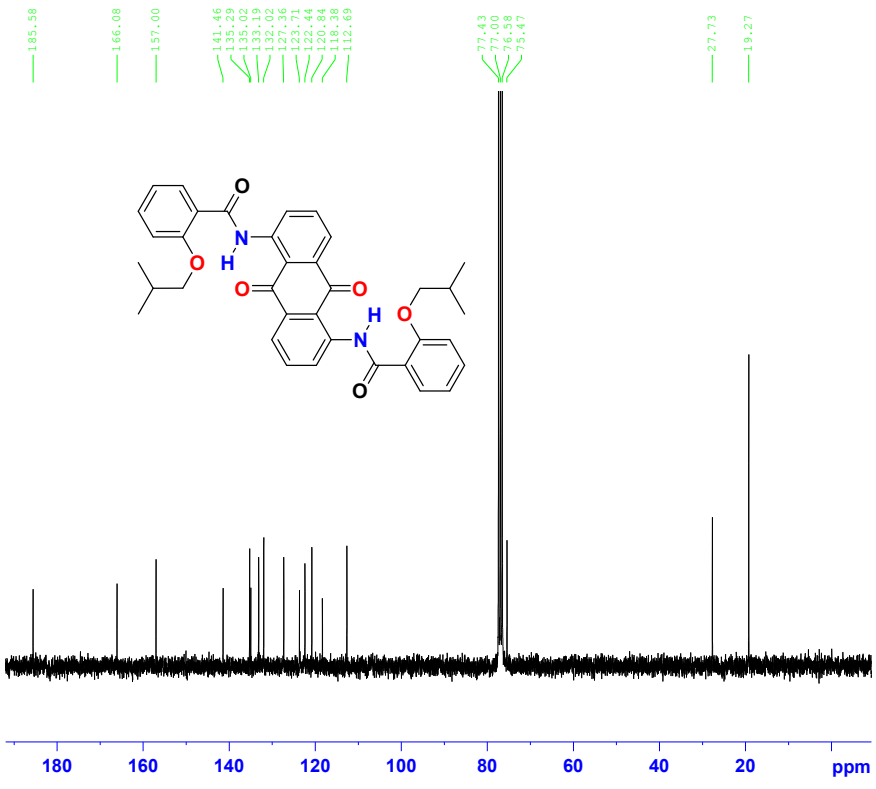
Graphic Abstract:





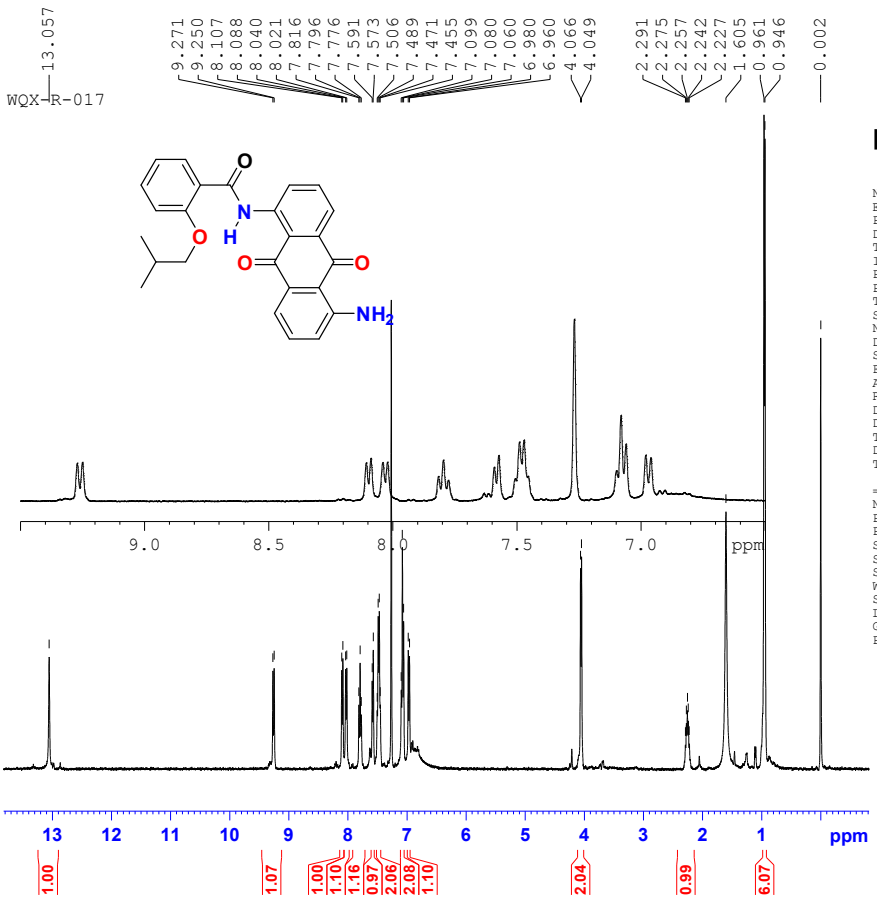
BRUKER

NAME yangyong-N-81
EXPNO 40
PROCNO 1



BRUKER

NAME yangyong-N-81
EXPNO 30
PROCNO 1



BRUKER

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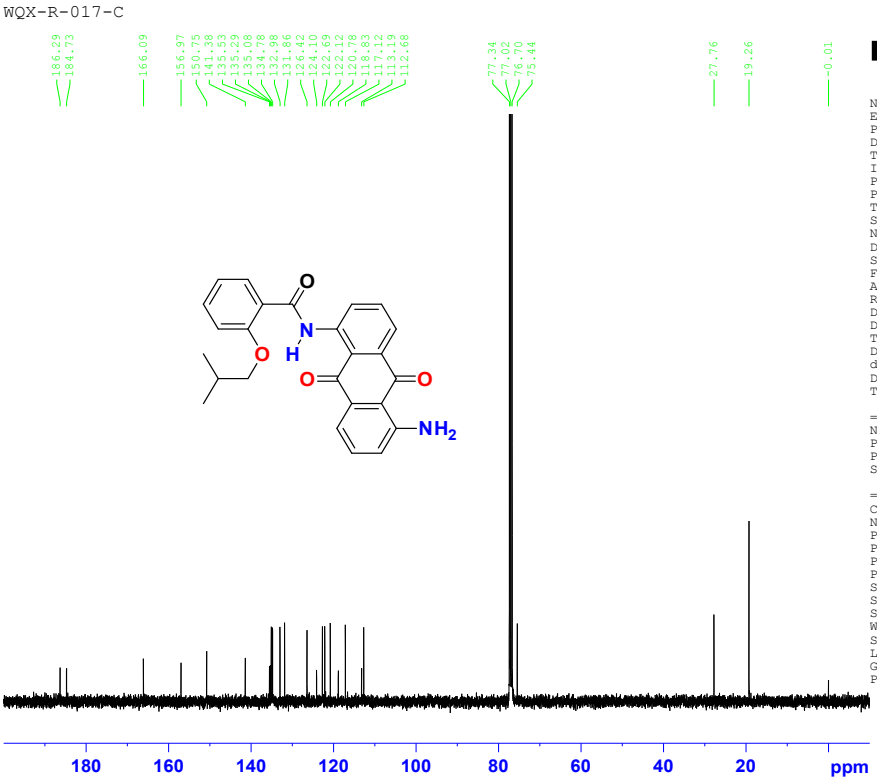
NAME                WQX-R-017
EXPNO                       1
PROCNO                      1
Date_                20140111
Time                    10.38
INSTRUM                 spect
PROBHD    5 mm PAQNP Swi
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                3.9846387 sec
RG                       287
DW                    60.800 usec
DE                     6.00 usec
TE                    287.5 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      10.90 usec
PL1                     -3.00 dB
SFO1             400.1324710 MHz
SI                       32768
SF               400.1300090 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```

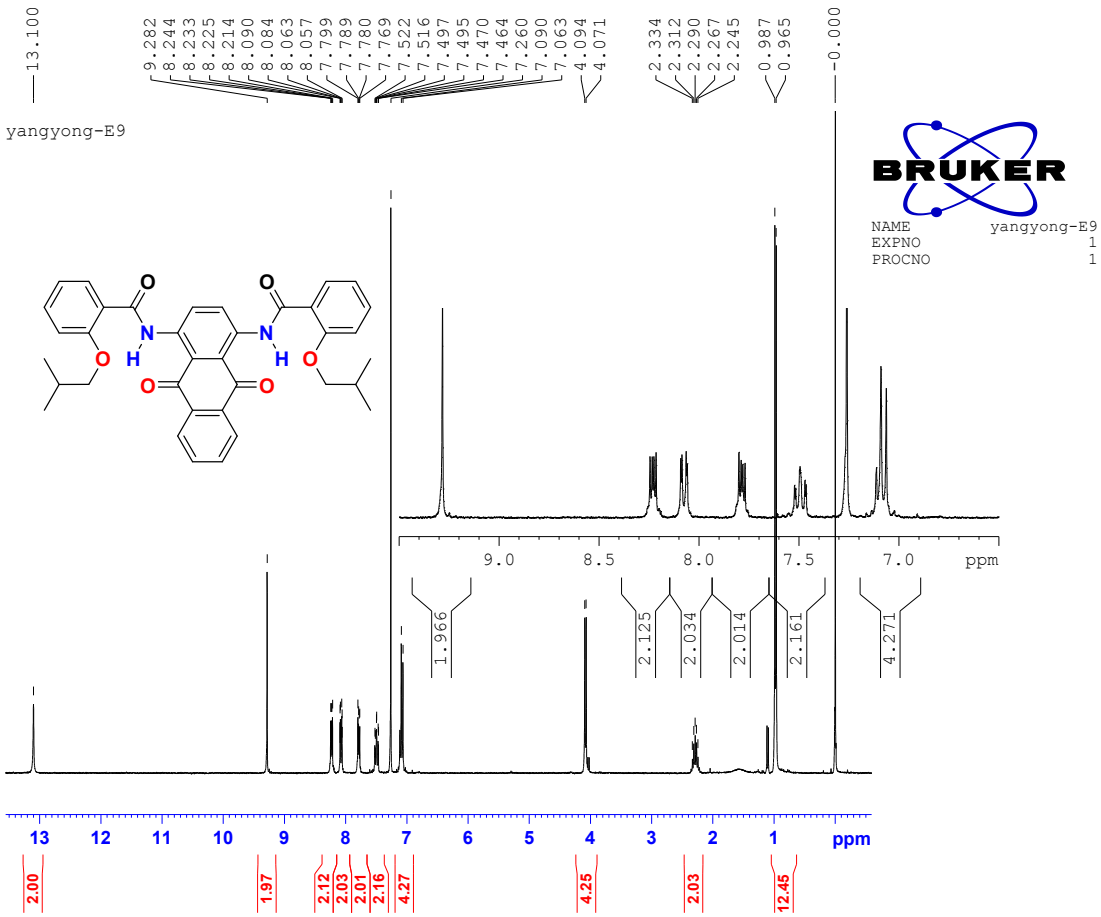


BRUKER

```
NAME              WQX-R-017-C
EXPNO                       1
PROCNO                      1
Date_                20140114
Time                    11.27
INSTRUM                 spect
PROBHD    5 mm PAQNP Swi
PULPROG              zgpg30
TD                     65536
SOLVENT                CDCl3
NS                        1005
DS                           4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                1.3631988 sec
RG                        2050
DW                    20.800 usec
DE                     6.00 usec
TE                    298.1 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                       9.56 usec
PL1                     -1.00 dB
SFO1             100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   80.00 usec
PL2                     -3.00 dB
PL12                    13.48 dB
PL13                    14.00 dB
SFO2             400.1316005 MHz
SI                       32768
SF               100.6127690 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```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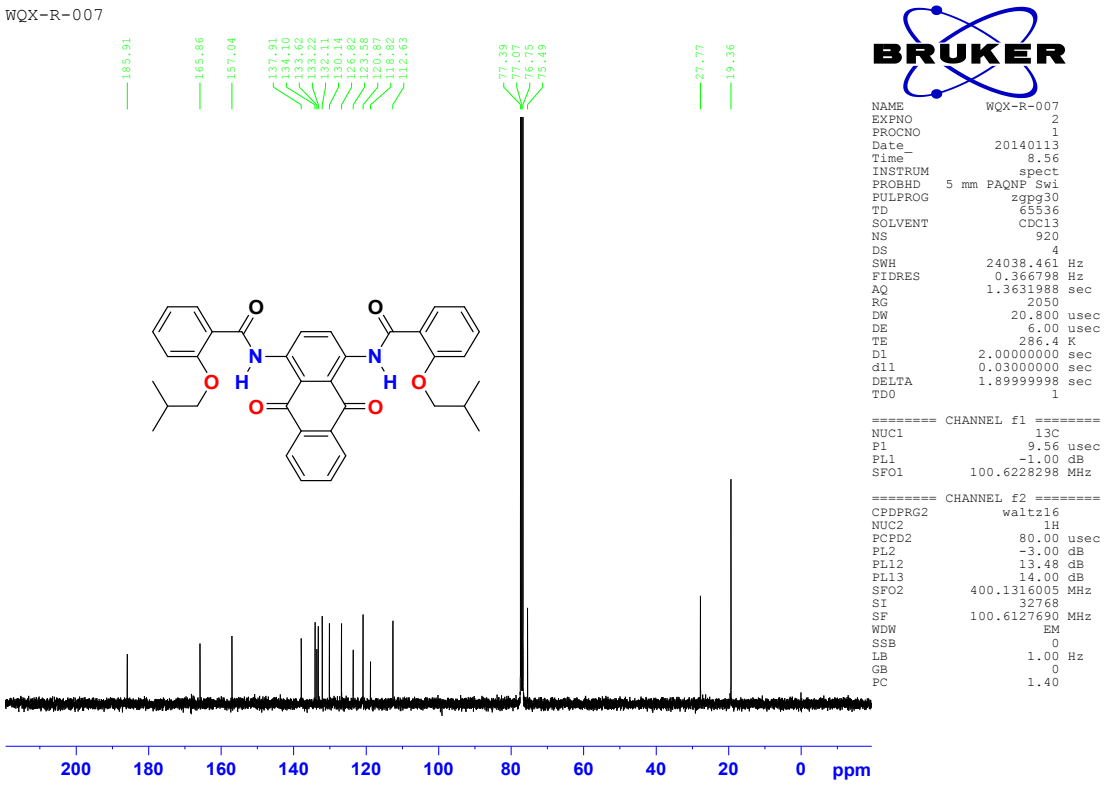
8.244
8.233
8.225
8.214
8.090
8.084
8.063
8.057
7.799
7.789
7.780
7.769
7.522
7.516
7.497
7.495
7.470
7.464
7.260
7.090
7.063
4.094
4.071
2.334
2.312
2.290
2.267
2.245
0.987
0.965
0.000
yangyong-E9
BRUKER
NAME yangyong-E9
EXPNO 1
PROCNO 1
9.0
8.5
8.0
7.5
7.0
ppm
1.966
2.125
2.034
2.014
2.161
4.271
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
2.00
1.97
2.12
2.03
2.01
2.16
4.27
4.25
2.03
12.45


WQX-R-007
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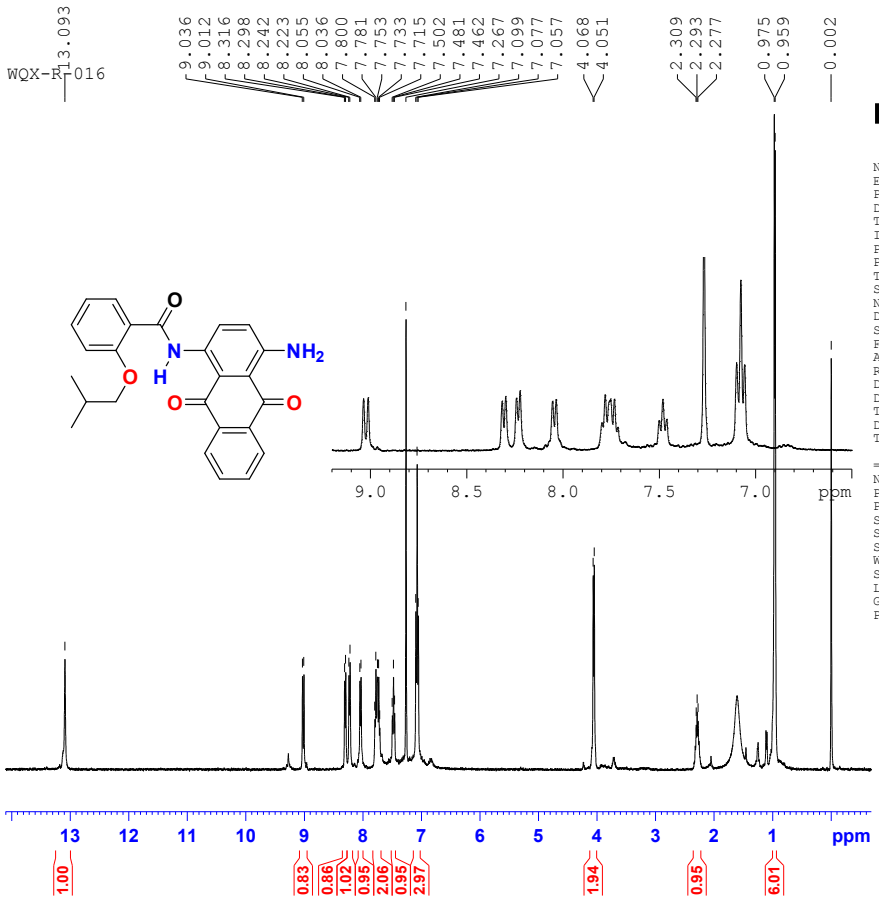
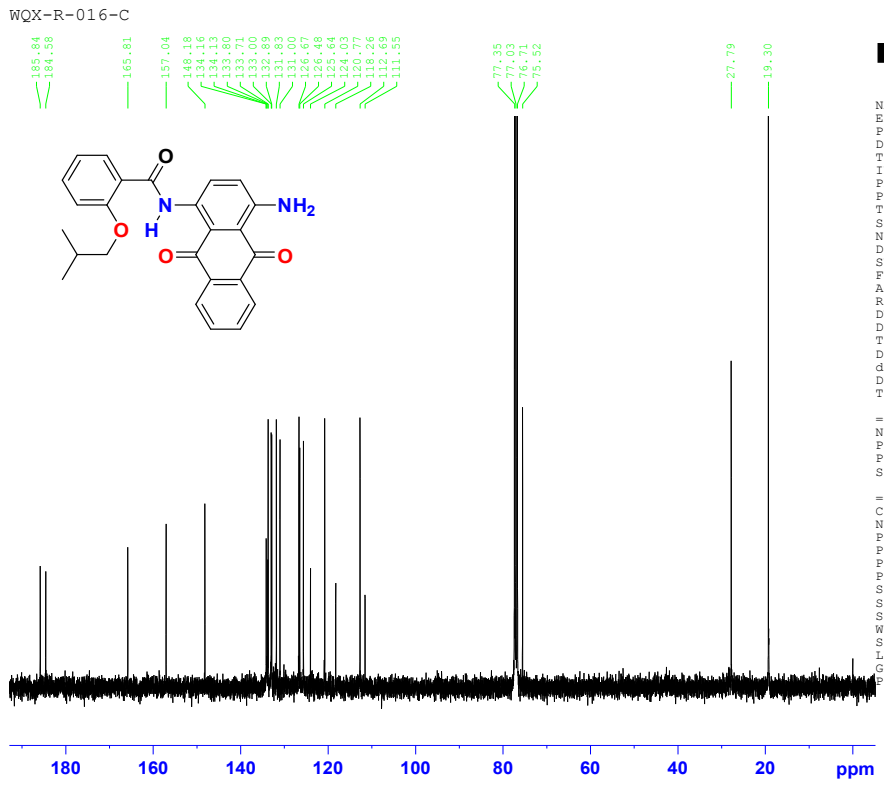
165.86
157.04
137.91
134.10
133.62
133.22
132.11
130.14
126.82
123.58
120.87
118.83
112.63
77.39
77.07
76.75
75.49
27.77
19.36
BRUKER
NAME WQX-R-007
EXPNO 2
PROCNO 1
Date_ 20140113
Time 8.56
INSTRUM spect
PROBHD 5 mm PAQNP Swi
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 920
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 286.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.56 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 13.48 dB
PL13 14.00 dB
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm



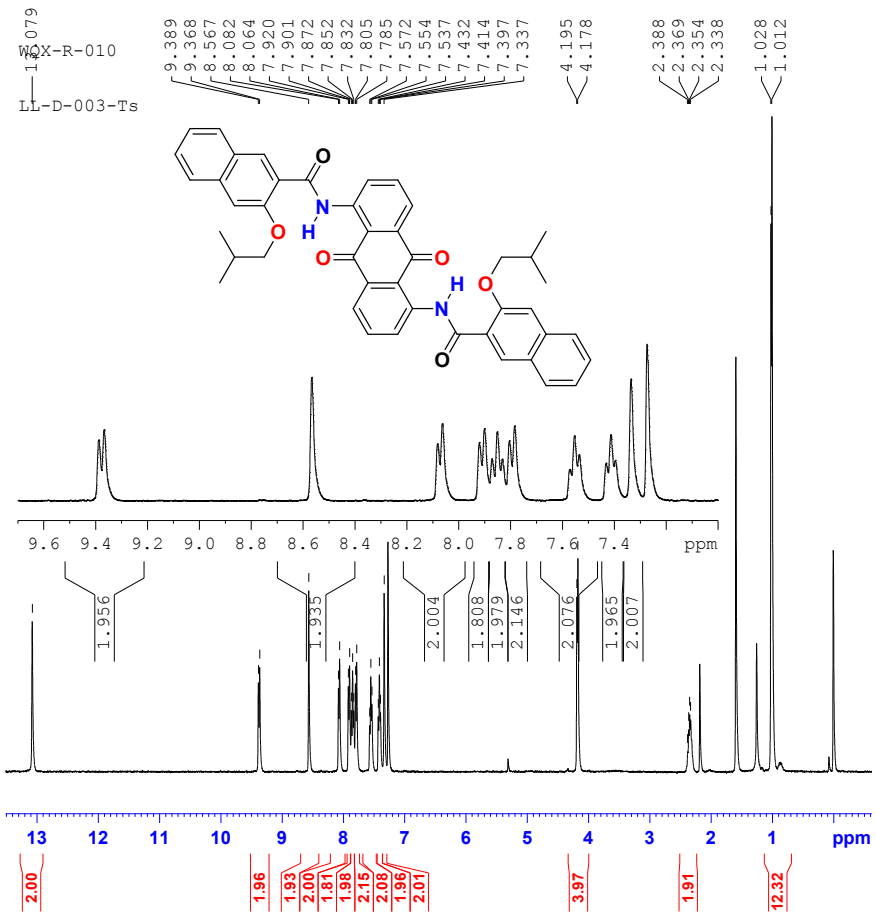
BRUKER

NAME	WQX-R-016
EXPNO	1
PROCNO	1
Date_	20140111
Time	10.33
INSTRUM	spect
PROBHD	5 mm PAQNP Swi
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	287
DW	60.800 usec
DE	6.00 usec
TE	287.7 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.90 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz
SI	32768
SF	400.1300090 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



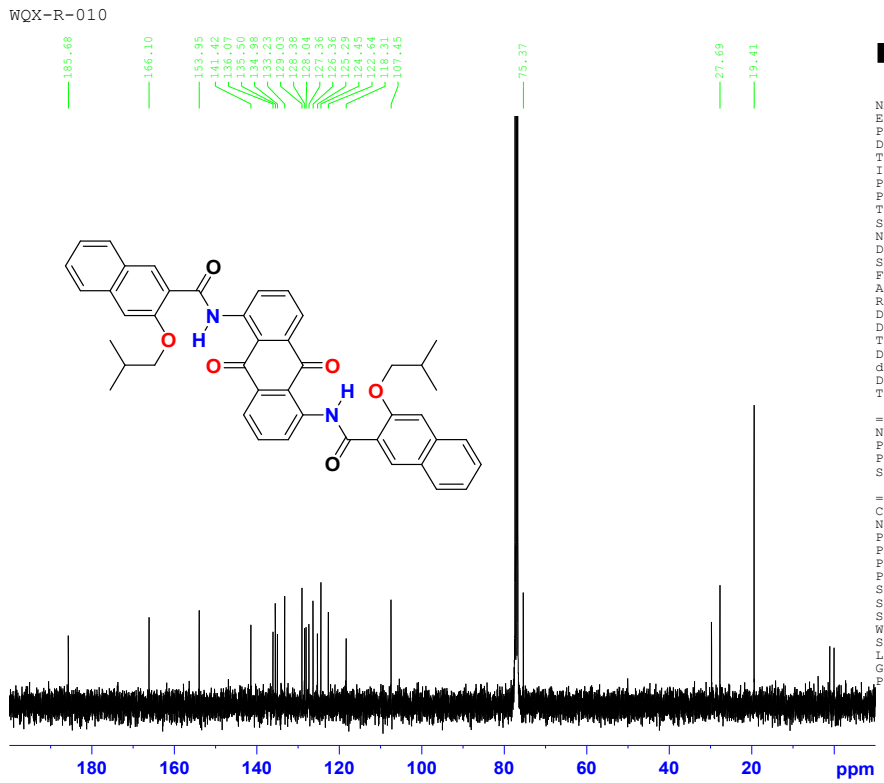
BRUKER

NAME	WQX-R-016-C
EXPNO	1
PROCNO	1
Date_	20140114
Time	10.26
INSTRUM	spect
PROBHD	5 mm PAQNP Swi
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1168
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.00 usec
TE	298.1 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.56 usec
PL1	-1.00 dB
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	13.48 dB
PL13	14.00 dB
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



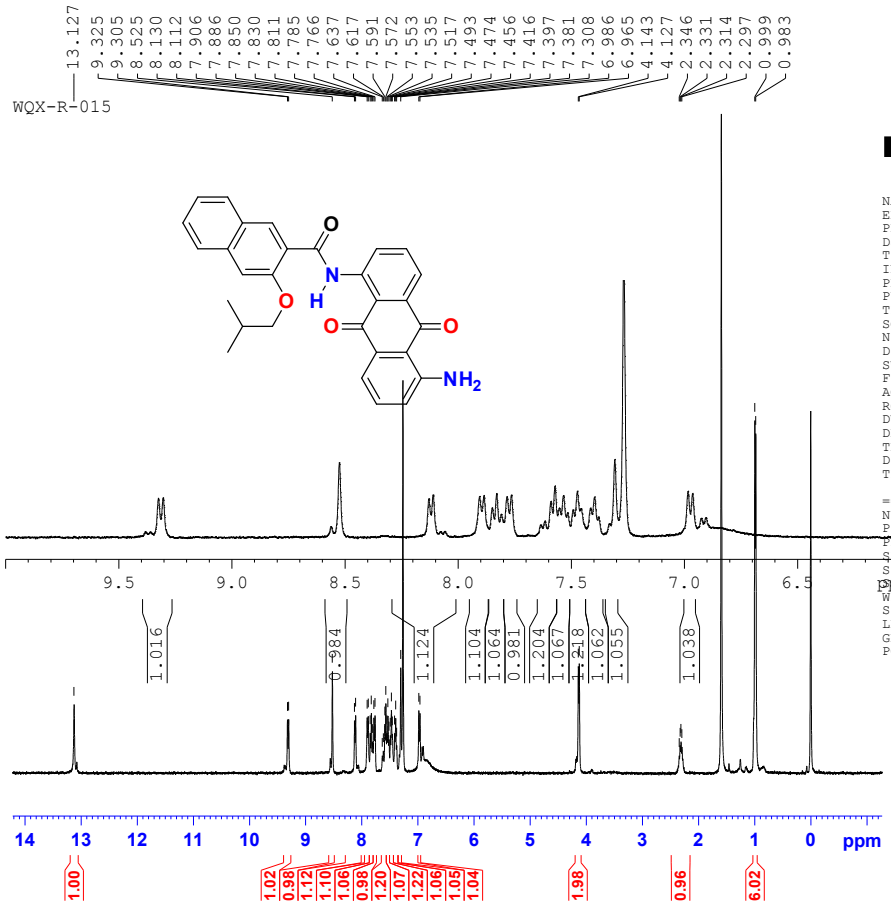
BRUKER

NAME	WQX-R-010
EXPNO	1
PROCNO	1
Date_	20131201
Time	16.48
INSTRUM	spect
PROBHD	5 mm PAQNP Swi
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	20
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	512
DW	60.800 usec
DE	6.00 usec
TE	289.5 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.90 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz
SI	32768
SF	400.1300090 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

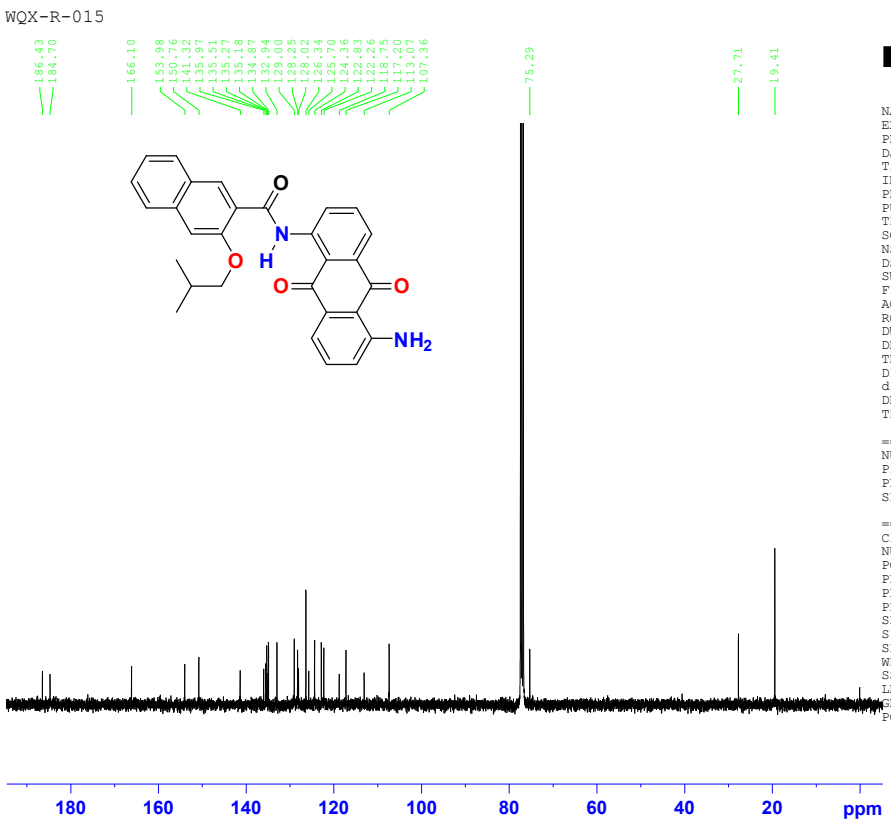
NAME	WQX-R-010
EXPNO	2
PROCNO	1
Date_	20140115
Time	10.02
INSTRUM	spect
PROBHD	5 mm PAQNP Swi
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1300
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.00 usec
TE	290.7 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.56 usec
PL1	-1.00 dB
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	13.48 dB
PL13	14.00 dB
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



BRUKER

```
NAME                WQX-R-015
EXPNO                       1
PROCNO                      1
Date_                20140111
Time                    10.27
INSTRUM                 spect
PROBHD   5 mm PAQNP Swi
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                3.9846387 sec
RG                        287
DW                   60.800 usec
DE                    6.00 usec
TE                    287.9 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                    10.90 usec
PL1                   -3.00 dB
SFO1           400.1324710 MHz
SI                      32768
SF             400.1300090 MHz
WDW                        EM
SSB                         0
LB                     0.30 Hz
GB                          0
PC                       1.00
```

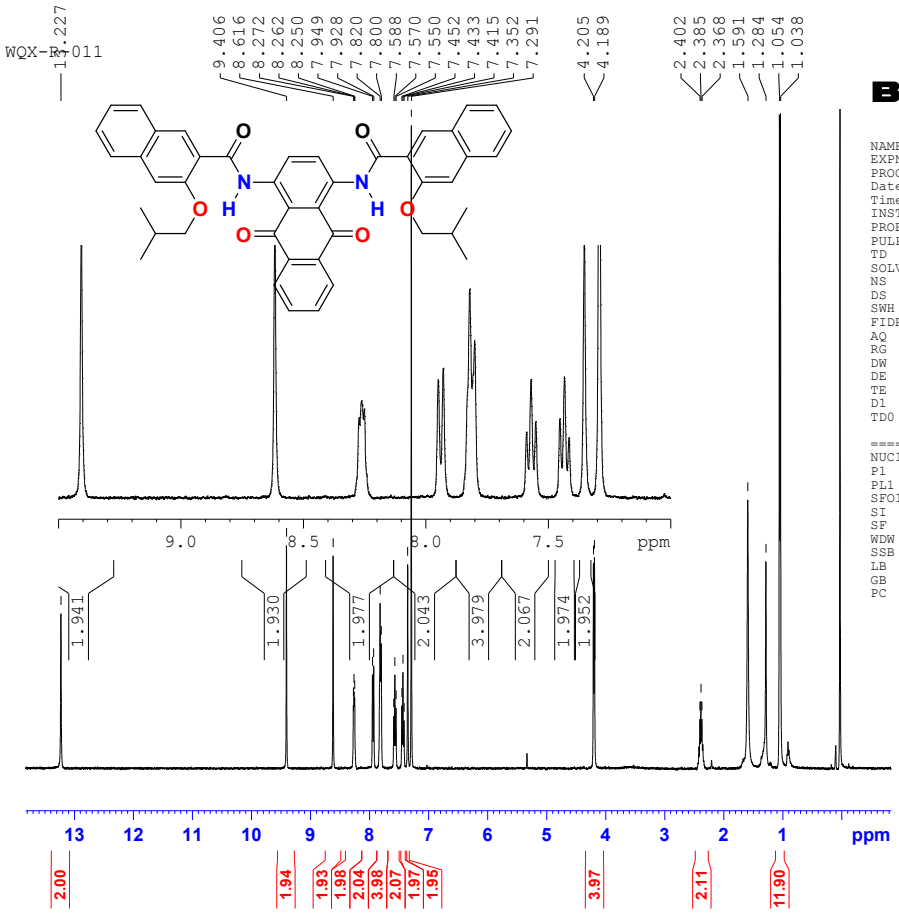


BRUKER

```
NAME                WQX-R-015
EXPNO                       2
PROCNO                      1
Date_                20140113
Time                    10.35
INSTRUM                 spect
PROBHD   5 mm PAQNP Swi
PULPROG              zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       1500
DS                          4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                1.3631988 sec
RG                       2050
DW                   20.800 usec
DE                    6.00 usec
TE                    286.7 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                    9.56 usec
PL1                  -1.00 dB
SFO1           100.6228298 MHz

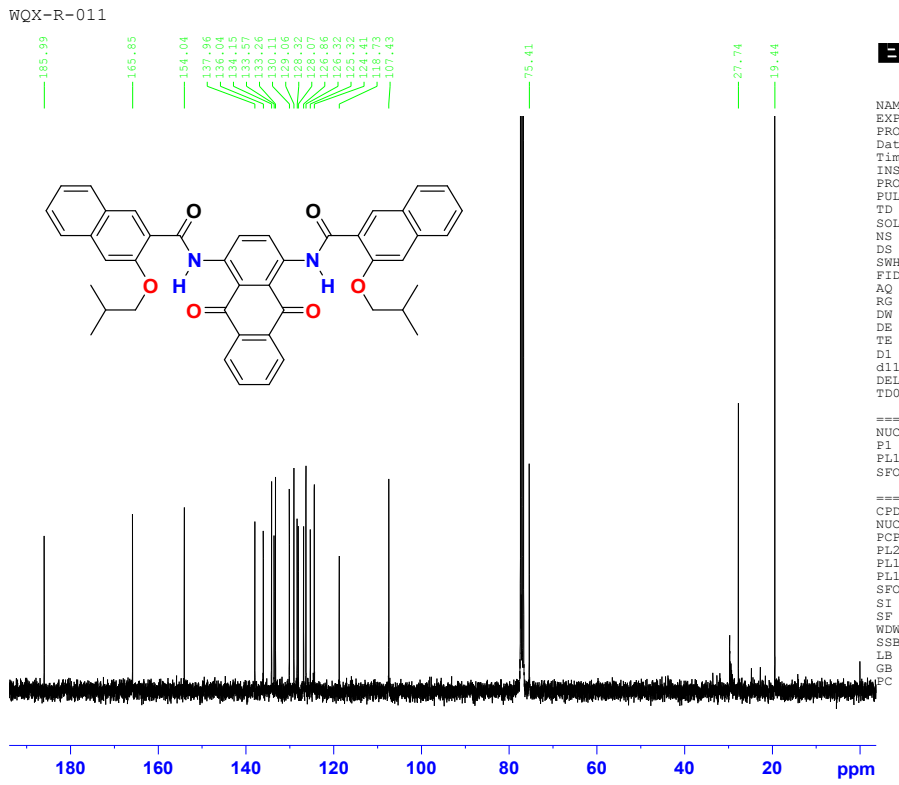
======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                       1H
PCPD2                80.00 usec
PL2                   -3.00 dB
PL12                  13.48 dB
PL13                  14.00 dB
SFO2           400.1316005 MHz
SI                      32768
SF             100.6127690 MHz
WDW                        EM
SSB                         0
LB                     1.00 Hz
GB                          0
PC                       1.40
```



BRUKER

```
NAME                WQX-R-011
EXPNO                       1
PROCNO                      1
Date_                20131113
Time                    19.29
INSTRUM                 spect
PROBHD   5 mm PAQNP Swi
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        23
DS                         2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                3.9846387 sec
RG                       575
DW                    60.800 usec
DE                     6.00 usec
TE                    293.9 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      10.90 usec
PL1                     -3.00 dB
SFO1             400.1324710 MHz
SI                       32768
SF               400.1300000 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```

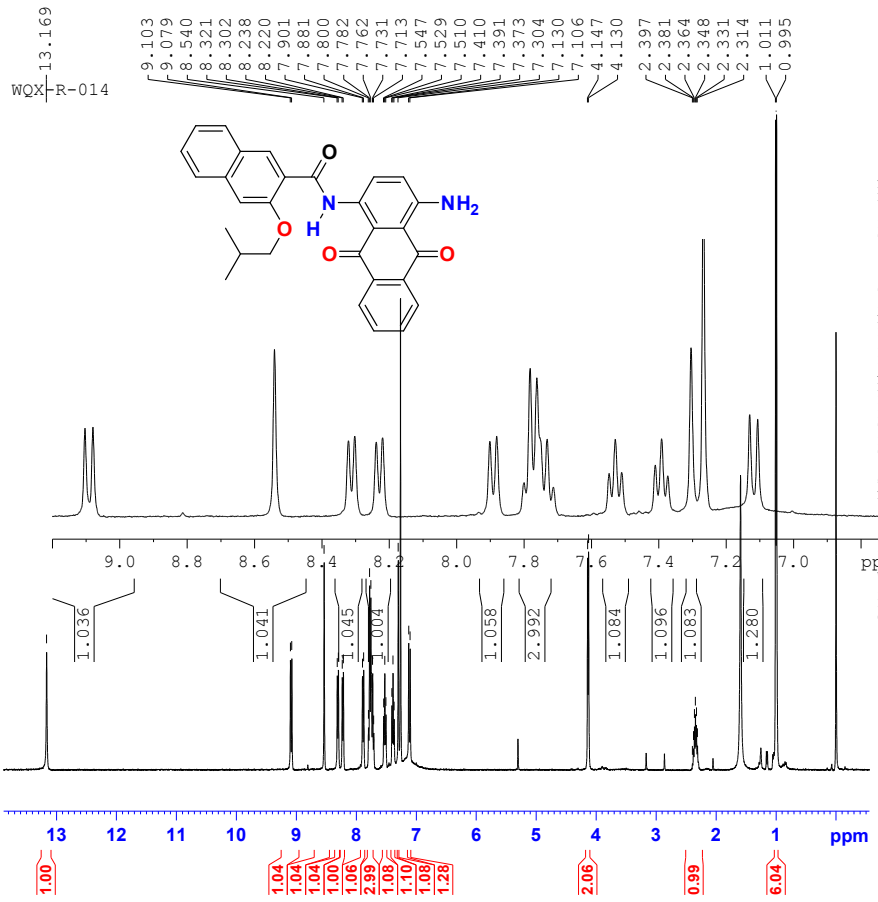


BRUKER

```
NAME                WQX-R-011
EXPNO                       3
PROCNO                      1
Date_                20140115
Time                    11.20
INSTRUM                 spect
PROBHD   5 mm PAQNP Swi
PULPROG                 zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       1283
DS                          4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                1.3631988 sec
RG                       2050
DW                    20.800 usec
DE                     6.00 usec
TE                    290.8 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                      9.56 usec
PL1                    -1.00 dB
SFO1            100.6228298 MHz

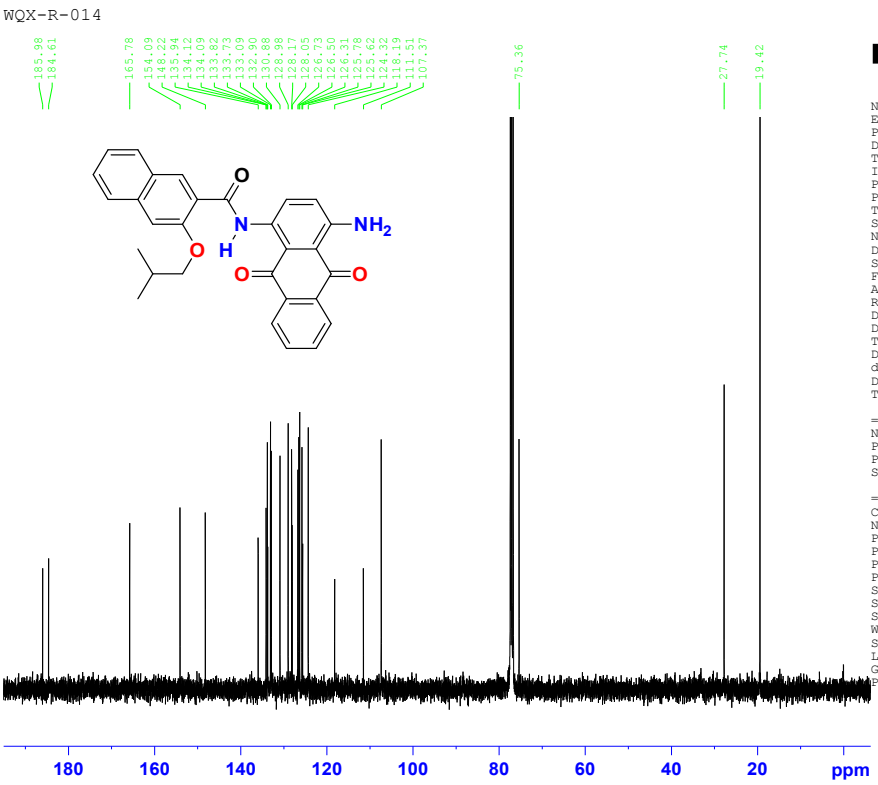
======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   80.00 usec
PL2                     -3.00 dB
PL12                    13.48 dB
PL13                    14.00 dB
SFO2             400.1316005 MHz
SI                       32768
SF               100.6127690 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```



BRUKER

```
NAME                WQX-R-014
EXPNO                       1
PROCNO                      1
Date_                20131219
Time                    18.12
INSTRUM                 spect
PROBHD    5 mm PAQNP Swi
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                         32
DS                          2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9846387 sec
RG                        456
DW                   60.800 usec
DE                    6.00 usec
TE                    289.5 K
D1                 1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                    10.90 usec
PL1                   -3.00 dB
SFO1           400.1324710 MHz
SI                      32768
SF             400.1300090 MHz
WDW                        EM
SSB                         0
LB                    0.30 Hz
GB                          0
PC                    1.00
```

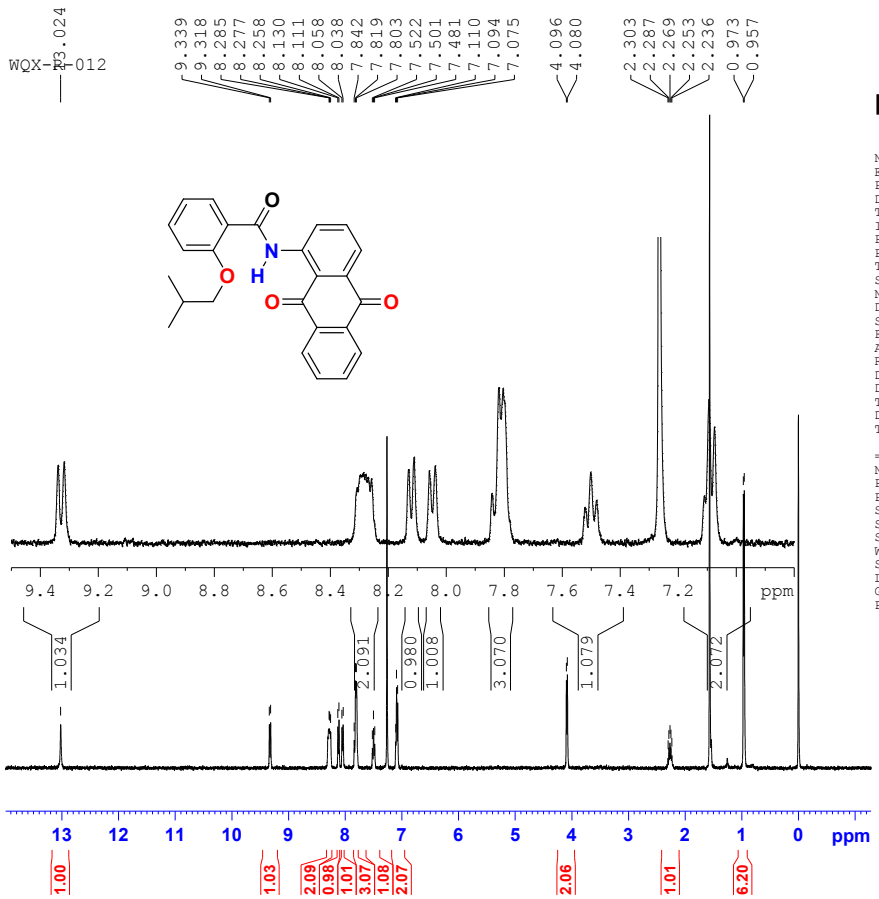


BRUKER

```
NAME                WQX-R-014
EXPNO                       2
PROCNO                      1
Date_                20140115
Time                    19.35
INSTRUM                 spect
PROBHD    5 mm PAQNP Swi
PULPROG                zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       1614
DS                          4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                       2050
DW                   20.800 usec
DE                    6.00 usec
TE                    291.0 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       13C
P1                     9.56 usec
PL1                   -1.00 dB
SFO1          100.6228298 MHz

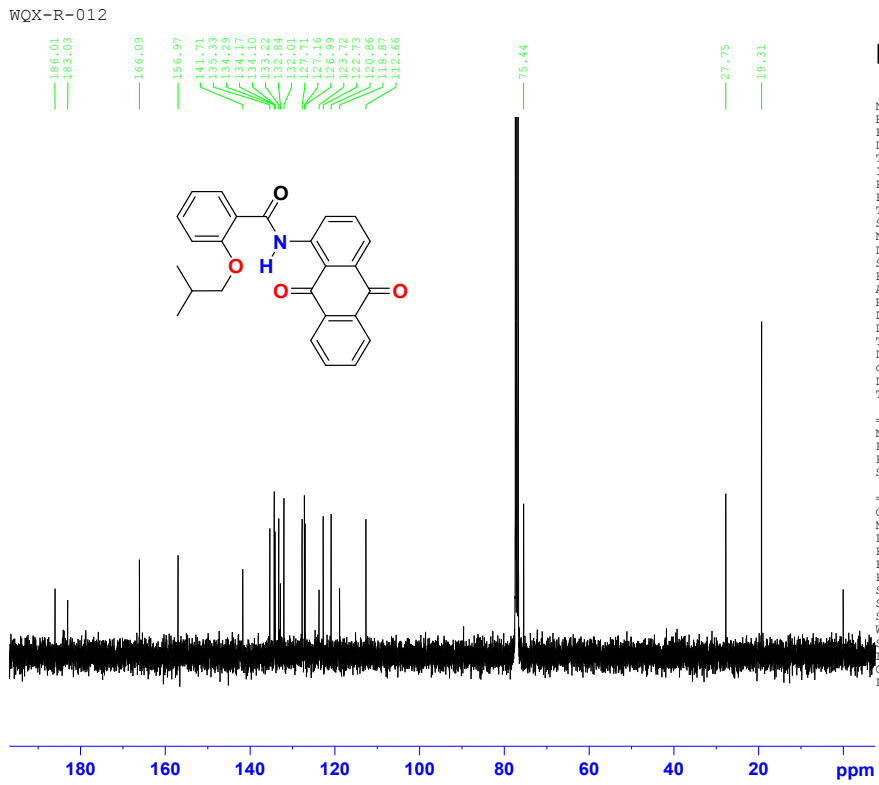
======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                 80.00 usec
PL2                   -3.00 dB
PL12                  13.48 dB
PL13                  14.00 dB
SFO2          400.1316005 MHz
SI                      32768
SF            100.6127690 MHz
WDW                        EM
SSB                         0
LB                    1.00 Hz
GB                          0
PC                    1.40
```



BRUKER

```
NAME                WQX-R-012
EXPNO                       1
PROCNO                      1
Date_                20131023
Time_                   19.35
INSTRUM                 spect
PROBHD   5 mm PAQNP Swi
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                       128
DS                         2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                  3.9846387 sec
RG                      1620
DW                    60.800 usec
DE                     6.00 usec
TE                    295.0 K
D1                 1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      10.90 usec
PL1                     -3.00 dB
SFO1               400.1324710 MHz
SI                       32768
SF                 400.1300090 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```

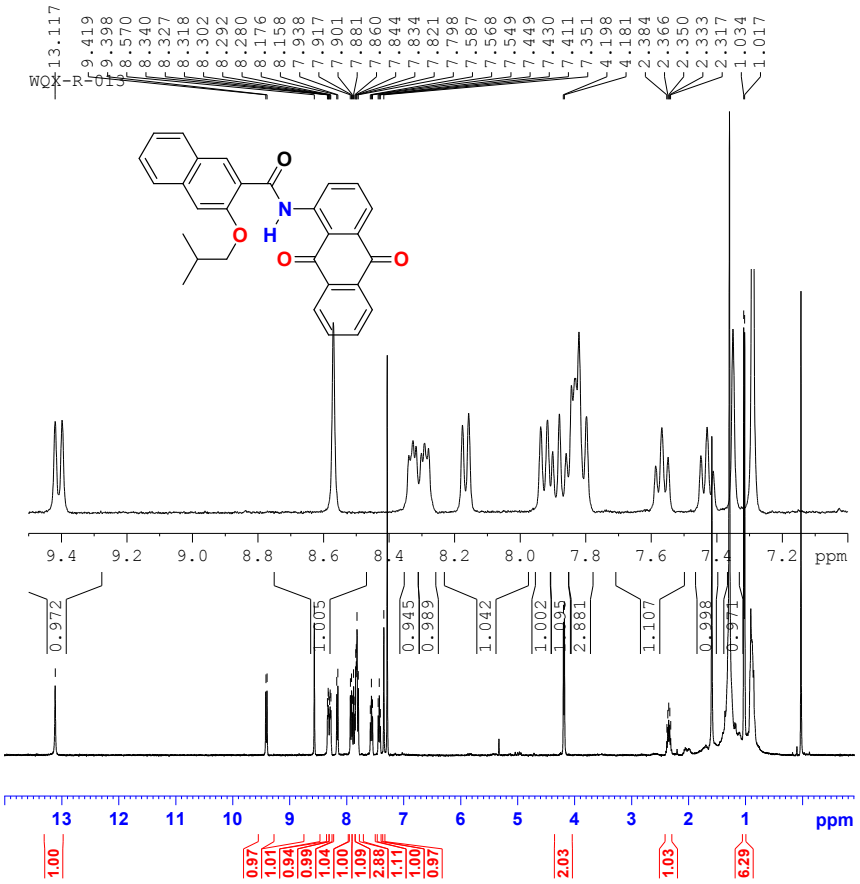


BRUKER

```
NAME                WQX-R-012
EXPNO                       3
PROCNO                      1
Date_                20140115
Time_                   12.45
INSTRUM                 spect
PROBHD   5 mm PAQNP Swi
PULPROG                zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       1200
DS                          4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631988 sec
RG                       2050
DW                    20.800 usec
DE                     6.00 usec
TE                    290.9 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                         1

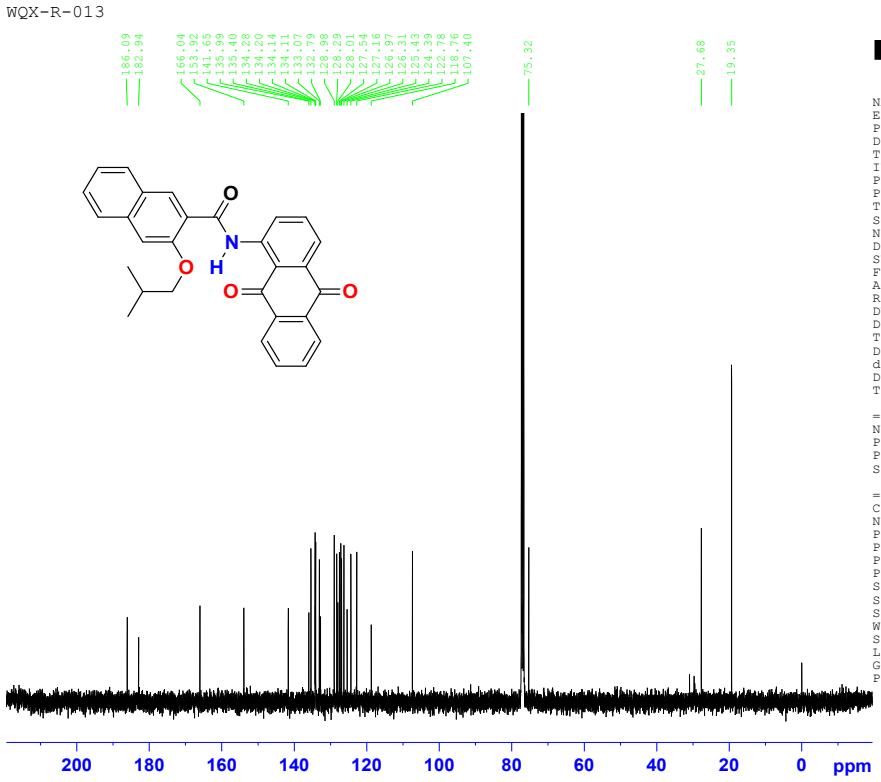
======== CHANNEL f1 ========
NUC1                       13C
P1                      9.56 usec
PL1                    -1.00 dB
SFO1               100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  80.00 usec
PL2                    -3.00 dB
PL12                   13.48 dB
PL13                   14.00 dB
SFO2               400.1316005 MHz
SI                       32768
SF                 100.6127690 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```



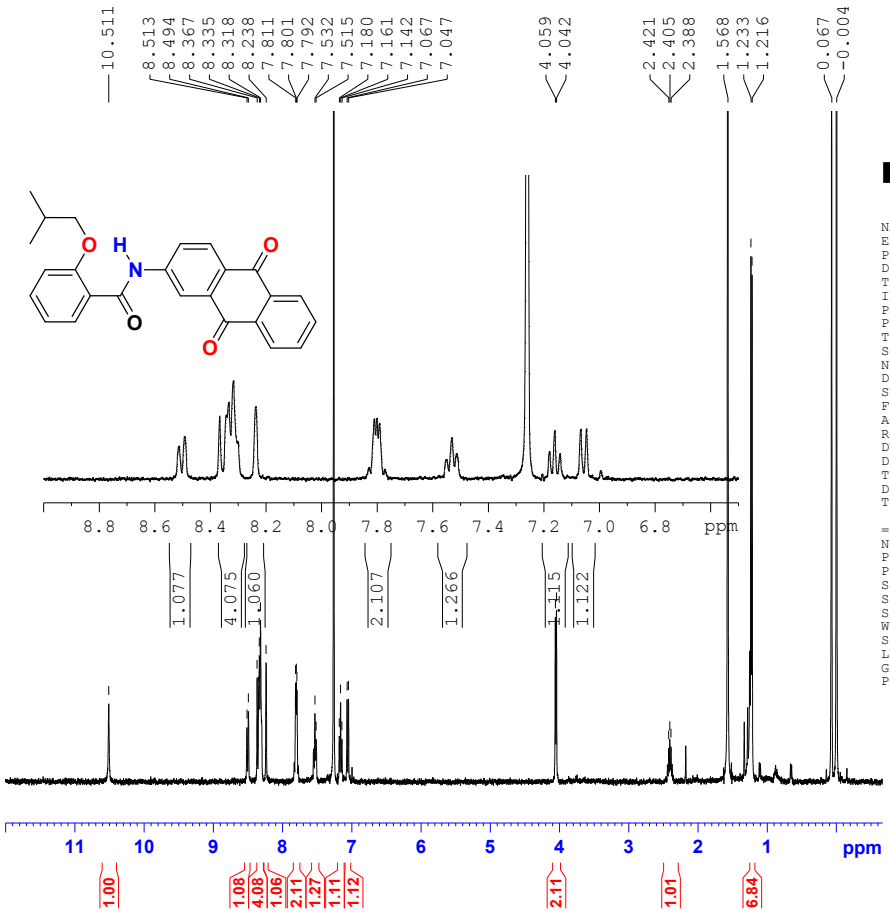
BRUKER

NAME	WQX-R-013
EXPNO	1
PROCNO	1
Date_	20131113
Time	19.22
INSTRUM	spect
PROBHD	5 mm PAQNP Swi
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	17
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	575
DW	60.800 usec
DE	6.00 usec
TE	293.9 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.90 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

NAME	WQX-R-013
EXPNO	3
PROCNO	1
Date_	20140115
Time	14.05
INSTRUM	spect
PROBHD	5 mm PAQNP Swi
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1299
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.00 usec
TE	291.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.56 usec
PL1	-1.00 dB
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	13.48 dB
PL13	14.00 dB
SFO2	400.1316005 MHz
SI	32768
SF	100.6127727 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



BRUKER

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EXPNO                        1
PROCNO                       1
Date_               20150314
Time                   10.01
INSTRUM                spect
PROBHD    5 mm PABBI 1H/
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                         8
DS                         2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                3.9846387 sec
RG                       812
DW                    60.800 usec
DE                     6.00 usec
TE                    291.1 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     7.00 usec
PL1                   -2.00 dB
SFO1           400.1324710 MHz
SI                     32768
SF             400.1300099 MHz
WDW                       EM
SSB                        0
LB                     0.30 Hz
GB                         0
PC                     1.00
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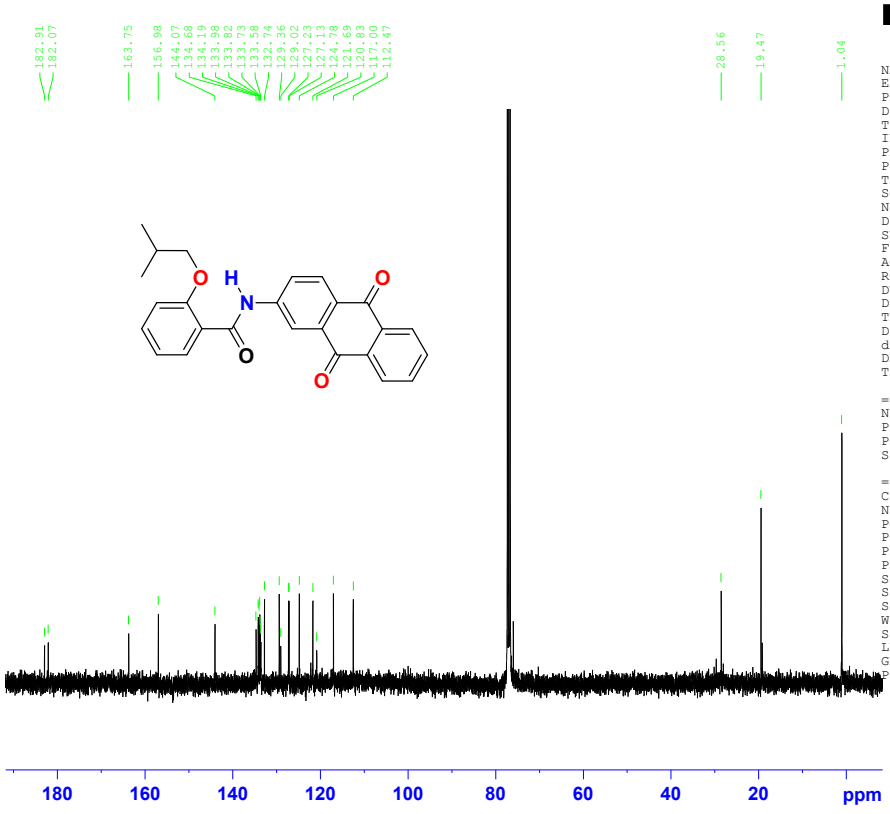

BRUKER

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NAME          WQX-R-015-20150315C
EXPNO                        1
PROCNO                       1
Date_               20150317
Time                   10.37
INSTRUM                spect
PROBHD    5 mm PABBI 1H/
PULPROG              zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      3226
DS                         4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                1.3631988 sec
RG                      50.8
DW                    20.800 usec
DE                     6.00 usec
TE                    292.0 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                    14.90 usec
PL1                   -3.00 dB
SFO1           100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                 80.00 usec
PL2                   -2.00 dB
PL12                  18.50 dB
PL13                  18.50 dB
SFO2           400.1316005 MHz
SI                     32768
SF             100.6127690 MHz
WDW                       EM
SSB                        0
LB                     1.00 Hz
GB                         0
PC                     1.40
```

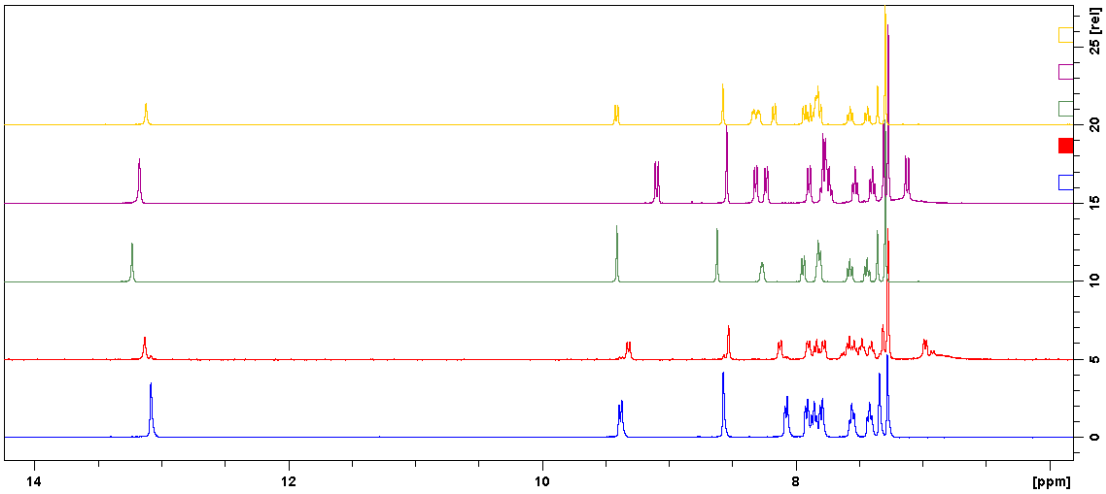

Fig. S1 Stacked partial ^{1}H NMR spectra of dye **8**, **9**, **10**, **11** and **13**, from bottom up, $CDCl_3$, 400 MHz, 298 K.

Fig. S2 Photoes for dyes (from left to right) **1** orange, **2** purple, **3** orange, **4** light yellow, **5** orange, **6** jacinth, **7** claret-red, **8** bright yellow, **9** orange, **10** jacinth, **11** claret-red, **12** bright yellow, **13** bright yellow, **14** light yellow, **15** colorless, in 5×10^{-5} M chloroform solution.

Fig. S3 Photoes taken in 1×10^{-5} M $CHCl_3$ solutions, under UV lamp (254 nm), from left to right, dye **1**~**7**.

Fig. S4 Photoes taken in 1×10^{-5} M $CHCl_3$ solutions, under UV lamp (254 nm), from left to right, dye **8**~**15**.