

# Supporting information

## Design of dyes based on the quinoline or quinoxaline skeleton towards visible light photoinitiators

Ilona Pyszka <sup>1</sup>, Beata Jędrzejewska <sup>1</sup>

<sup>1</sup> Faculty of Chemical Technology and Engineering, Bydgoszcz University of Science and Technology, 85-326 Bydgoszcz, Poland

\* Correspondence: Ilona.Pyszka@pbs.edu.pl; Tel.: +48-52-374-9039

Table of contents	Page
<sup>1</sup> H and <sup>13</sup> C NMR spectra.....	S2
Normalized electronic absorption spectra of synthesized dyes in ethyl acetate – Figure S1.....	S12
Normalized (a) fluorescence and (b) phosphorescence spectra of the synthesized dyes in 2-methyltetrahydrofuran at room temperature – Figure S2.....	S13
Electronic absorption spectrum, fluorescence and phosphorescence spectra of synthesized dyes in 2-methyltetrahydrofuran. – Figure S3.....	S13
Absorption spectrum of the triplet state of the tested dyes recorded in deoxygenated acetonitrile – Figure S4.....	S14
Kinetic curves of the disappearance of the triplet state recorded for the tested dyes at DQ2 - 430 nm, DQ3 - 370 nm, DQ4 - 360 nm, DQ5 - 340 nm – Figure S5.....	S14

# <sup>1</sup>H spectrum of IPB

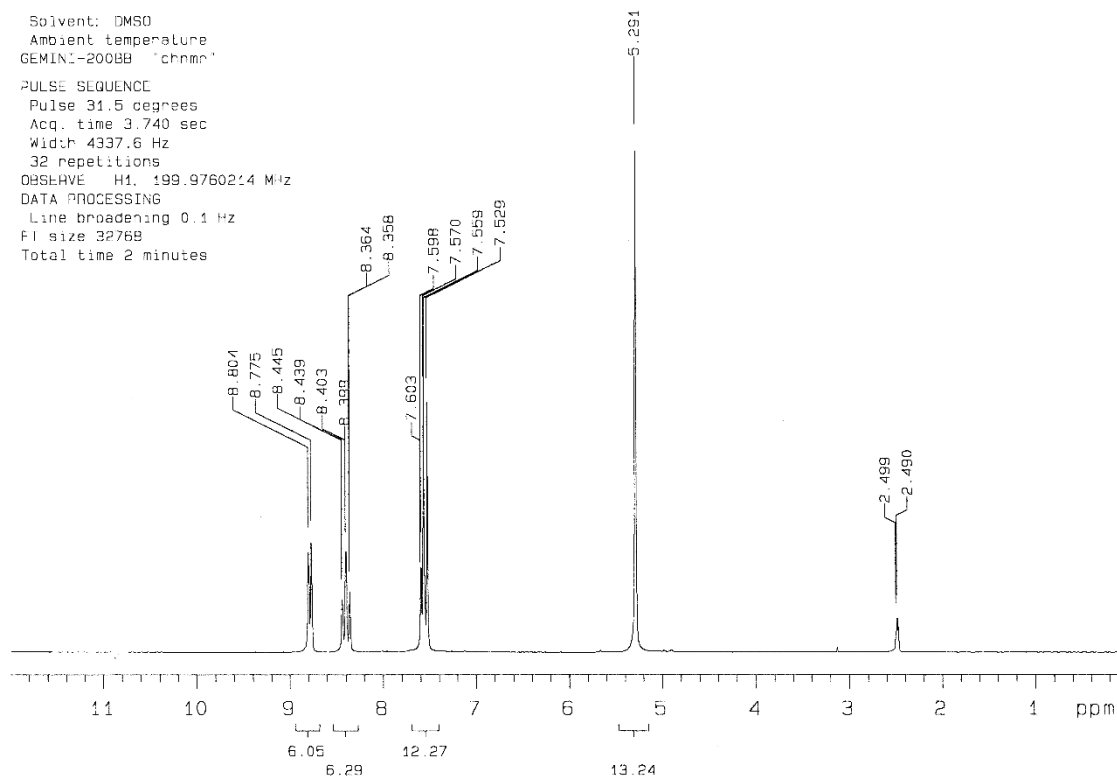
No.180

ZK - SA

Solvent: DMSO  
Ambient temperature  
GEMINI-200BB "chnmr"

## PULSE SEQUENCE

Pulse 31.5 degrees  
Acq. time 3.740 sec  
Width 4337.6 Hz  
32 repetitions  
OBSERVE H1, 199.9760214 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FI size 32768  
Total time 2 minutes



# <sup>13</sup>C spectrum of IPB

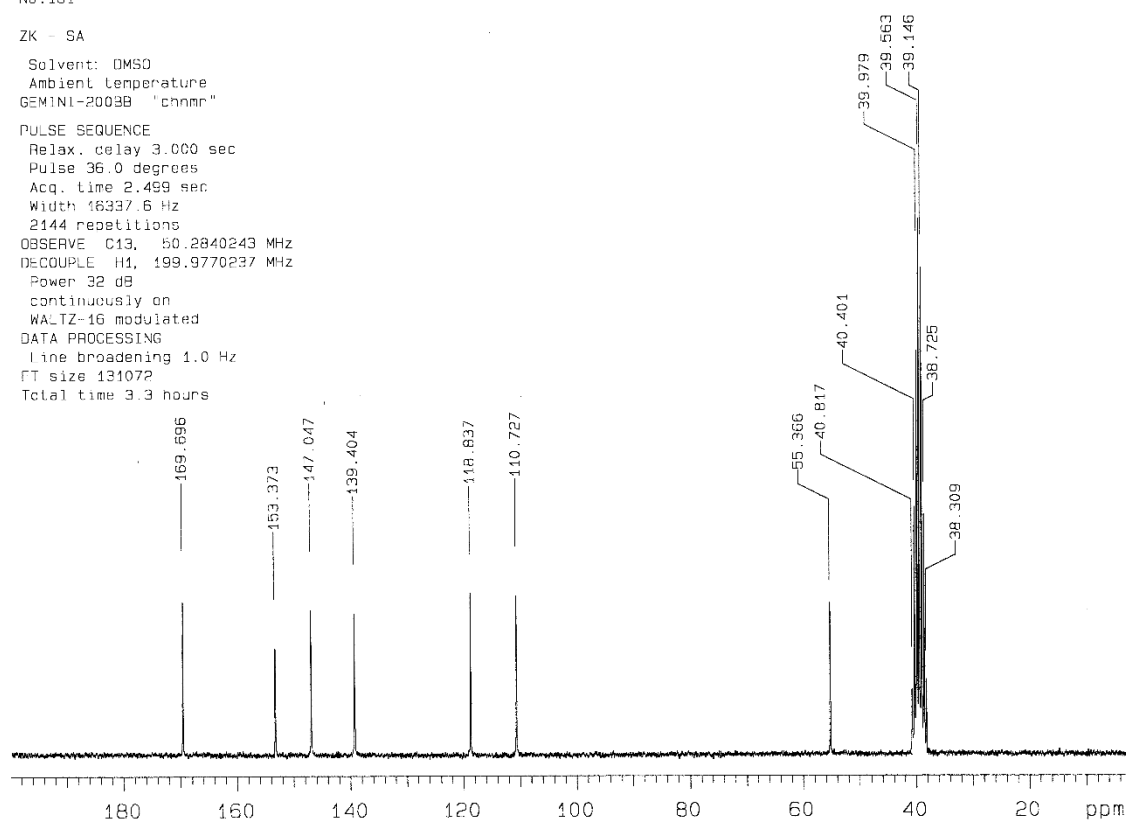
No.181

ZK - SA

Solvent: DMSO  
Ambient temperature  
GEMINI-200BB "chnmr"

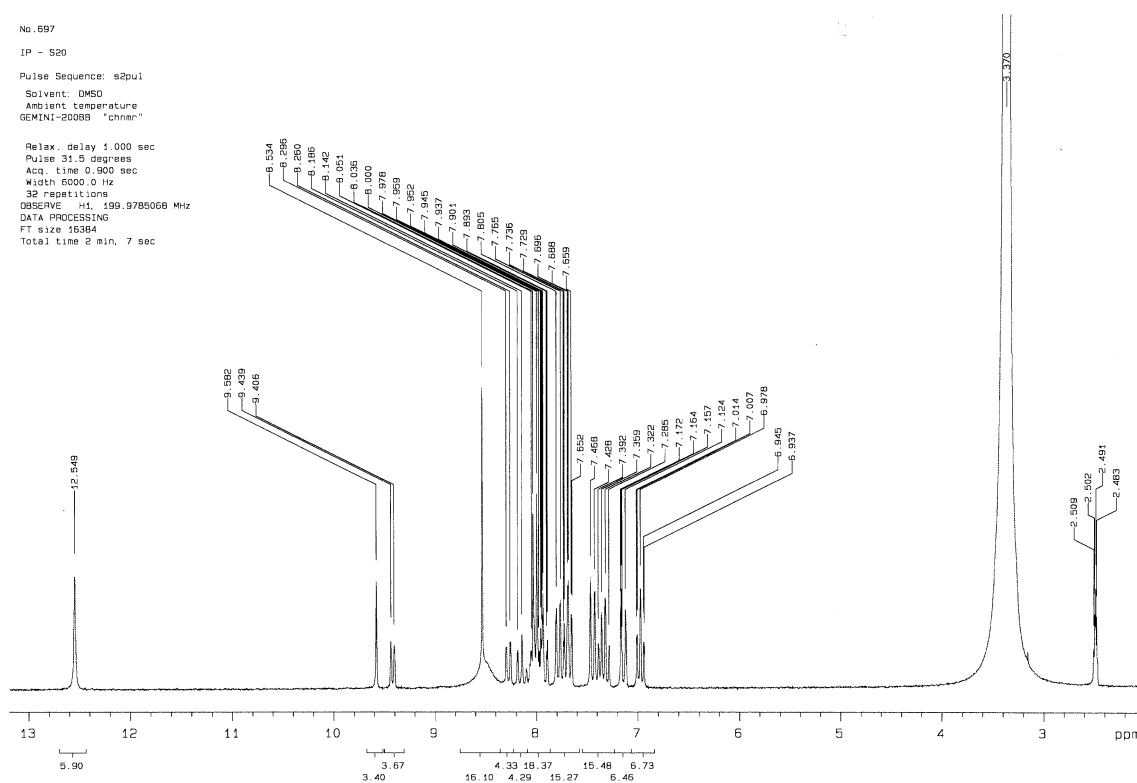
## PULSE SEQUENCE

Relax. delay 3.000 sec  
Pulse 36.0 degrees  
Acq. time 2.499 sec  
Width 16337.6 Hz  
2144 repetitions  
OBSERVE C13, 50.2840243 MHz  
DECOUPLE H1, 199.9770237 MHz  
Power 32 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
line broadening 1.0 Hz  
FT size 131072  
Total time 3.3 hours



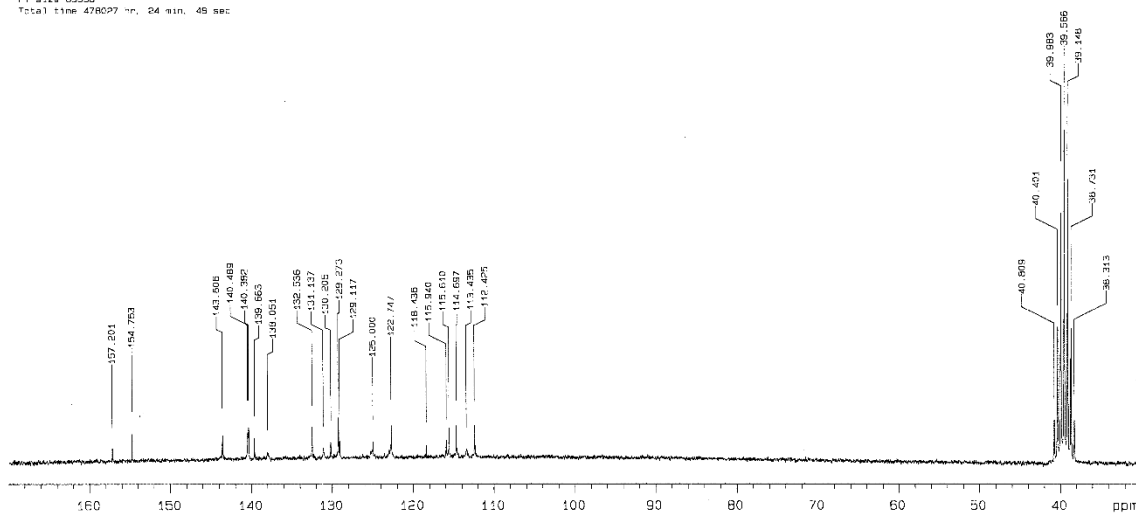
# <sup>1</sup>H spectrum of DQ1

No. 697  
IP - S20  
Pulse Sequence: s2pul  
Solvent: DMSO  
Ambient temperature  
GEMINI-200BB "chman"  
Relax. delay 1.000 sec  
Pulse 31.5 degrees  
Acq. time 0.900 sec  
Width 6000.0 Hz  
32 repetitions  
OBSERVE H1 199.9785058 MHz  
DATA PROCESSING  
FT size 16384  
Total time 2 min. 7 sec



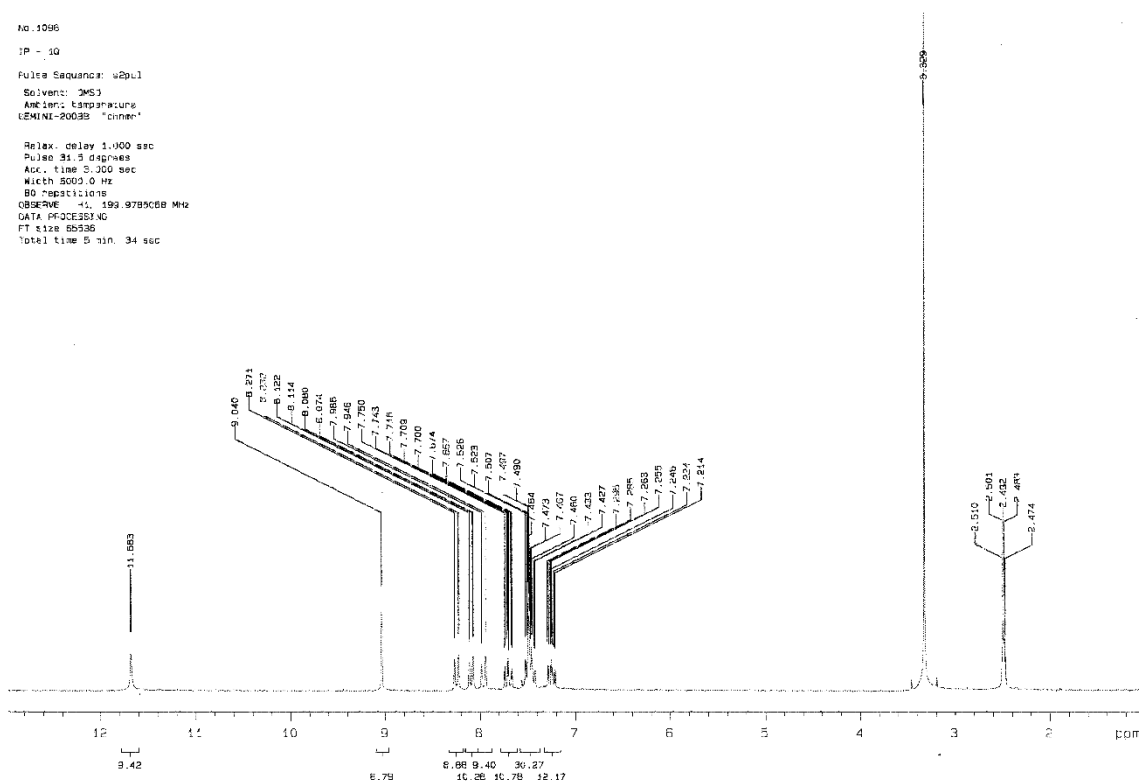
# <sup>13</sup>C spectrum of DQ1

No. 698  
IP - S20  
Pulse Sequence: s2pul  
Solvent: DMSO  
Ambient temperature  
GEMINI-200BB "chman"  
Pulse 60.0 degrees  
Acq. time 1.498 sec  
Width 16000.0 Hz  
47804 repetitions  
OBSERVE C13 50.2845554 MHz  
DECOUPLE H1 199.9795085 MHz  
Power 30 dB  
Continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 1.0 Hz  
FT size 65536  
Total time 478027 hr, 24 min, 48 sec



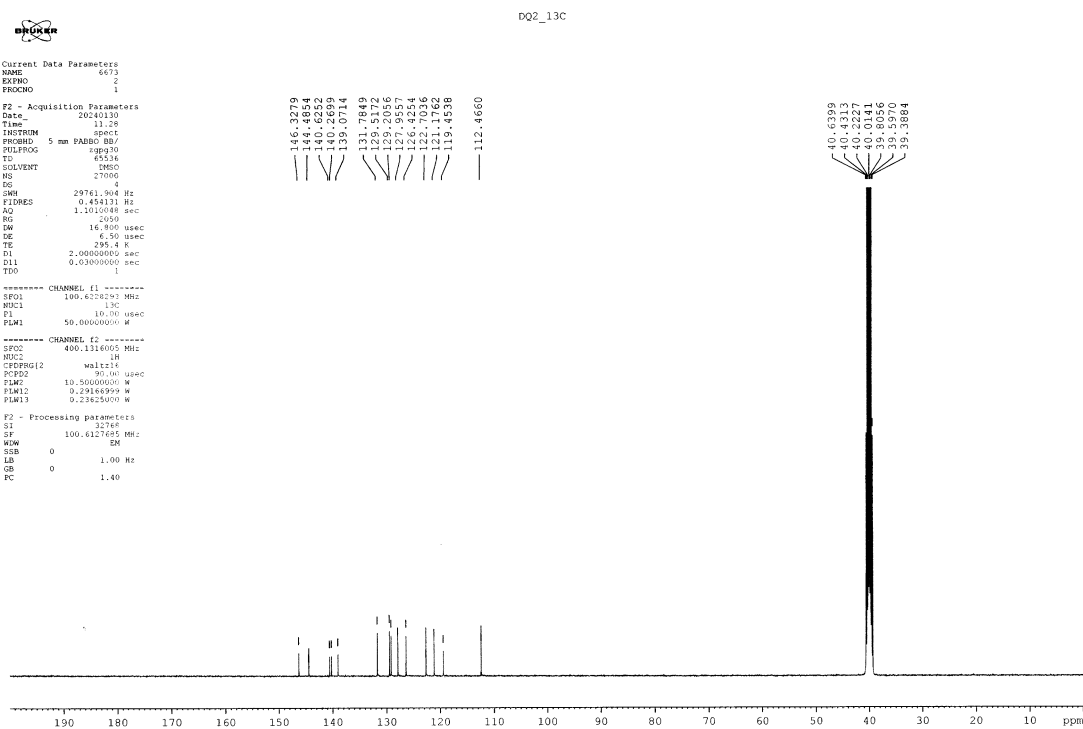
# <sup>1</sup>H spectrum of DQ2

NO.1096  
IP - 1Q  
Pulse Sequence: w2pul  
Solvent: DMSO  
Ambient Temperature  
CEMINT-20033 "cinnar"  
Relax. delay 1.000 sec  
Pulse 31.5 degrees  
Acc. time 3.000 sec  
Width 5000.0 Hz  
SFO 400.131013  
OBSERVE 40.199.9785008 MHz  
DATA PROCESSING  
F1 size 65536  
Total time 5 min. 34 sec

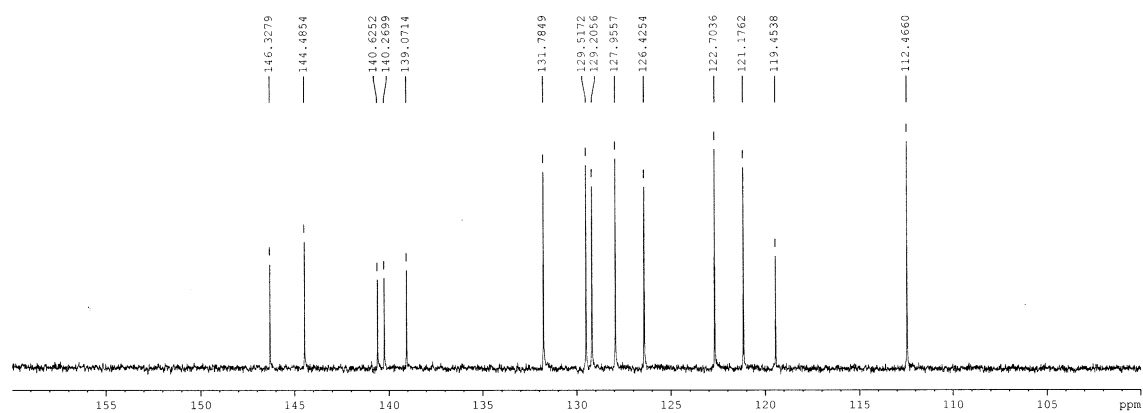


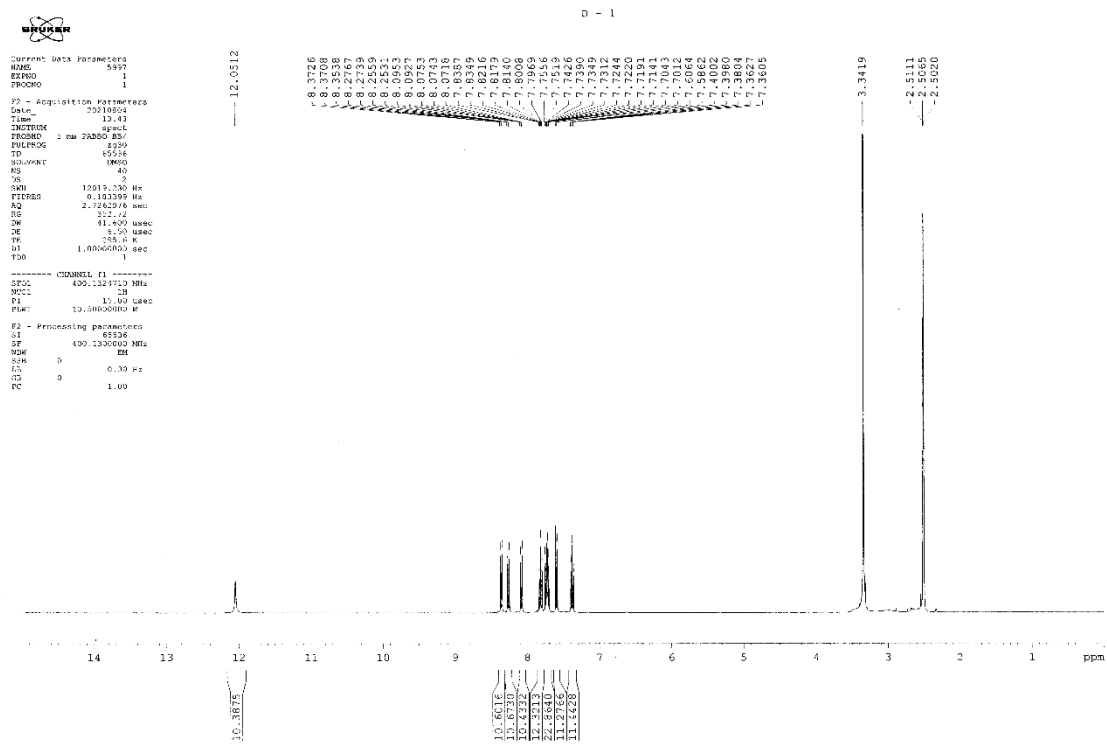
# <sup>13</sup>C spectrum of DQ2

Current Data Parameters  
NAME 6673  
EXPNO 2  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20240110  
Time 11.28  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 27000  
DS 4  
SWH 29761.994 Hz  
FIDRES 0.454131 Hz  
AQ 1.1010088 sec  
RG 2050  
DM 16.850 usec  
DE 6.50 usec  
TE 295.4 K  
D1 2.00000000 sec  
d11 0.63000000 sec  
TD0 1  
----- CHANNEL f1 -----  
SFO1 100.6261200 MHz  
NUC1 13C  
P1 10.00 usec  
PLM1 50.00000000 W  
----- CHANNEL f2 -----  
SFO2 400.1310130 MHz  
NUC2 1H  
PCPDG12 waltz16  
PCPDG13 30.00 usec  
PLM2 10.50000000 W  
PLM12 0.29146909 W  
PLM13 0.23625000 W  
F2 - Processing parameters  
SI 32768  
SF 100.6127695 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

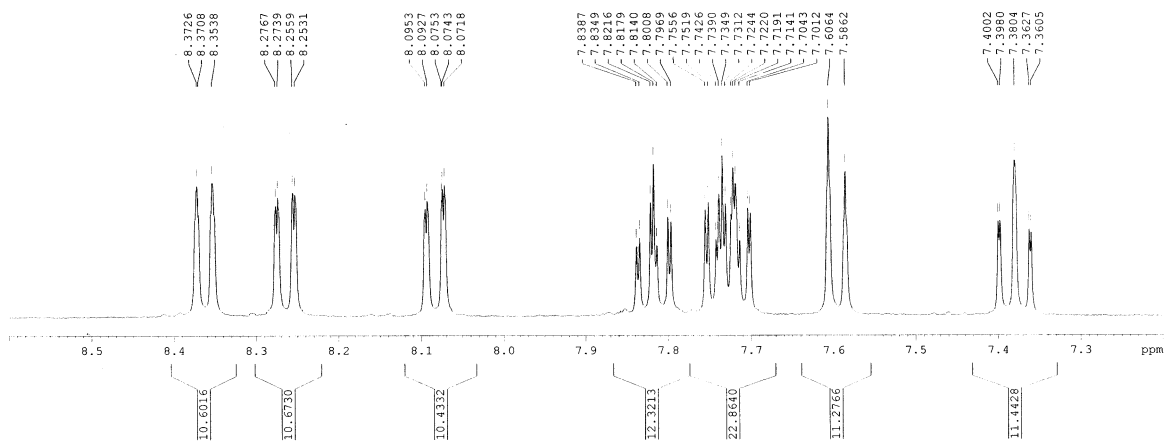


Enlarged spectrum in the range of 110-150 ppm.

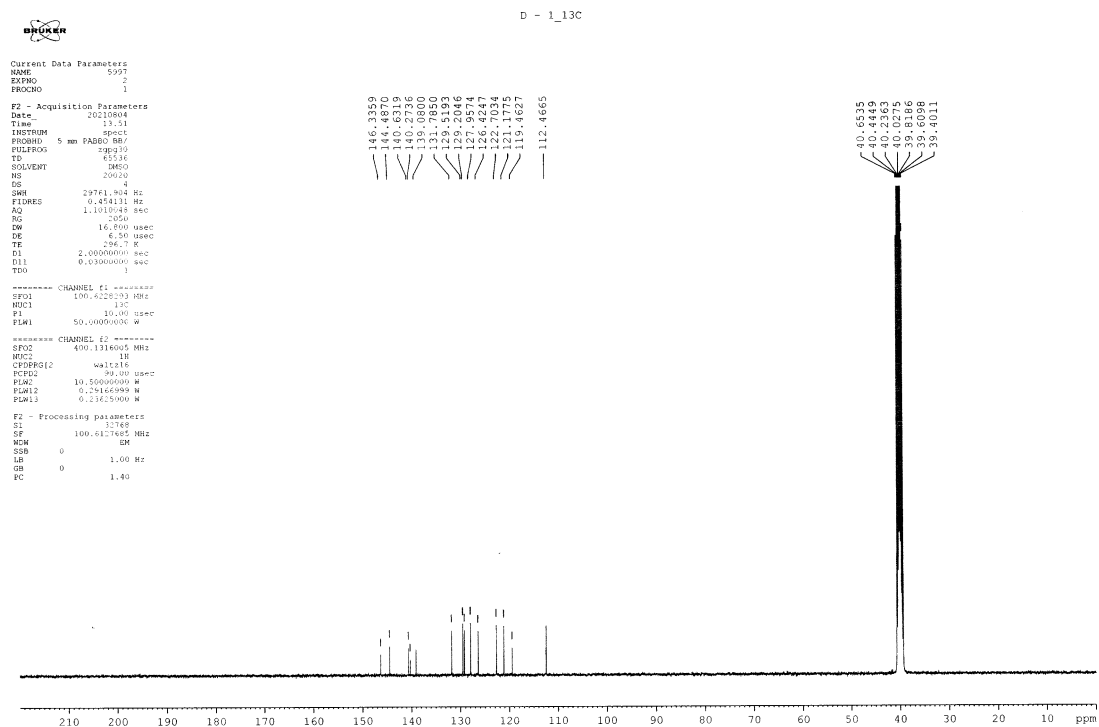


<sup>1</sup>H spectrum of DQ3

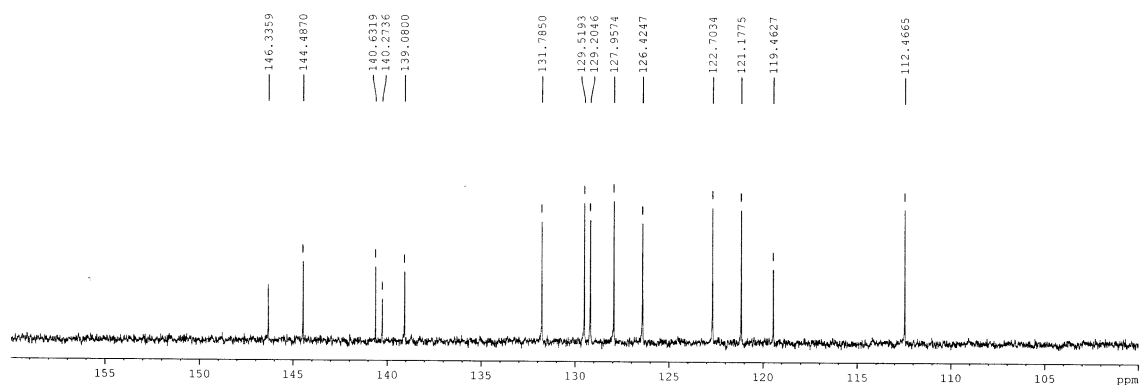
Enlarged spectrum in the range of 7-9.



# <sup>13</sup>C spectrum of DQ3

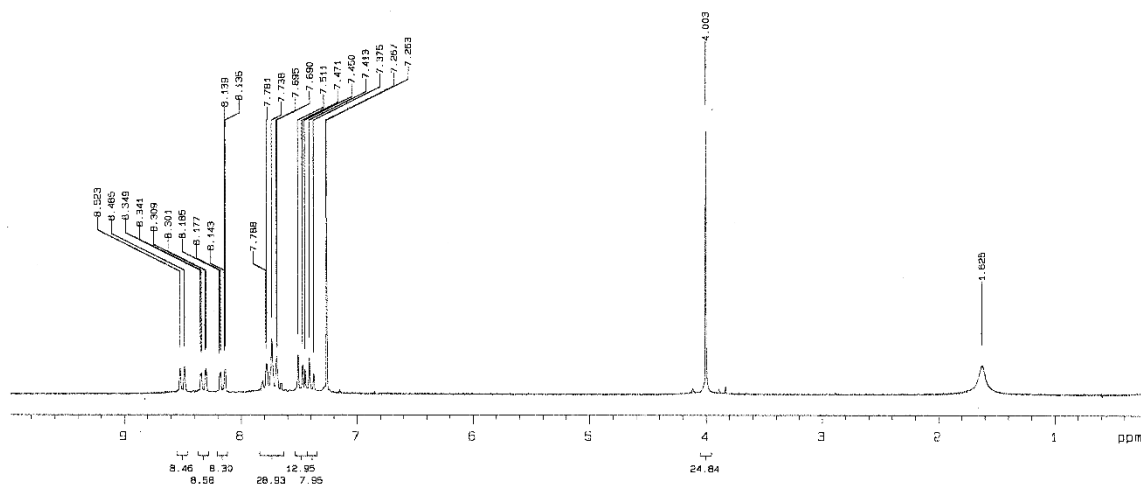


Enlarged spectrum in the range of 110-150 ppm.



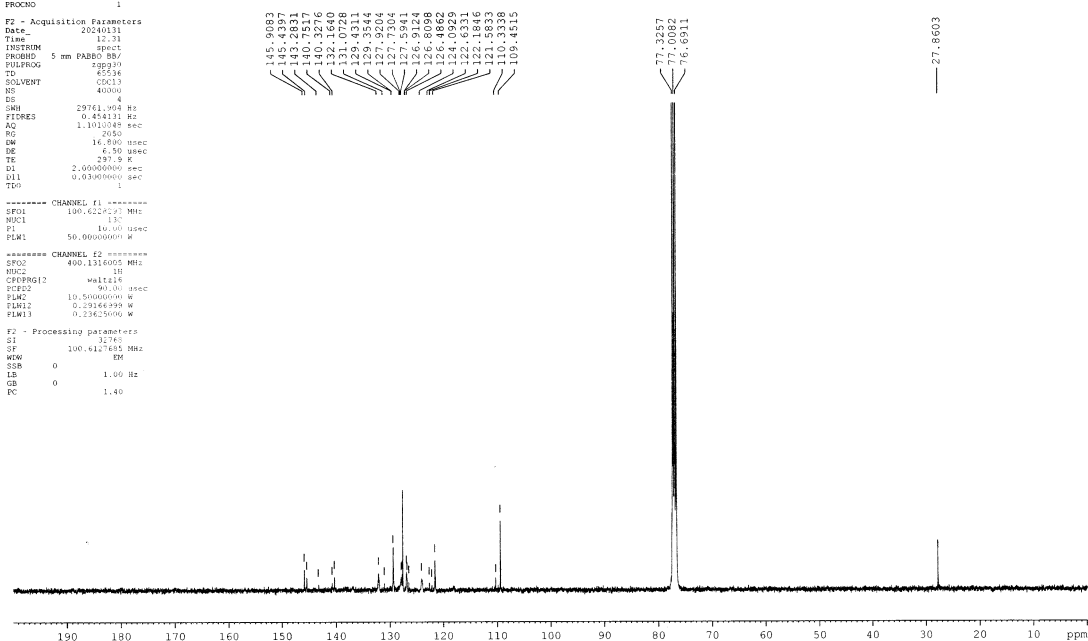
# <sup>1</sup>H spectrum of DQ4

No.1065  
IP  
Pulse Sequence: s2su1  
Solvent: CDCl3  
Ambient temperature  
GEMINI-20098 "chsm"  
Relax. delay 1.000 sec  
Pulse 27.0 degrees  
Acq. time 2.800 sec  
Width 4408.4 Hz  
80 repetitions  
OBSERVE H1, 199.9775573 MHz  
DATA PROCESSING  
F1 size 32768  
Total time 10 min. 30 sec



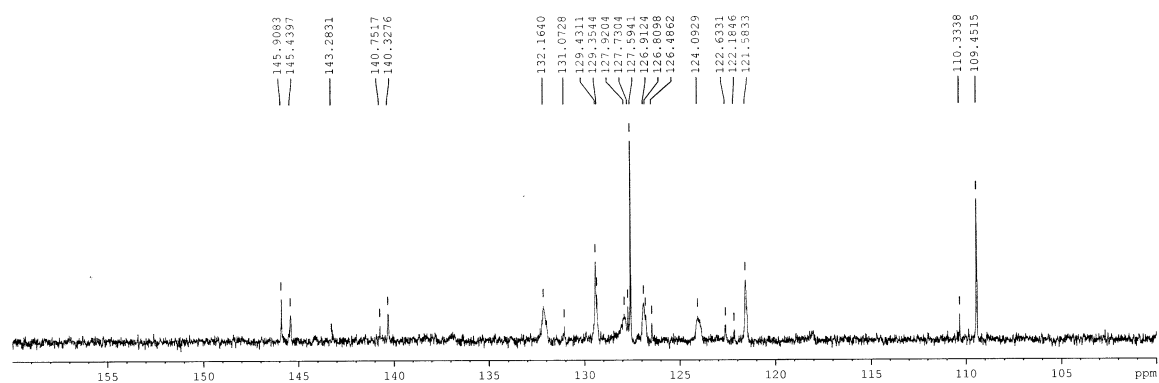
# <sup>13</sup>C spectrum of DQ4

Current Data Parameters  
NAME 6616  
EXPNO 2  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20240131  
Time 12.31  
INSTRUM spect  
PROBHD 5 mm PABO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 4000  
DS 4  
SWH 29741.904 Hz  
FIDRES 0.454331 Hz  
AQ 1.1010349 sec  
RG 2050  
CW 16.890 usec  
DE 6.90 usec  
TE 297.3 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
TD0 1  
----- CHANNEL f1 -----  
SFO1 100.625127 MHz  
NUC1 13C  
P1 10.00 usec  
PLM1 50.00000000 W  
----- CHANNEL f2 -----  
SFO2 400.131800 MHz  
NUC2 1H  
CPRPG12 waltz16  
F2F2 90.00 usec  
PLM2 10.50000000 W  
PLM12 0.2316499 W  
PLM13 0.23625000 W  
F2 - Processing parameters  
SI 32768  
SF 100.6127483 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

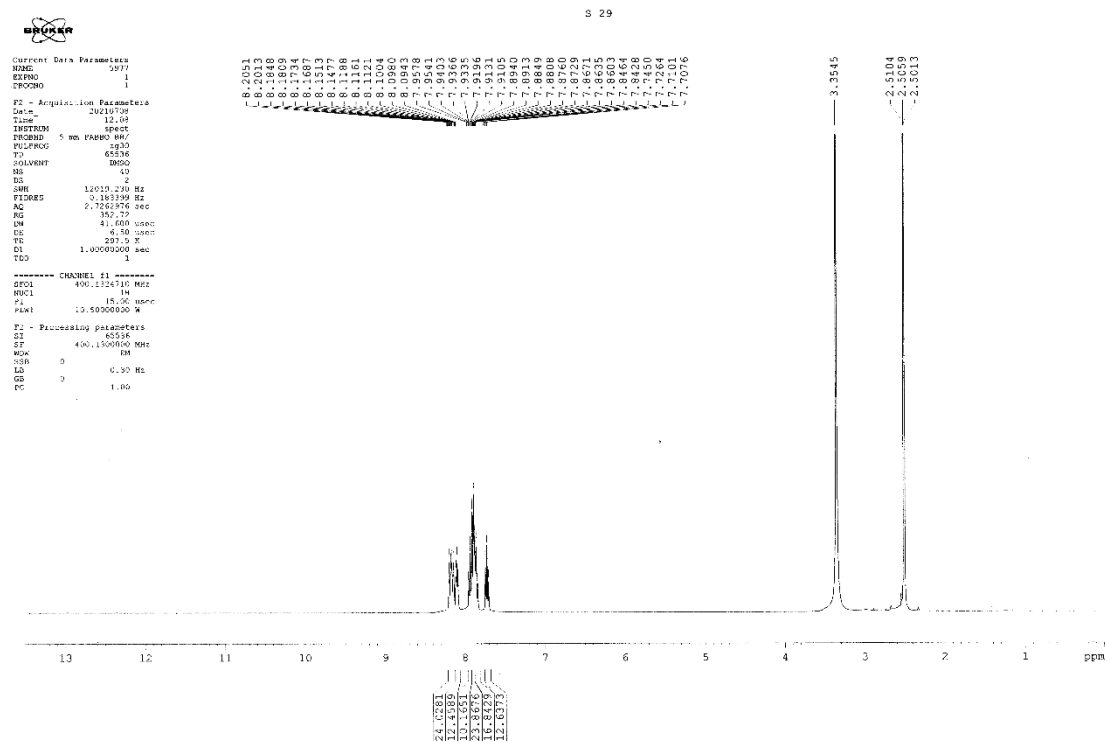




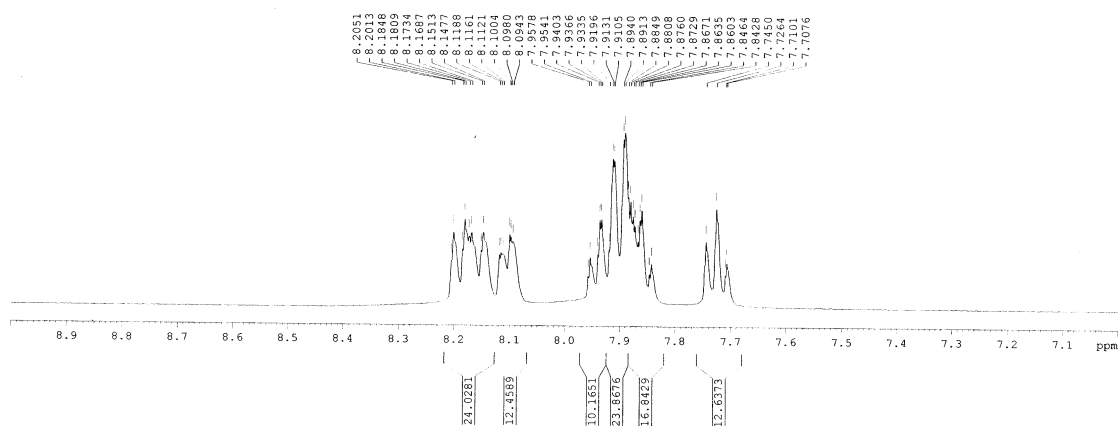
Enlarged spectrum in the range of 10-150 ppm.



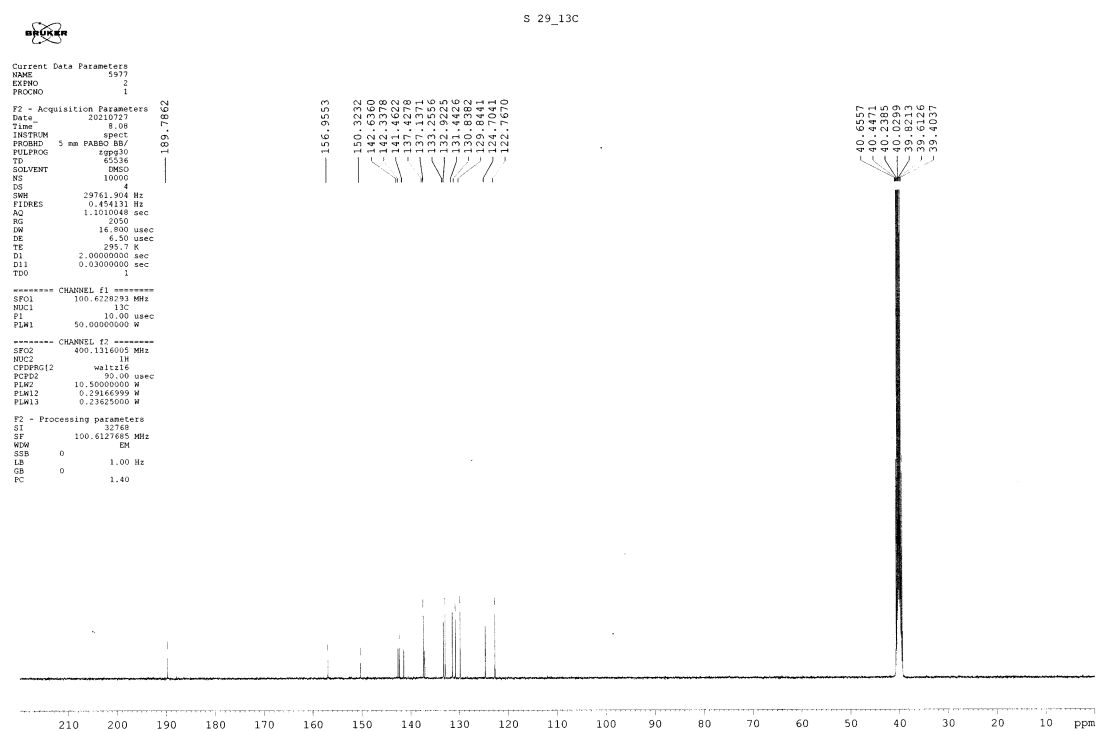
# <sup>1</sup>H spectrum of DQ5



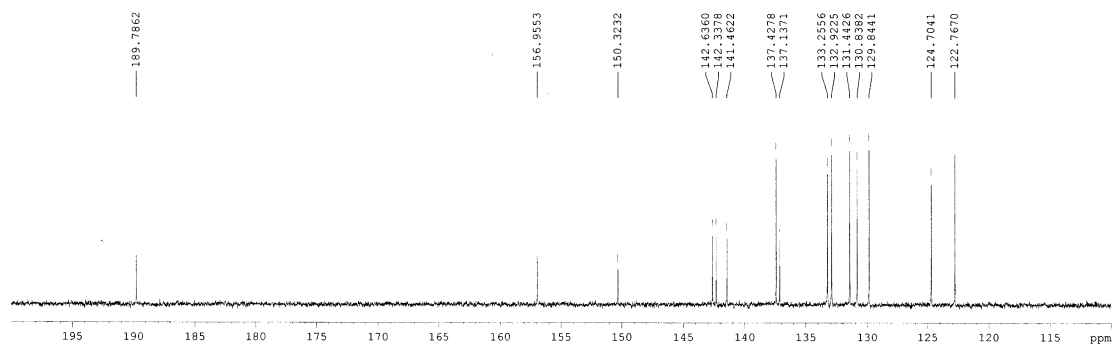
Enlarged spectrum in the range of 7-9.

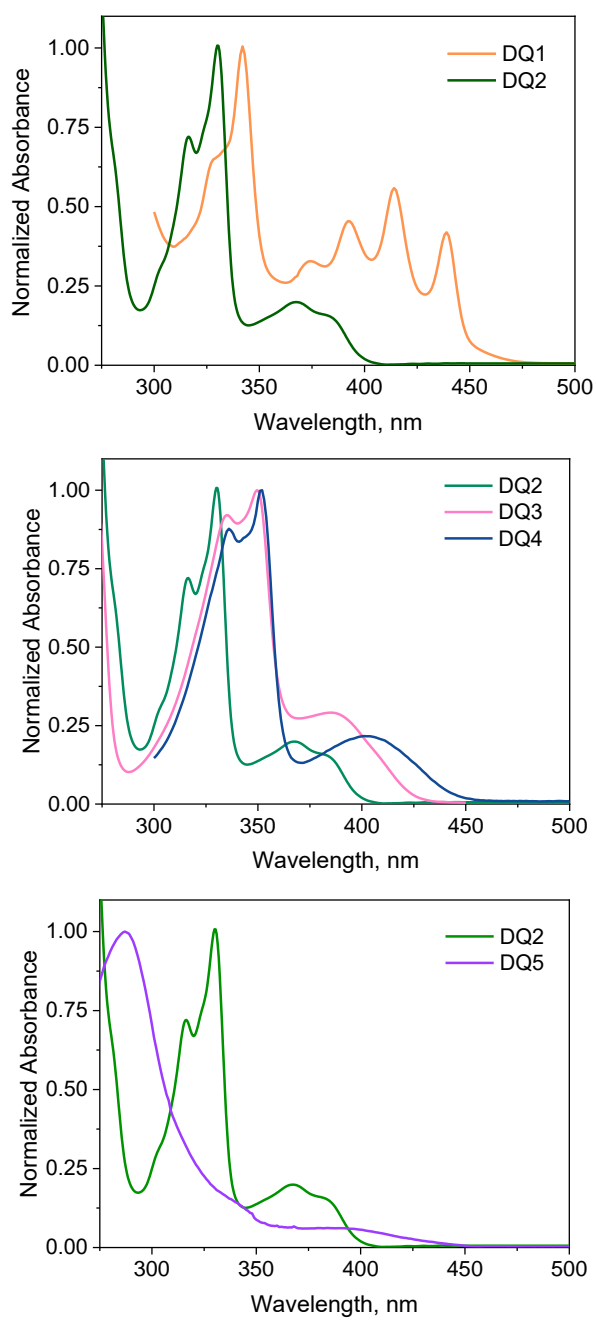


# <sup>13</sup>C spectrum of DQ5

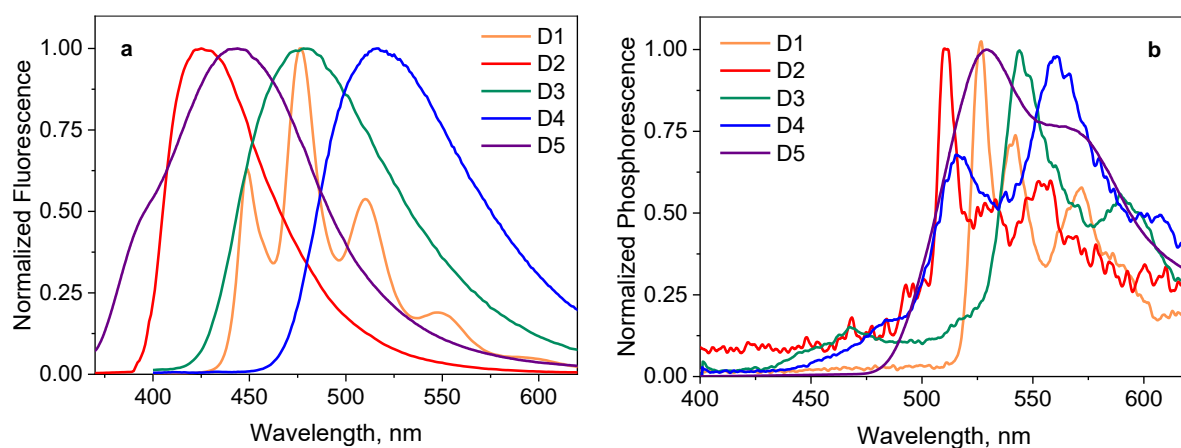


Enlarged spectrum in the range of 110-180 ppm.

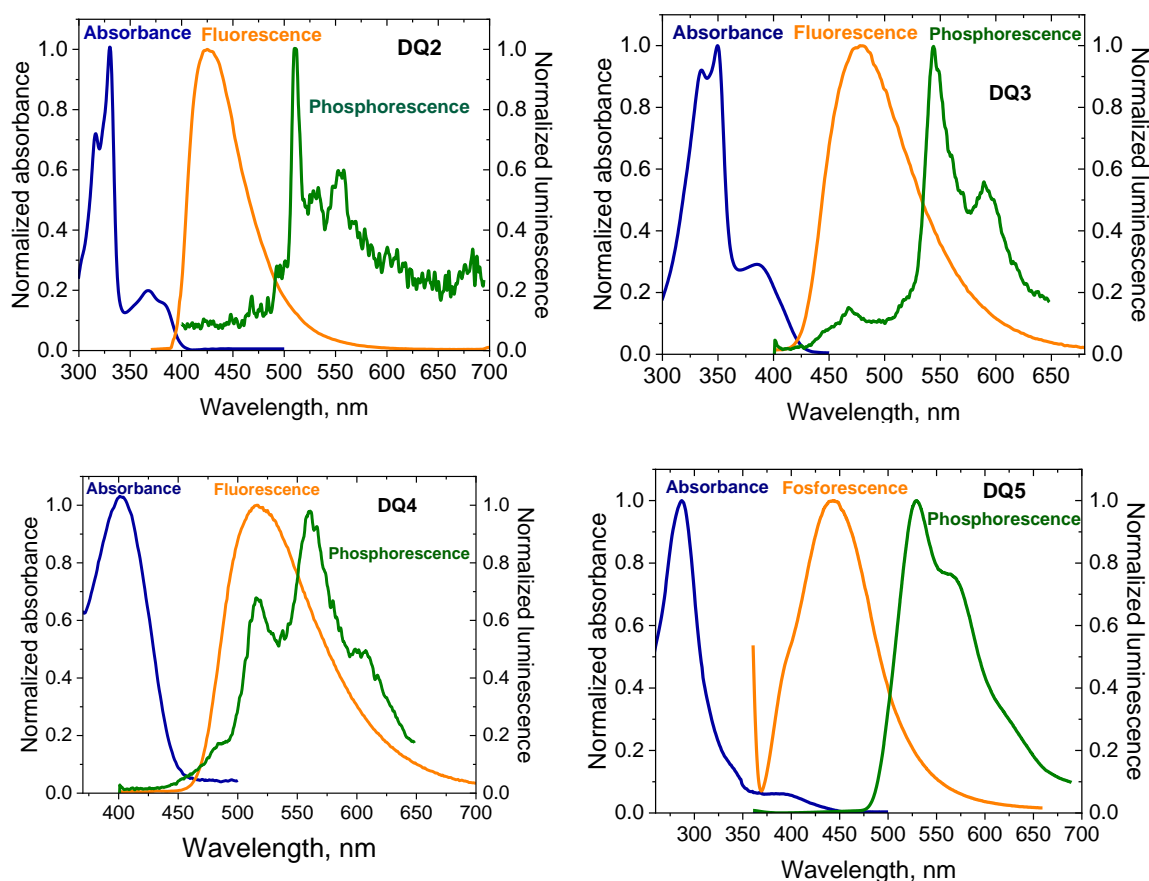




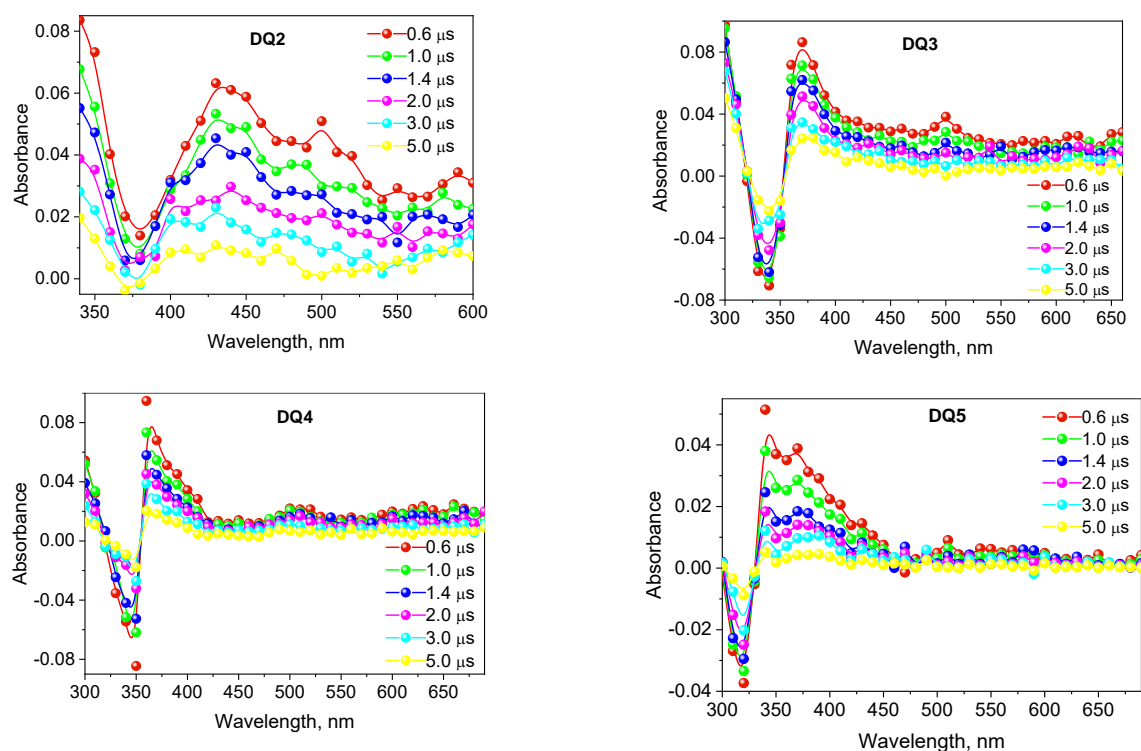
**Figure S1.** Normalized electronic absorption spectra of synthesized dyes in ethyl acetate.



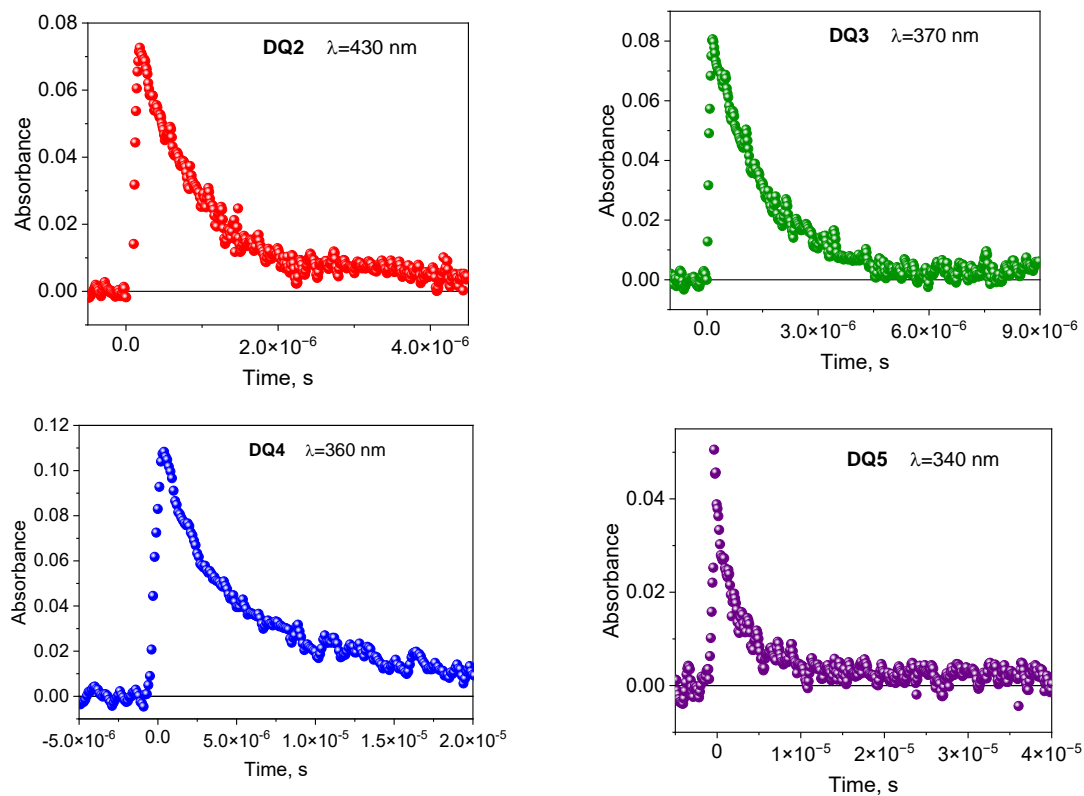
**Figure S2.** Normalized (a) fluorescence and (b) phosphorescence spectra of the synthesized dyes in 2-methyltetrahydrofuran at room temperature and at liquid nitrogen temperature, respectively.



**Figure S3.** Electronic absorption spectrum, fluorescence and phosphorescence spectra of the tested dyes in 2-methyltetrahydrofuran.



**Figure S4.** Absorption spectrum of the triplet state of the tested dyes recorded in deoxygenated acetonitrile.



**Figure S5.** Kinetic curves of the disappearance of the triplet state recorded for the tested dyes at DQ2 - 430 nm, DQ3 - 370 nm, DQ4 - 360 nm, DQ5 - 340 nm.