Supplementary Material for PCCP

Supplementary information for

Fluorescence and chemiluminescence properties of indolylmaleimides: experimental and theoretical studies

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Contents

Experimental Section

Reagents and solutions

Deionized and distilled water purified by a Milli-Q system (Japan Millipore, Tokyo, Japan) was used. 2,3-Dibromomaleimide, potassium *tert*-butoxide (THF), methyl magnesium chloride (3M in THF), Iron (II) bromide were purchased from Aldrich (Milwaukee, USA). Indole, 2-phenylindole, 2-acetonaphthone, 2-iodoaniline, ammonium nitrate, palladium black, palladium acetate, tetrakis(triphenylphosphine)palladium, acetone, benzene, chloroform, dichloromethane, dimethylformamide, ethyl acetate, hexane, methanol, sodium hydroxide, toluene and hydrogen peroxide (30 %) were purchased from Wako Chemicals (Osaka, Japan). 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (98%, DDQ), *p*-toluenesulfonic acid monohydrate (*p*-TsOH), acetonitrile, ethanol and tetrahydrofuran were purchased from Nacalai Tesque (Kyoto, Japan). All other chemicals and solvents were of analytical reagent grade.

Apparatus and its operations

The ^{1}H-NMR spectra were obtained using a Varian UNITY plus (USA) spectrometer at 500 MHz. The FAB MS spectra of **1**－**15** were obtained using a JEOL JMS 600 (Tokyo, Japan). The absorbance and fluorescence spectra of **1**－**15** were obtained using a Jasco V-530 absorptiometer and an FP-6500 fluorometer (Tokyo, Japan).

Spectra data of compounds **1**, **2**, **4**, **7** and **13**

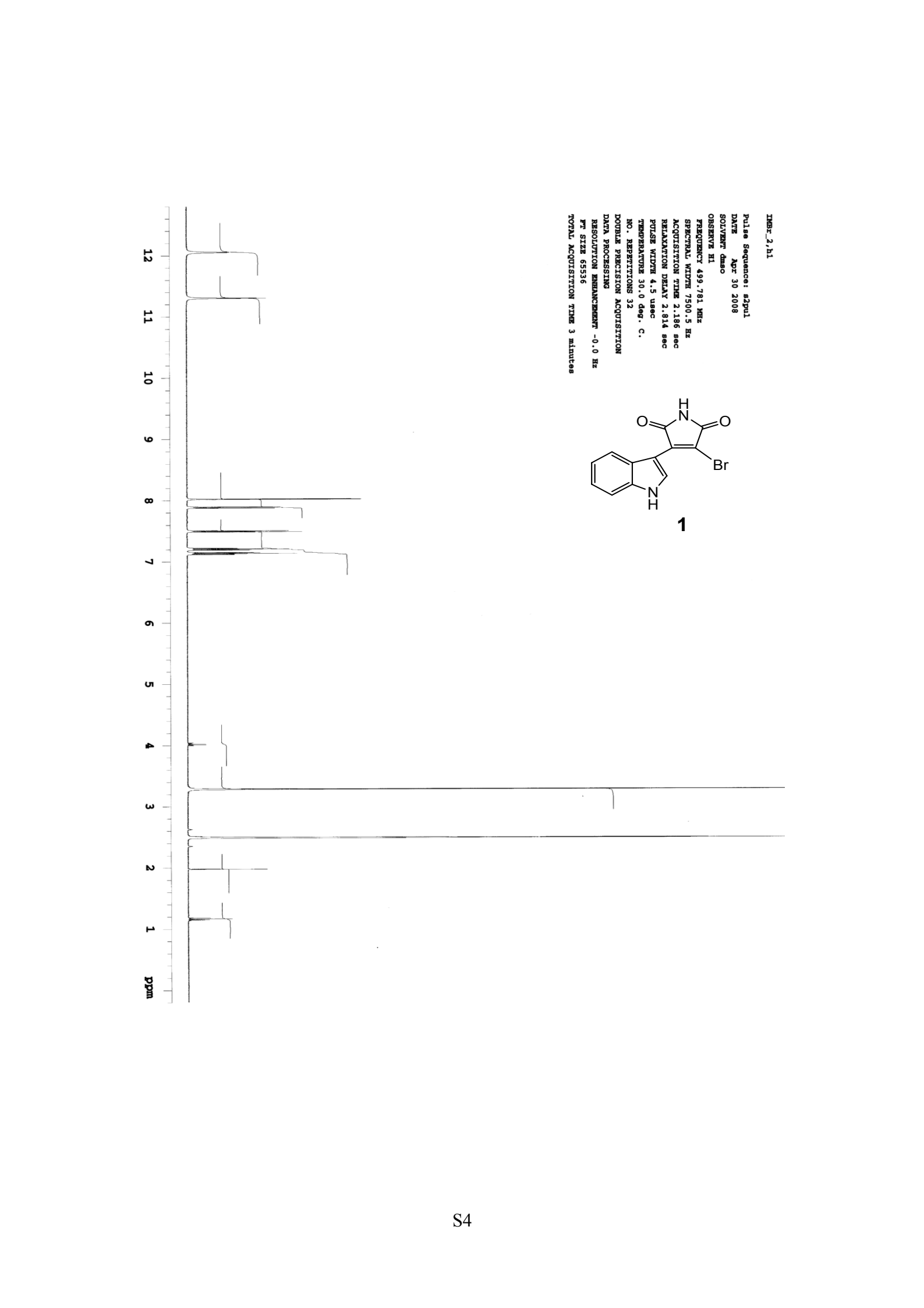
3-Bromo-4-(1H-3-indolyl)-2,5-dihydro-1H-pyrroledione (**1**). m.p.: 182–184℃. ^{1}H-NMR (DMSO-d_6): 7.11–7.19 (m, 1H, ArH), 7.2–7.22 (m, 1H, ArH), 7.48–7.50 (t, *J* = 8 Hz, 1H, ArH), 7.87–7.89 (d, *J* = 8 Hz, 1H, ArH), 8.01–8.02 (d, *J* = 3 Hz, 1H, ArH), 11.3 (s, 1H, maleimide NH), 12 (s, 1H, indole NH), FAB MS: m/z = 292.05 $[M+H]^+$, $C_{12}H_7BrN_2O_2$, calc. (%): H; 2.42 , C; 49.51, N; 9.62. Found (%): H; 2.58, C; 49.86, N; 9.34.

3-Bromo-4-(2-phenyl-1H-3-indolyl)-2,5-dihydro-1H-pyrroledione (**2**). m.p.: 245–247℃. ^{1}H-NMR(DMSO-d_6): 7.08–7.11 (m, 1H, ArH), 7.19–7.22 (m, 1H, ArH), 7.35–7.38 (t, *J* = 7.5Hz, 1H, ArH), 7.44–7.48 (m, 4H, ArH), 7.54 (d, *J* = 7.5 Hz, 2H, ArH), 11.3 (s, 1H, maleimide NH), 12 (s, 1H, indole NH), FAB MS: m/z = 368.1 $[M+H]^+$, $C_{18}H_{11}BrN_2O_2$, calc. (%): H; 3.02, C; 58.88, N; 7.63. Found (%): H; 3.26, C; 59.29, N; 7.36.

3-(1H-3-indolyl)-2,5-pyrrolidinedione (**4**). m.p.: 108–111℃. ^{1}H-NMR(DMSO-d_6): 2.72–2.77 (dd, *J* = 5.5 Hz, 1H, H), 3.14–3.20 (dd, *J* = 9.5 Hz, 1H), 4.3–4.33 (m, 1H), 6.96–6.98 (m, 1H, ArH), 7.07–7.10 (m, 1H, ArH), 7.29–7.30 (d, *J* = 2.5 Hz, 1H, ArH), 7.35–7.36 (d, *J* = 8 Hz, 1H, ArH), 7.40–7.41 (d, *J* = 7.5 Hz, 1H, ArH), 10.9 (s, 1H, maleimide NH), 11.2 (s, 1H, indole NH). FAB MS: m/z = 214.16 $[M]^+$, $C_{12}H_{10}N_2O_2 \cdot 3 / 4\ H_2O$, calc. (%): H; 5.09, C; 63.29, N; 12.30. Found (%): H; 4.96, C; 63.17, N; 11.54.

3-(1H-3-indolyl)-2,5-dihydro-1H-2,5-pyrroledione (**7**). m.p.: 200–203℃. ^{1}H-NMR (DMSO–d_6): 6.76 (s, 1H, Olefin H), 7.17–7.26 (m, 2H, ArH), 7.50–7.51 (d, *J* = 7.5 Hz, 1H, ArH), 7.93–7.95 (d, *J* = 8 Hz, 1H, ArH), 8.33–8.34 (d, *J* = 3 Hz, 1H, ArH), 10.70 (s, 1H, maleimide NH), 11.97 (s, 1H, indole NH), FAB MS: m/z = 213.15 $[M+H]^+$, $C_{12}H_8N_2O_2$, calc. (%): H; 3.80, C; 67.92, N; 13.20. Found (%): H; 3.92, C; 67.69, N; 13.05.

Methyl-3-(indole-3-yl)pyruvic acid (**13**). m.p.: 165–168℃. ^{1}H-NMR(DMSO–d_6): 3.78 (s, 1H, -OCH_3), 6.81 (s, 1H, ArH), 7.04–7.07 (t, *J* = 7.5 Hz, 1H,ArH), 7.11–7.14 (t, *J* = 7.5 Hz, 1H, ArH), 7.39–7.40 (d, *J* = 8 Hz, 1H,ArH), 7.69–7.71 (d, *J* = 8 Hz, 1H, ArH), 7.879–7.884 (d, *J* = 2.5 Hz, 1H, -CH_2-), 8.916–8.919 (d, *J* = 1.5 Hz, 1H, -CH_2-), 11.39 (s, 1H, indole NH), FAB MS: m/z = 217.14 $[M+H]^+$, $C_{12}H_{11}NO_3$, calc. (%): C; 66.35, H; 5.10, N; 6.45. Found (%): C; 66.27, H; 5.15, N; 6.44.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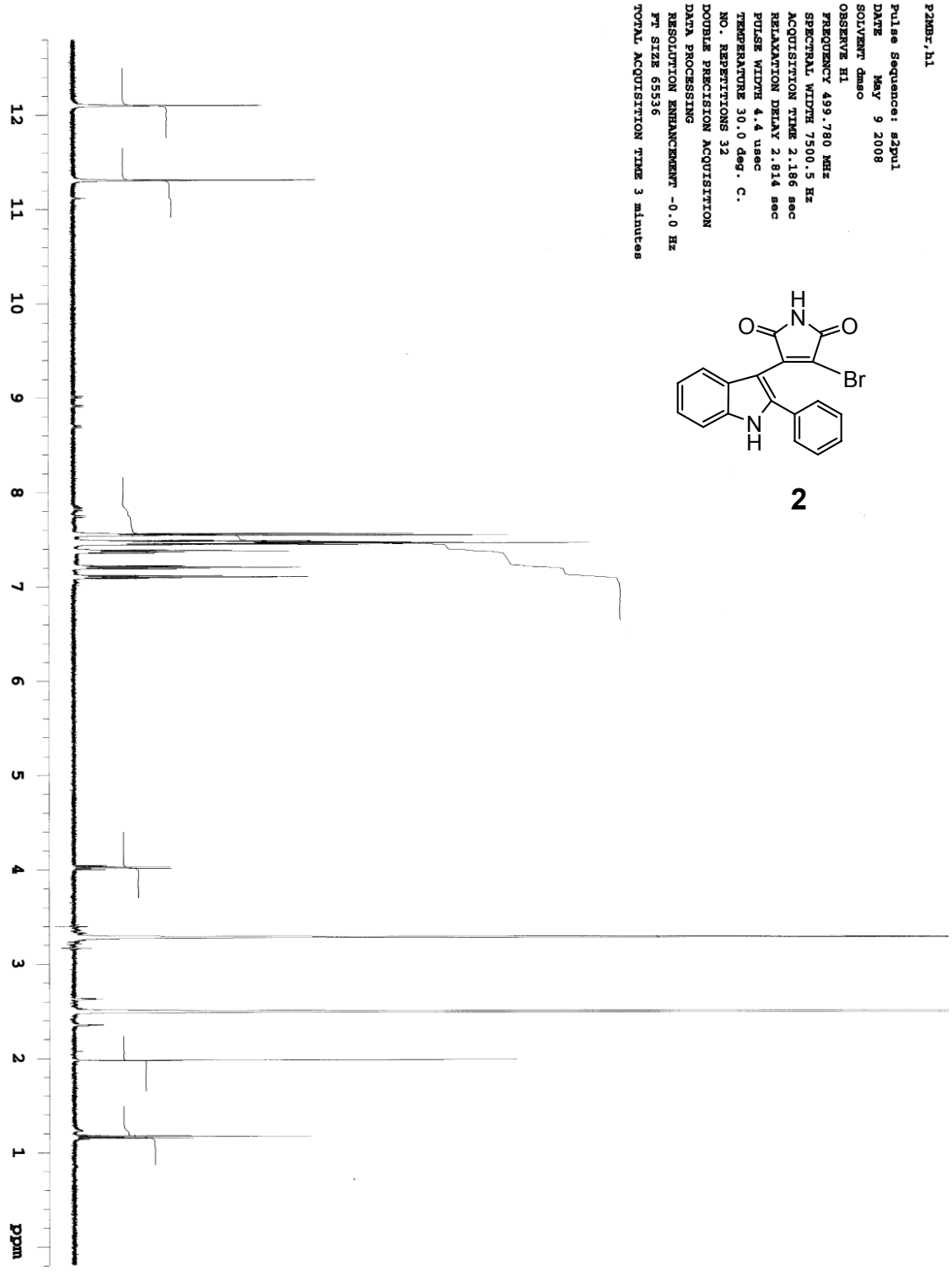
RELAXATION DELAY 2.814 sec
PULSE WIDTH 4.5 usec
TEMPERATURE 30.0 deg. C.
NO. REPETITIONS 32
DOUBLE PRECISION ACQUISITION
DATA PROCESSING
RESOLUTION ENHANCEMENT -0.0 Hz
FT SIZE 65536
TOTAL ACQUISITION TIME 3 minutes
O
H
N
O
Br
N
H
1
12
11
10
9
8
7
6
5
4
3
2
1
ppm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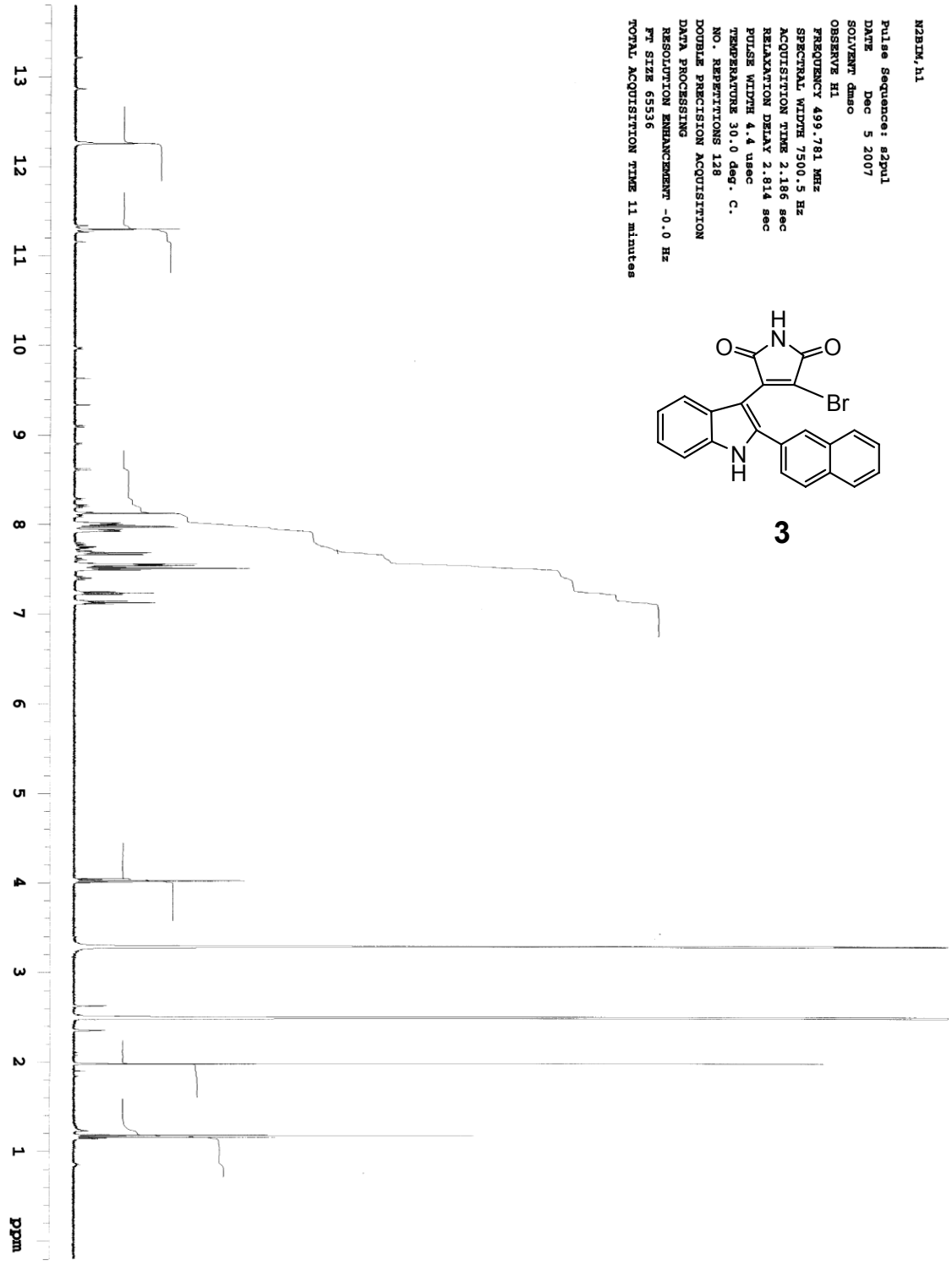
DATE May 9 2008
SOLVENT dmso
OBSERVE H1
FREQUENCY 499.780 MHz
SPECTRAL WIDTH 7500.5 Hz
ACQUISITION TIME 2.186 sec
RELAXATION DELAY 2.814 sec
PULSE WIDTH 4.4 usec
TEMPERATURE 30.0 deg. C.
NO. REPETITIONS 32
DOUBLE PRECISION ACQUISITION
DATA PROCESSING
RESOLUTION ENHANCEMENT -0.0 Hz
FT SIZE 65536
TOTAL ACQUISITION TIME 3 minutes
H
N
O
O
Br
N
H
2
12
11
10
9
8
7
6
5
4
3
2
1
ppm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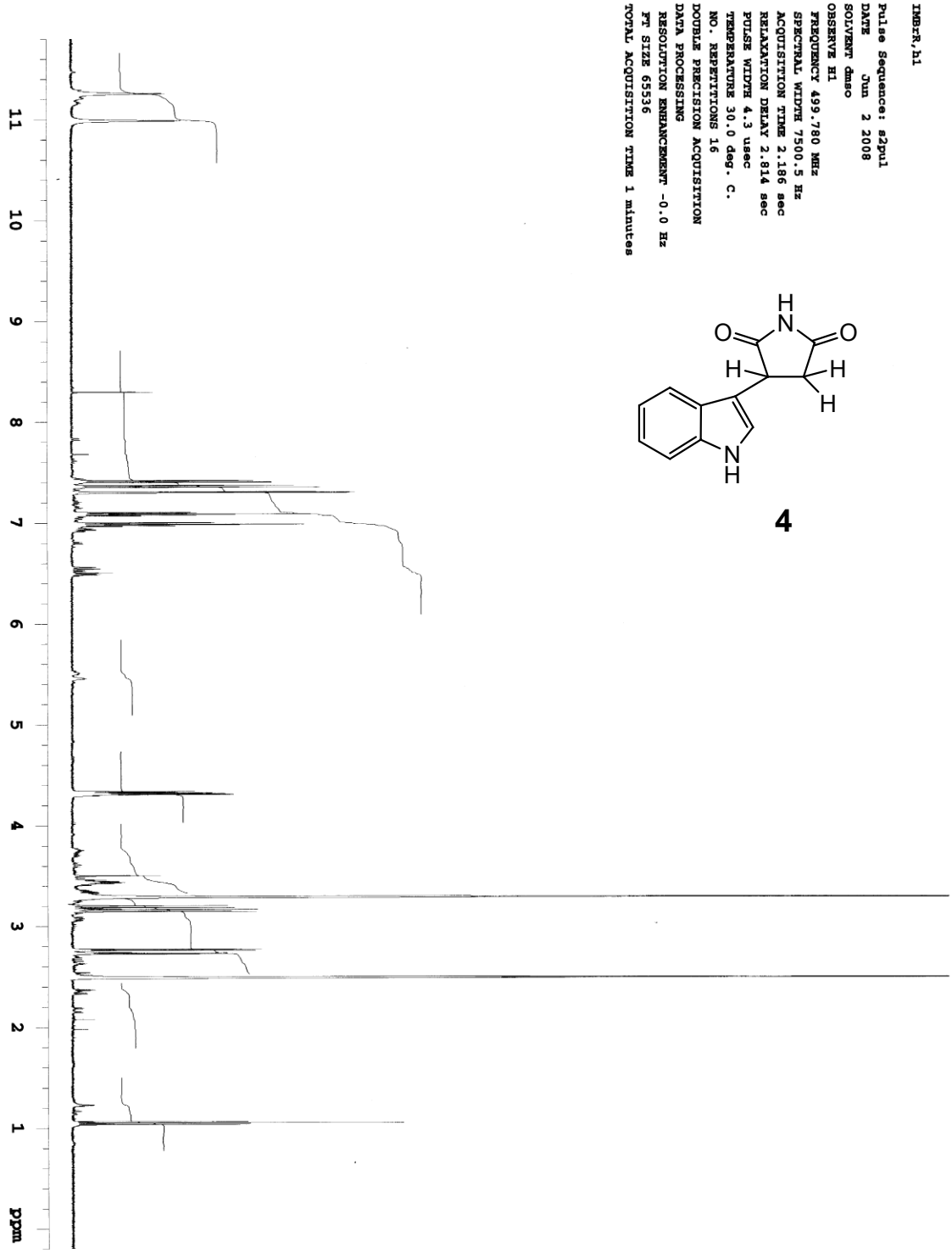
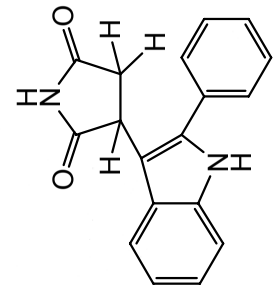
ACQUISITION TIME 2.186 sec
RELAXATION DELAY 2.814 sec
PULSE WIDTH 4.4 usec
TEMPERATURE 30.0 deg. C.
NO. REPETITIONS 128
DOUBLE PRECISION ACQUISITION
DATA PROCESSING
RESOLUTION ENHANCEMENT -0.0 Hz
FT SIZE 65536
TOTAL ACQUISITION TIME 11 minutes
O
N
H
O
Br
N
H
3
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm


IMBrR.h1
Pulse Sequence: s2pul
DATE Jun 2 2008
SOLVENT dmso
OBSERVE H1
FREQUENCY 499.780 MHz
SPECTRAL WIDTH 7500.5 Hz
ACQUISITION TIME 2.186 sec
RELAXATION DELAY 2.814 sec
PULSE WIDTH 4.3 usec
TEMPERATURE 30.0 deg. C.
NO. REPETITIONS 16
DOUBLE PRECISION ACQUISITION
DATA PROCESSING
RESOLUTION ENHANCEMENT -0.0 Hz
FT SIZE 65536
TOTAL ACQUISITION TIME 1 minutes
H
N
O
O
H
H
H
N
H
4
11
10
9
8
7
6
5
4
3
2
1
ppm

P2MBrR_2,h1

Pulse Sequence: s2pul
DATE Sep 17 2008
SOLVENT dmso
OBSERVE H1
FREQUENCY 499.781 MHz
SPECTRAL WIDTH 7500.5 Hz
ACQUISITION TIME 2.186 sec
RELAXATION DELAY 2.814 sec
PULSE WIDTH 4.1 usec
TEMPERATURE 30.0 deg. C.
NO. REPETITIONS 32
DOUBLE PRECISION ACQUISITION
DATA PROCESSING
RESOLUTION ENHANCEMENT -0.0 Hz
FT SIZE 65536
TOTAL ACQUISITION TIME 3 minutes



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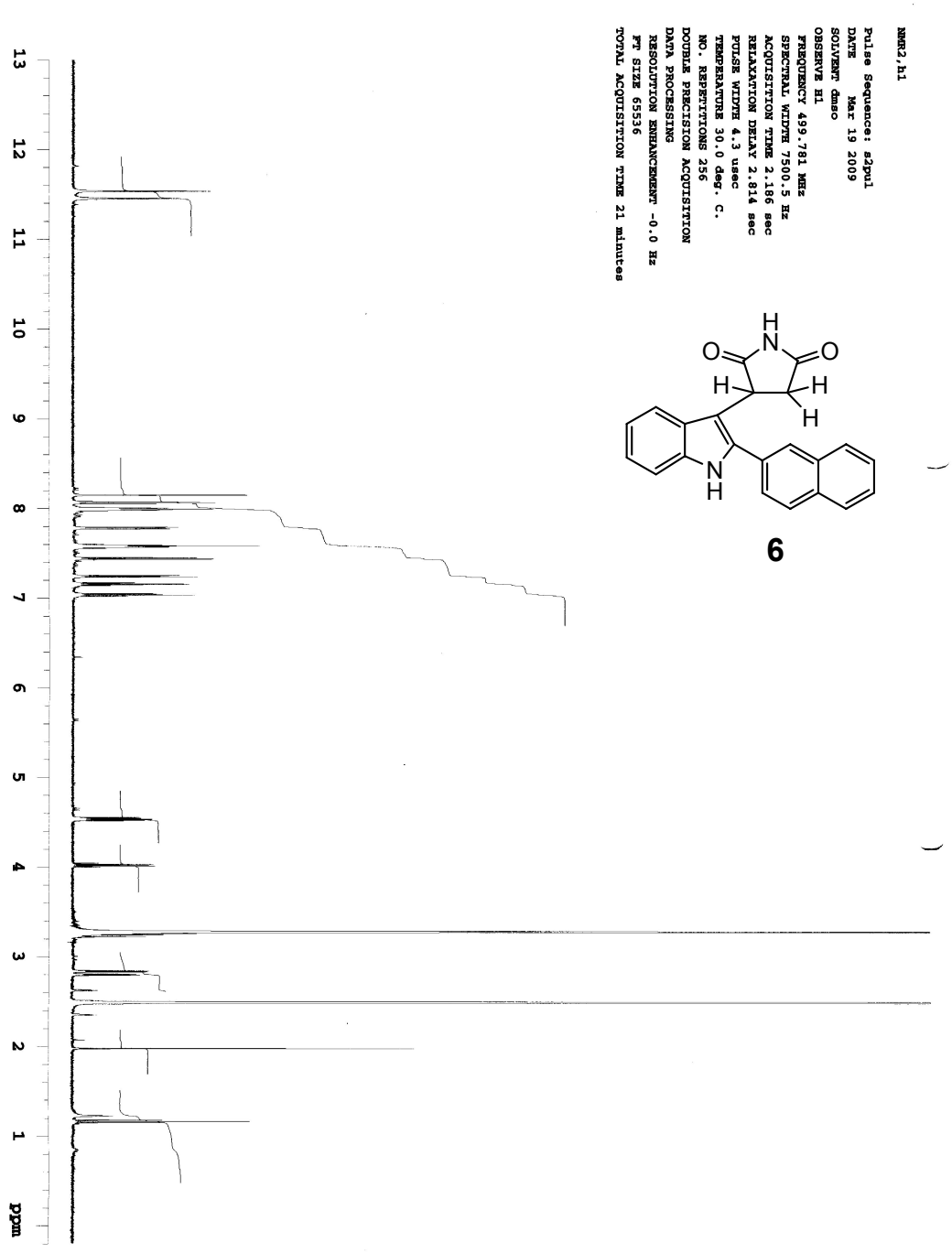
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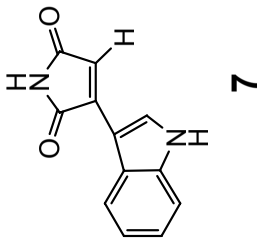
FREQUENCY 499.781 MHz
SPECTRAL WIDTH 7500.5 Hz
ACQUISITION TIME 2.186 sec
RELAXATION DELAY 2.814 sec
PULSE WIDTH 4.3 usec
TEMPERATURE 30.0 deg. C.
NO. REPETITIONS 256
DOUBLE PRECISION ACQUISITION
DATA PROCESSING
RESOLUTION ENHANCEMENT -0.0 Hz
FT SIZE 65536
TOTAL ACQUISITION TIME 21 minutes
H
N
O
O
H
H
H
N
H
6
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm

IMBrO,h1

Pulse Sequence: s2pul
DATE Jun 4 2008
SOLVENT dmso
OBSERVE H1
FREQUENCY 499.780 MHz
SPECTRAL WIDTH 7500.5 Hz
ACQUISITION TIME 2.186 sec
RELAXATION DELAY 2.814 sec
PULSE WIDTH 4.3 usec
TEMPERATURE 30.0 deg. C.
NO. REPETITIONS 20
DOUBLE PRECISION ACQUISITION
DATA PROCESSING
RESOLUTION ENHANCEMENT -0.0 Hz
FT SIZE 65536
TOTAL ACQUISITION TIME 2 minutes



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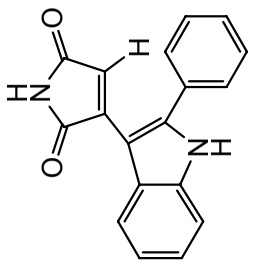
P2MBrO_1,h1

Pulse Sequence: s2pul
DATE Oct 21 2008
SOLVENT dmso
OBSERVE H1
FREQUENCY 499.781 MHz
SPECTRAL WIDTH 7500.5 Hz
ACQUISITION TIME 2.186 sec
RELAXATION DELAY 2.814 sec
PULSE WIDTH 4.4 usec
TEMPERATURE 30.0 deg. C.
NO. REPETITIONS 32
DOUBLE PRECISION ACQUISITION
DATA PROCESSING
RESOLUTION ENHANCEMENT -0.0 Hz
FT SIZE 65536
TOTAL ACQUISITION TIME 3 minutes



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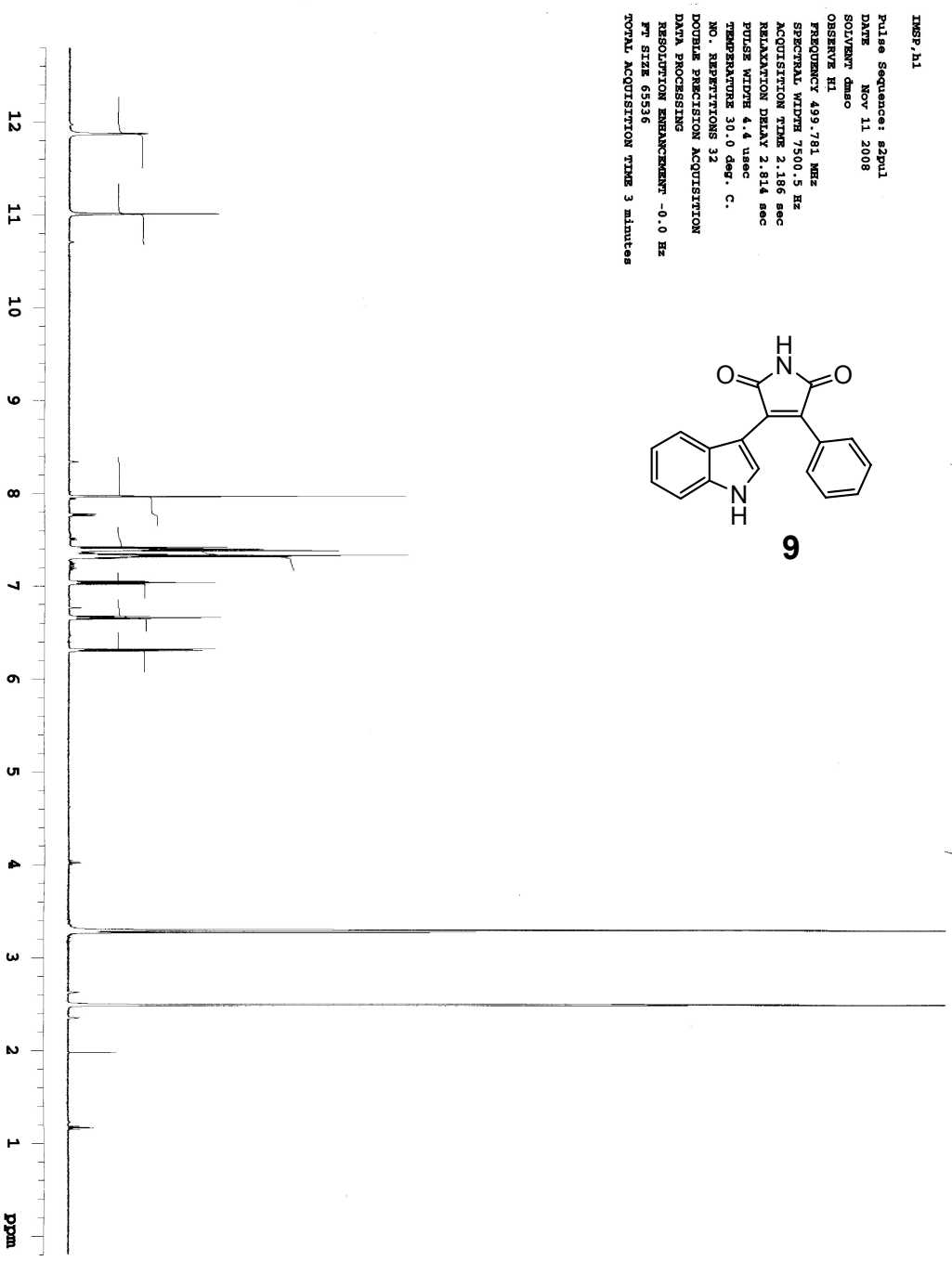
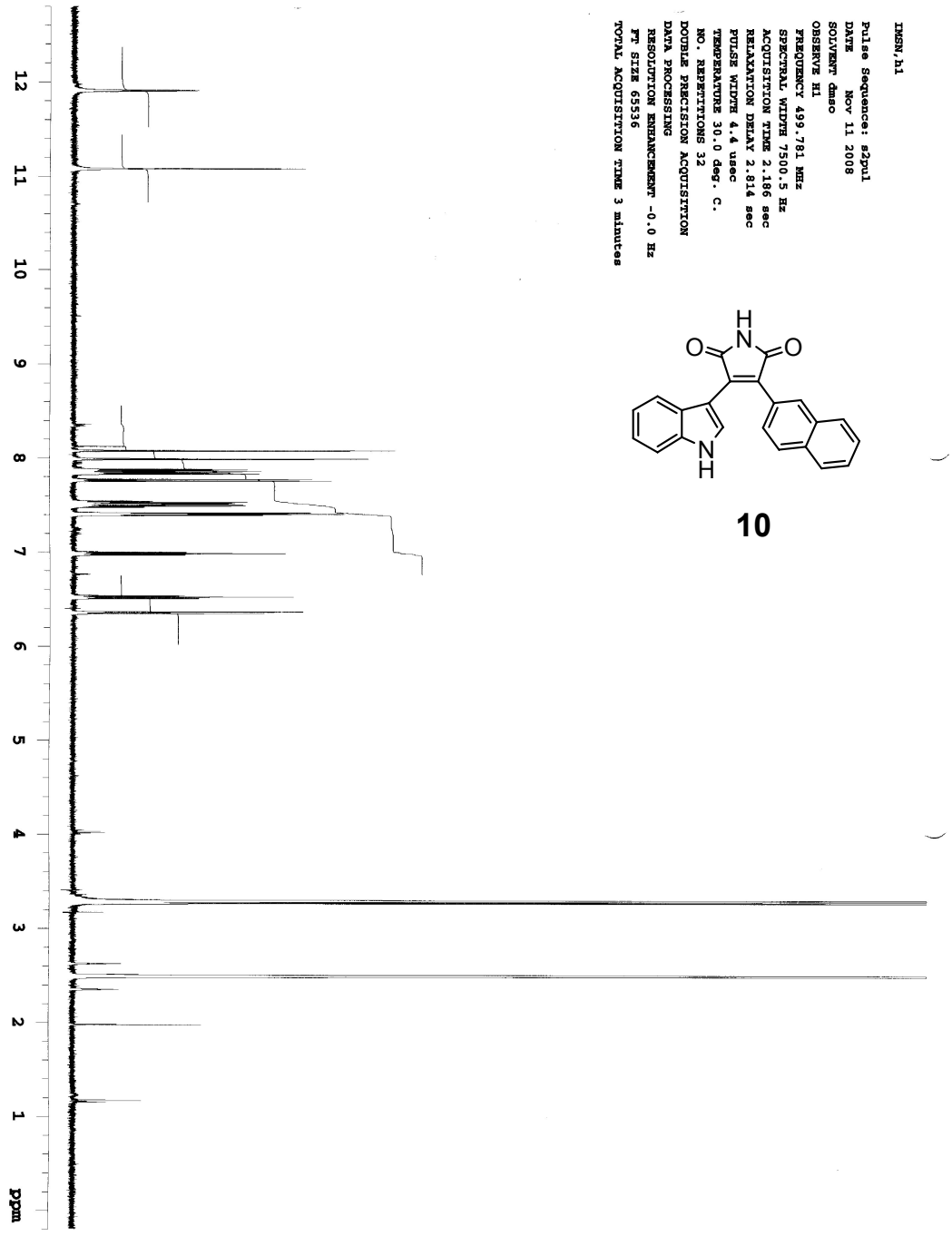

IMSP.h1
Pulse Sequence: s2pul
DATE Nov 11 2008
SOLVENT dmso
OBSERVE H1
FREQUENCY 499.781 MHz
SPECTRAL WIDTH 7500.5 Hz
ACQUISITION TIME 2.186 sec
RELAXATION DELAY 2.814 sec
PULSE WIDTH 4.4 usec
TEMPERATURE 30.0 deg. C.
NO. REPETITIONS 32
DOUBLE PRECISION ACQUISITION
DATA PROCESSING
RESOLUTION ENHANCEMENT -0.0 Hz
FT SIZE 65536
TOTAL ACQUISITION TIME 3 minutes
H
N
O
O
N
H
9
12
11
10
9
8
7
6
5
4
3
2
1
ppm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SOLVENT dmso
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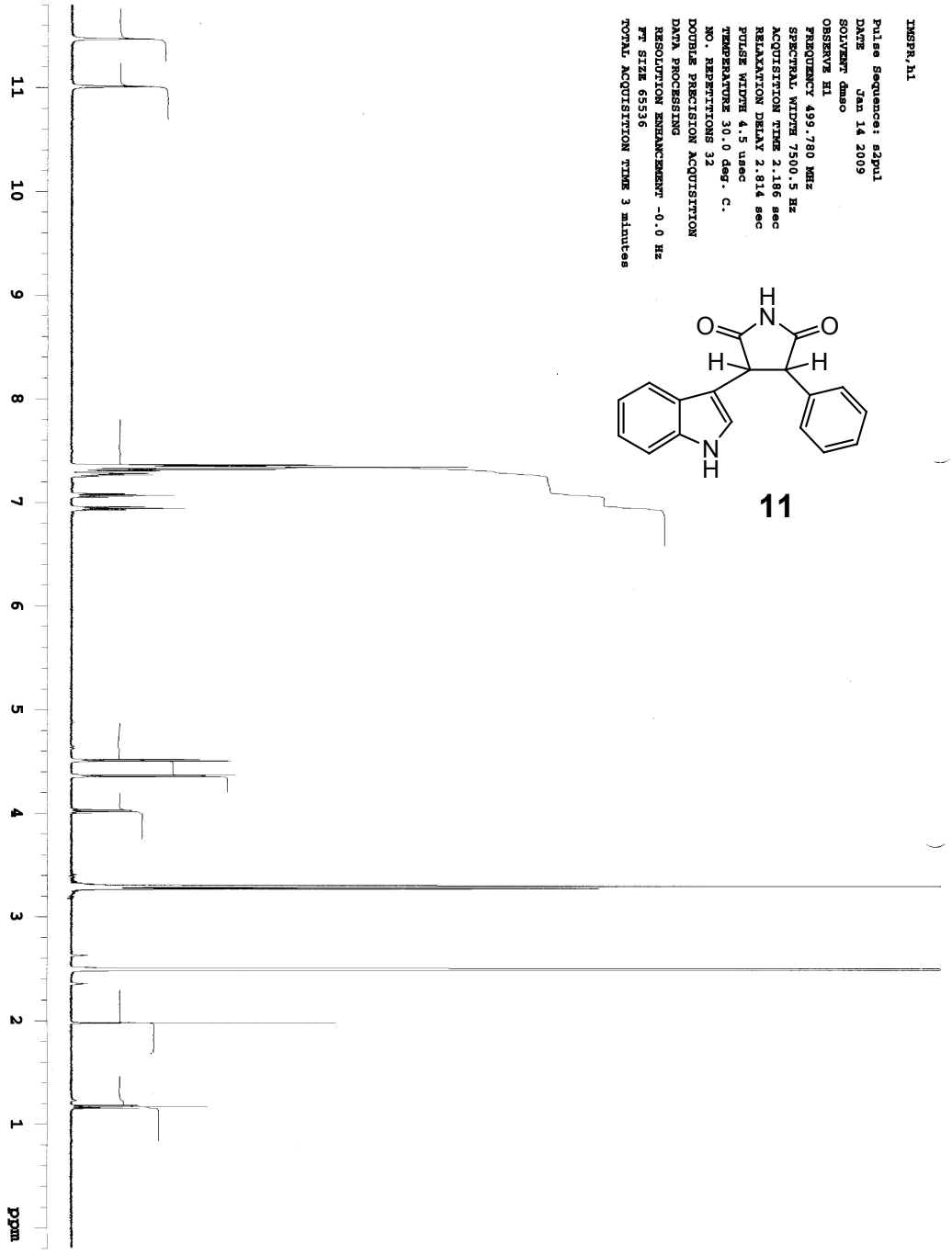
SPECTRAL WIDTH 7500.5 Hz
ACQUISITION TIME 2.186 sec
RELAXATION DELAY 2.814 sec
PULSE WIDTH 4.4 usec
TEMPERATURE 30.0 deg. C.
NO. REPETITIONS 32
DOUBLE PRECISION ACQUISITION
DATA PROCESSING
RESOLUTION ENHANCEMENT -0.0 Hz
FT SIZE 65536
TOTAL ACQUISITION TIME 3 minutes
O
N
H
O
O
NH
10
12
11
10
9
8
7
6
5
4
3
2
1
ppm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DATE Jan 14 2009
SOLVENT dmso
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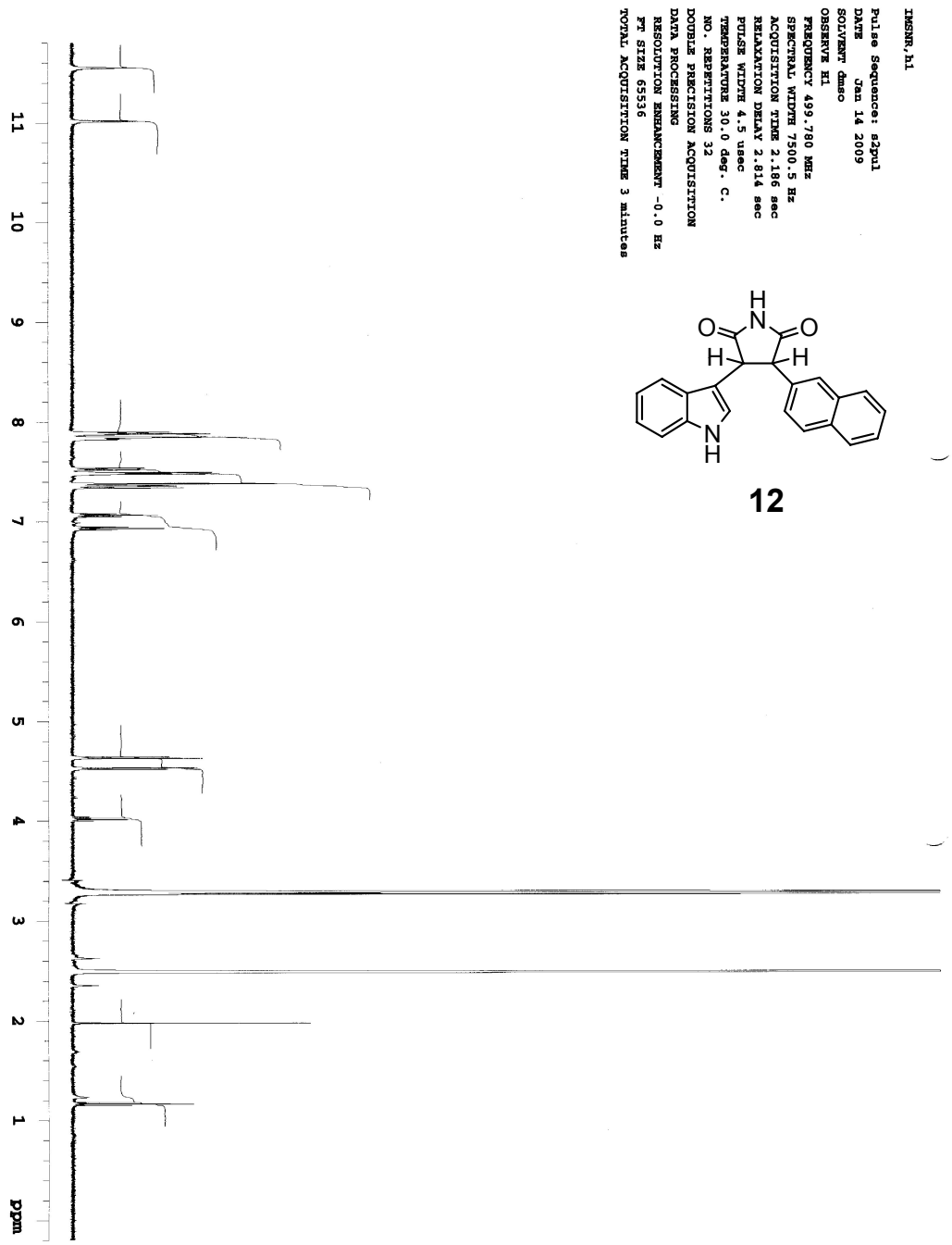
FREQUENCY 499.780 MHz
SPECTRAL WIDTH 7500.5 Hz
ACQUISITION TIME 2.186 sec
RELAXATION DELAY 2.814 sec
PULSE WIDTH 4.5 usec
TEMPERATURE 30.0 deg. C.
NO. REPETITIONS 32
DOUBLE PRECISION ACQUISITION
DATA PROCESSING
RESOLUTION ENHANCEMENT -0.0 Hz
FT SIZE 65536
TOTAL ACQUISITION TIME 3 minutes
H
N
O
O
H
H
N
H
11
11
10
9
8
7
6
5
4
3
2
1
ppm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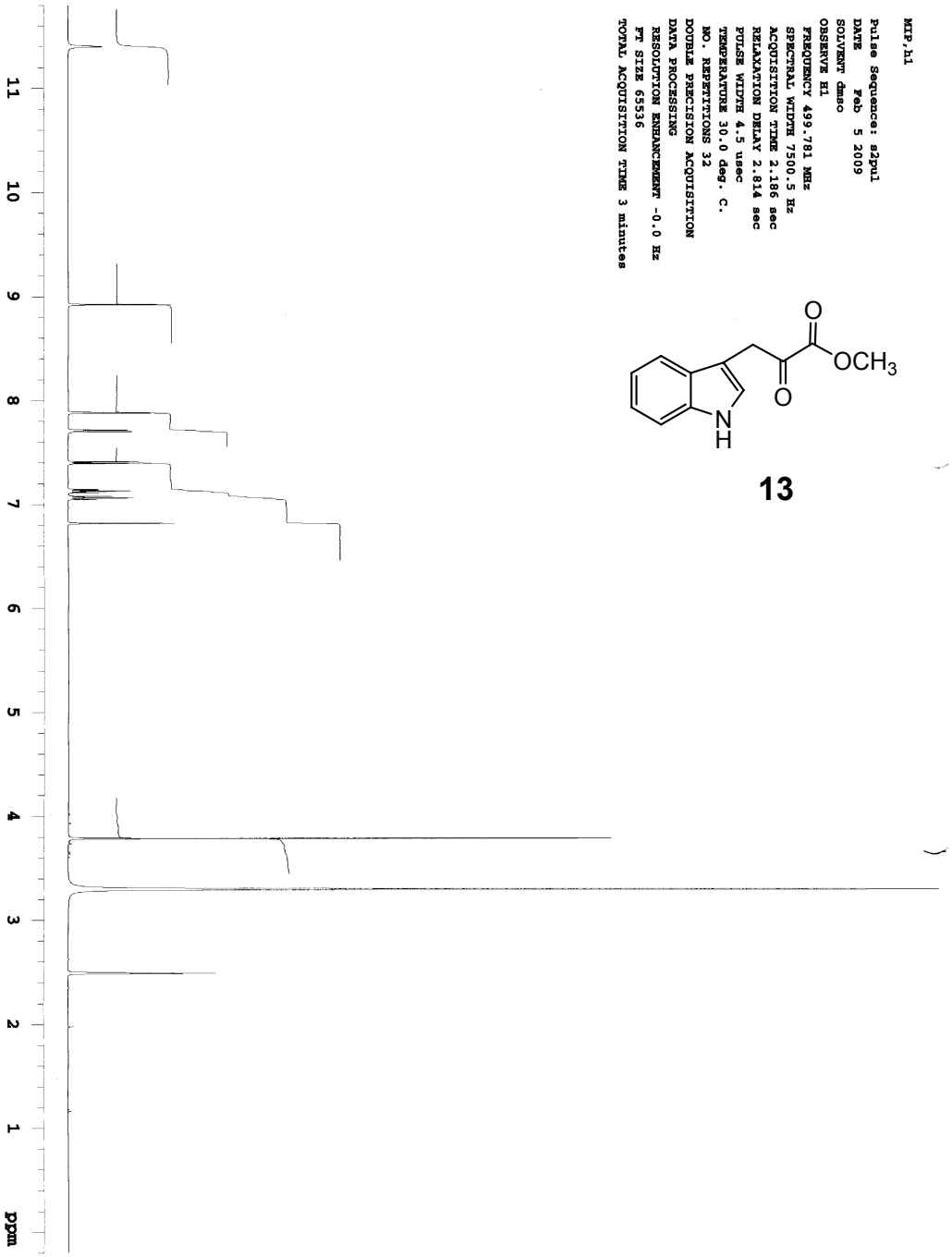
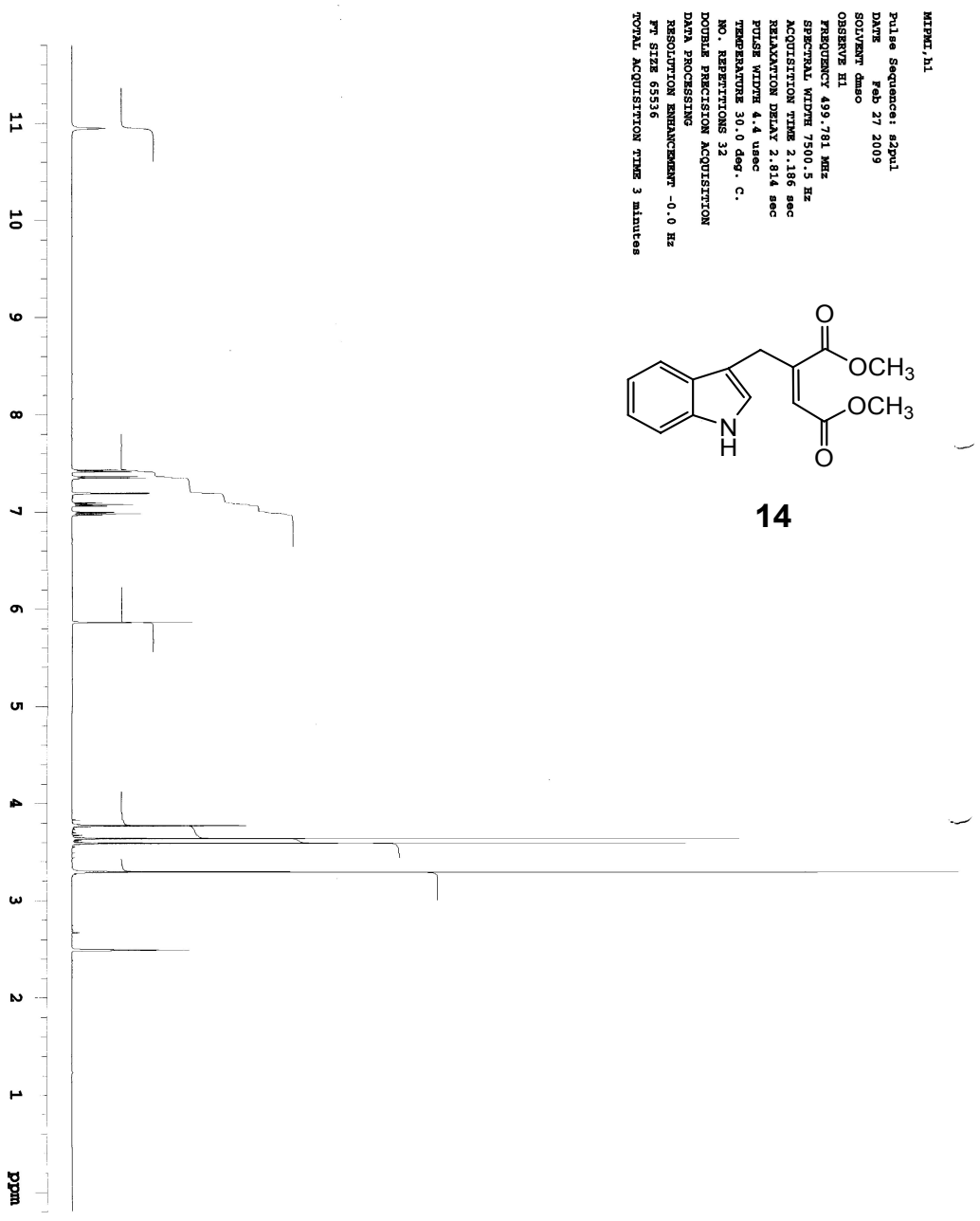
DATE Jan 14 2009
SOLVENT dmso
OBSERVE H1
FREQUENCY 499.780 MHz
SPECTRAL WIDTH 7500.5 Hz
ACQUISITION TIME 2.186 sec
RELAXATION DELAY 2.814 sec
PULSE WIDTH 4.5 usec
TEMPERATURE 30.0 deg. C.
NO. REPETITIONS 32
DOUBLE PRECISION ACQUISITION
DATA PROCESSING
RESOLUTION ENHANCEMENT -0.0 Hz
FT SIZE 65536
TOTAL ACQUISITION TIME 3 minutes
H
N
O
O
H
H
N
H
12
11
10
9
8
7
6
5
4
3
2
1
ppm


MIP,h1
Pulse Sequence: s2pul
DATE Feb 5 2009
SOLVENT dmso
OBSERVE H1
FREQUENCY 499.781 MHz
SPECTRAL WIDTH 7500.5 Hz
ACQUISITION TIME 2.186 sec
RELAXATION DELAY 2.814 sec
PULSE WIDTH 4.5 usec
TEMPERATURE 30.0 deg. C.
NO. REPETITIONS 32
DOUBLE PRECISION ACQUISITION
DATA PROCESSING
RESOLUTION ENHANCEMENT -0.0 Hz
FT SIZE 65536
TOTAL ACQUISITION TIME 3 minutes
O
OCH3
O
N
H
13
11
10
9
8
7
6
5
4
3
2
1
ppm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SOLVENT dmso
OBSERVE H1
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SPECTRAL WIDTH 7500.5 Hz
ACQUISITION TIME 2.186 sec
RELAXATION DELAY 2.814 sec
PULSE WIDTH 4.4 usec
TEMPERATURE 30.0 deg. C.
NO. REPETITIONS 32
DOUBLE PRECISION ACQUISITION
DATA PROCESSING
RESOLUTION ENHANCEMENT -0.0 Hz
FT SIZE 65536
TOTAL ACQUISITION TIME 3 minutes
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OCH3
OCH3
O
NH
14
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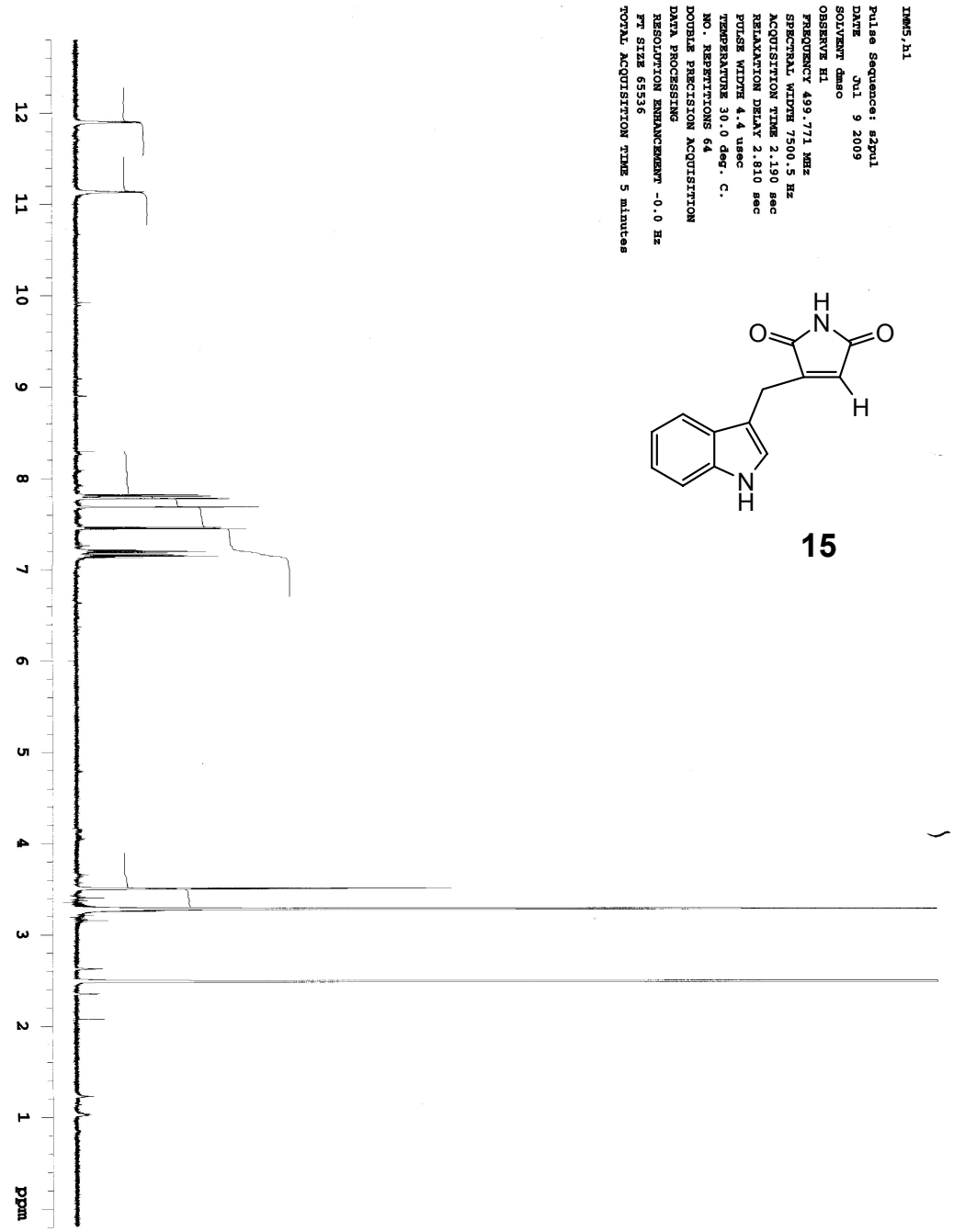
10
9
8
7
6
5
4
3
2
1
ppm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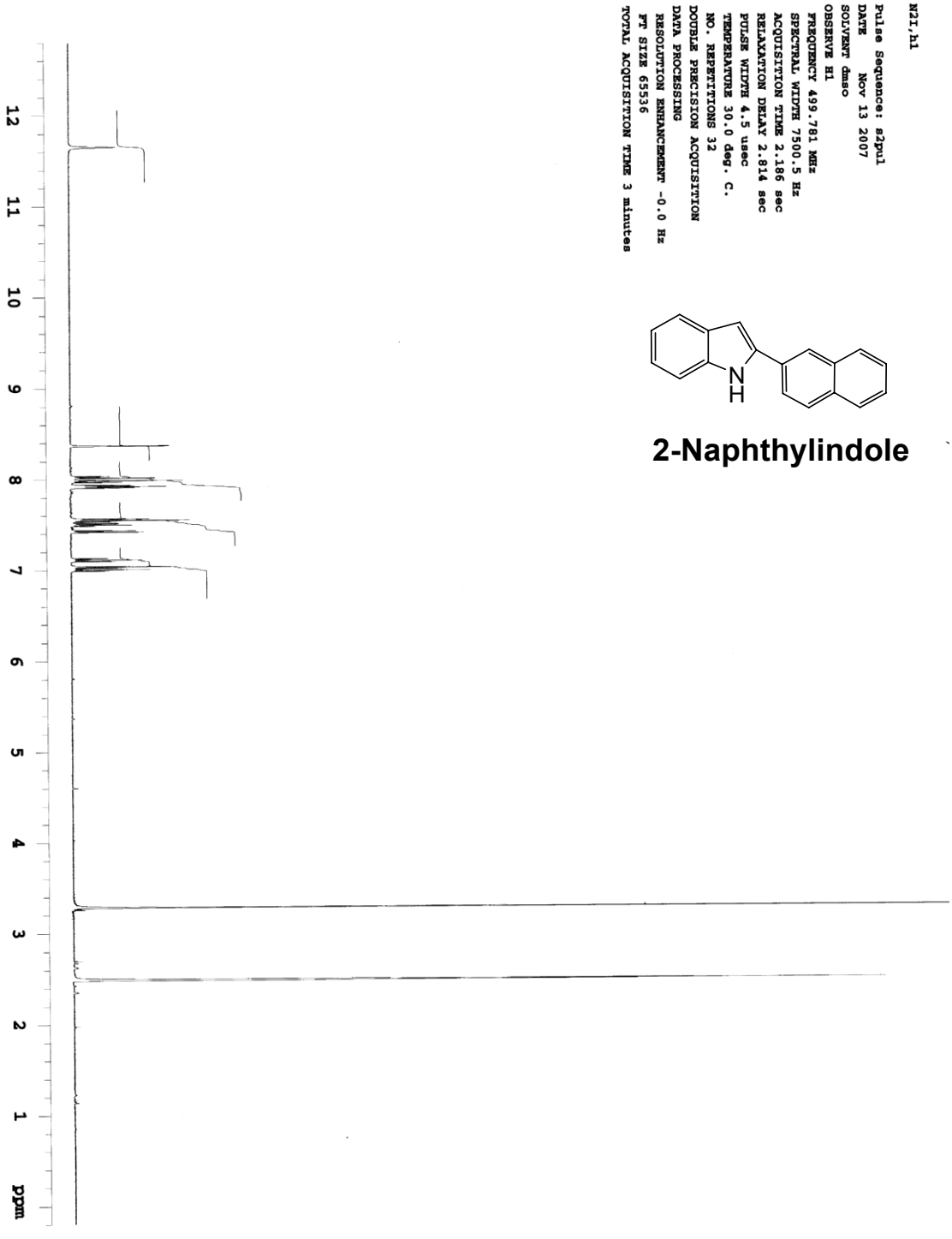
DATE Jul 9 2009
SOLVENT dmso
OBSERVE H1
FREQUENCY 499.771 MHz
SPECTRAL WIDTH 7500.5 Hz
ACQUISITION TIME 2.190 sec
RELAXATION DELAY 2.910 sec
PULSE WIDTH 4.4 usec
TEMPERATURE 30.0 deg. C.
NO. REPETITIONS 64
DOUBLE PRECISION ACQUISITION
DATA PROCESSING
RESOLUTION ENHANCEMENT -0.0 Hz
FT SIZE 65536
TOTAL ACQUISITION TIME 5 minutes
H
N
O
O
H
N
H
15
12
11
10
9
8
7
6
5
4
3
2
1
ppm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SPECTRAL WIDTH 7500.5 Hz
ACQUISITION TIME 2.186 sec
RELAXATION DELAY 2.814 sec
PULSE WIDTH 4.5 usec
TEMPERATURE 30.0 deg. C.
NO. REPETITIONS 32
DOUBLE PRECISION ACQUISITION
DATA PROCESSING
RESOLUTION ENHANCEMENT -0.0 Hz
FT SIZE 65536
TOTAL ACQUISITION TIME 3 minutes
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2-Naphthylindole
12
11
10
9
8
7
6
5
4
3
2
1
ppm

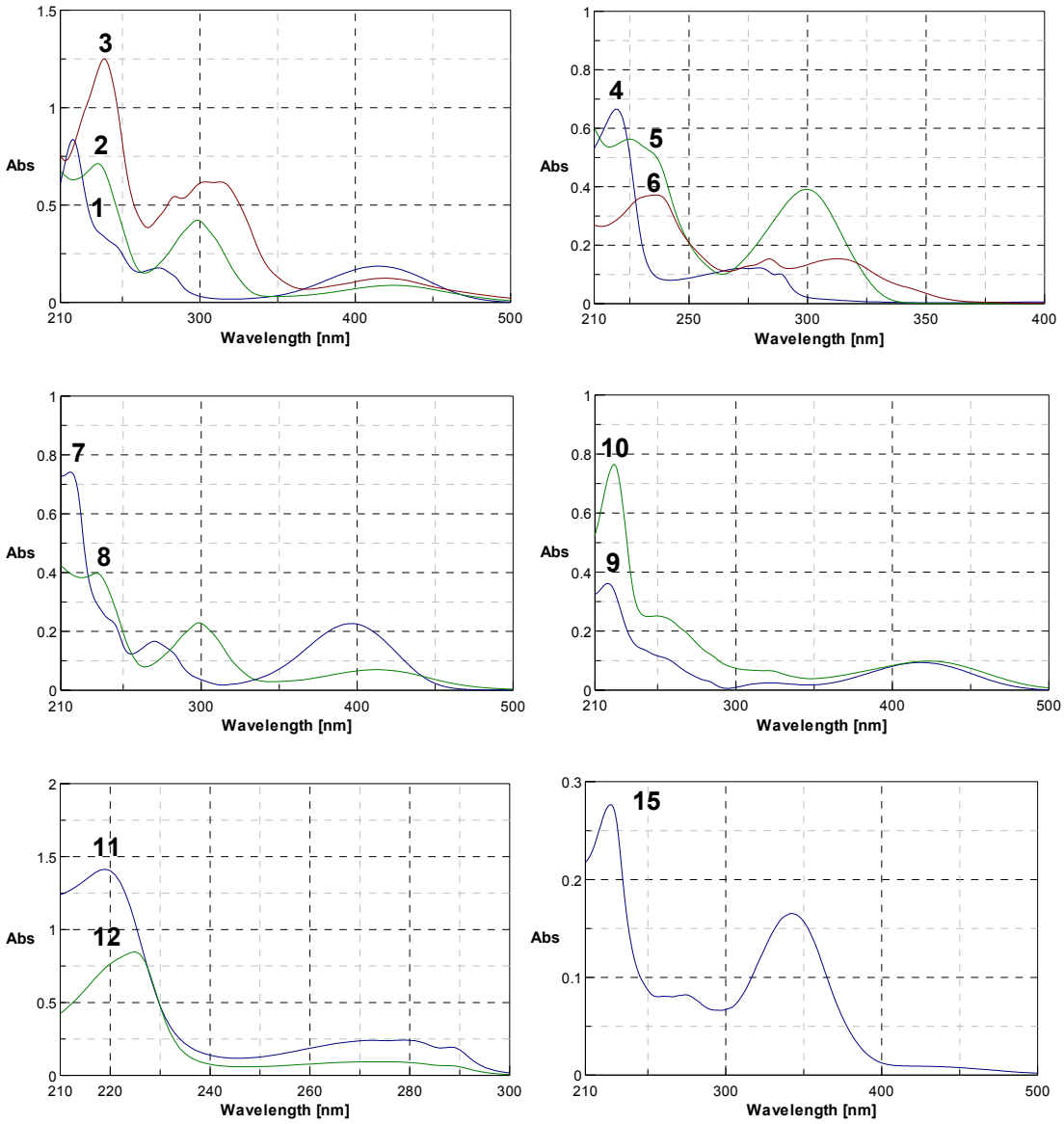
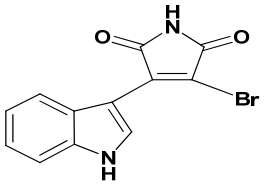
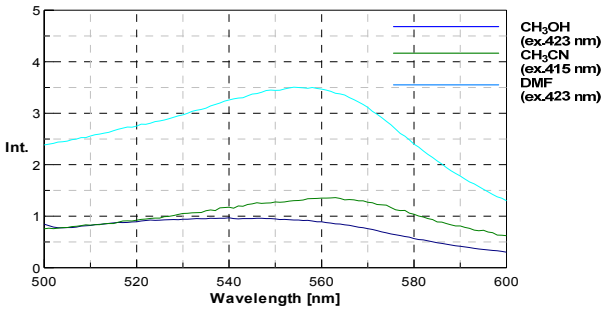


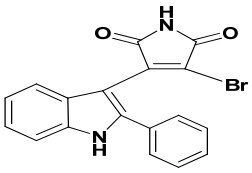
Fig. S1. Absorption spectra of compounds **1–12** and **15** in CH_3CN

The concentration of compounds **1–5** and **7** is 0.02 mM. The concentration of compounds **6**, **8**, **9**, **10**, **12** and **15** is 0.01 mM. The concentration of compound **11** is 0.1 mM.

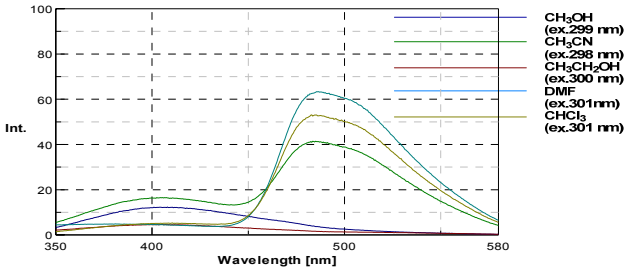

H
N
O
O
Br
N
H

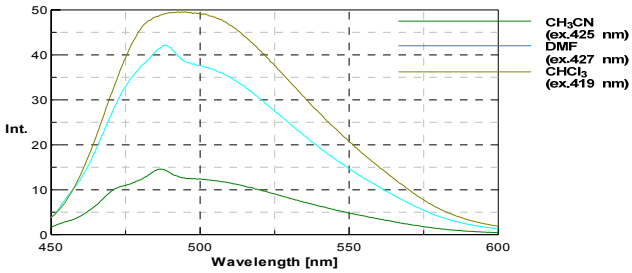
1

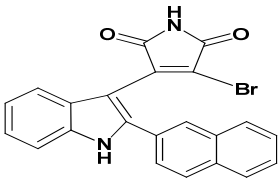

CH3OH
(ex.423 nm)
CH3CN
(ex.415 nm)
DMF
(ex.423 nm)
Int.
Wavelength [nm]


H
N
O
O
Br
N
H

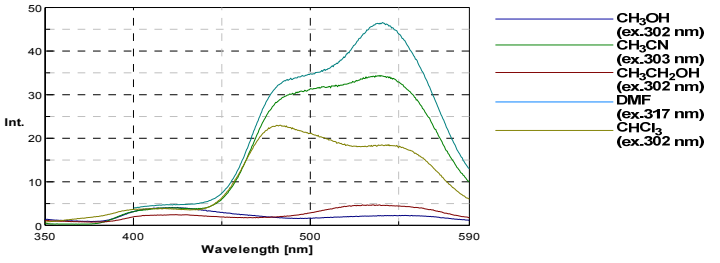
2

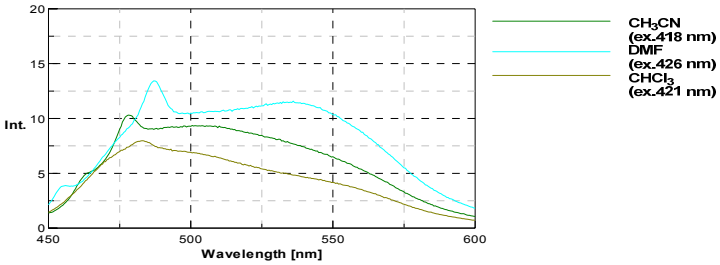

CH3OH
(ex.299 nm)
CH3CN
(ex.298 nm)
CH3CH2OH
(ex.300 nm)
DMF
(ex.301nm)
CHCl3
(ex.301 nm)
Int.
Wavelength [nm]

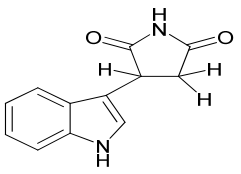

CH3CN
(ex.425 nm)
DMF
(ex.427 nm)
CHCl3
(ex.419 nm)
Int.
Wavelength [nm]


H
N
O
O
Br
N
H

3


CH3OH
(ex.302 nm)
CH3CN
(ex.303 nm)
CH3CH2OH
(ex.302 nm)
DMF
(ex.317 nm)
CHCl3
(ex.302 nm)
Int.
Wavelength [nm]


CH3CN
(ex.418 nm)
DMF
(ex.426 nm)
CHCl3
(ex.421 nm)
Int.
Wavelength [nm]



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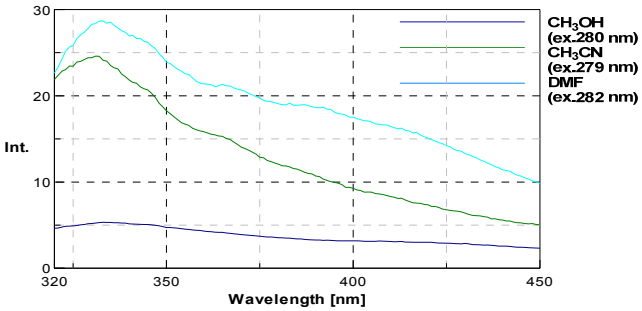
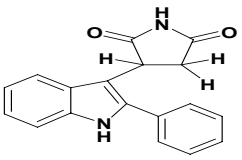

CH3OH
(ex.280 nm)
CH3CN
(ex.279 nm)
DMF
(ex.282 nm)
Int.
Wavelength [nm]



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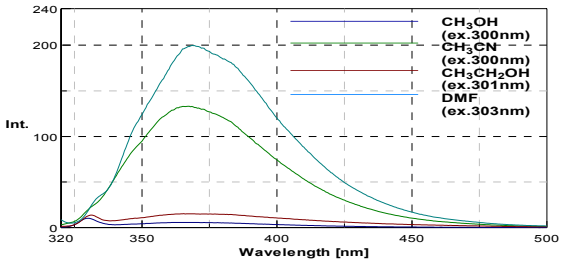
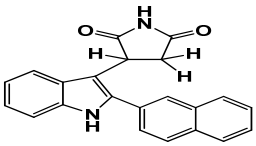

CH3OH
(ex.300nm)
CH3CN
(ex.300nm)
CH3CH2OH
(ex.301nm)
DMF
(ex.303nm)
Int.
Wavelength [nm]



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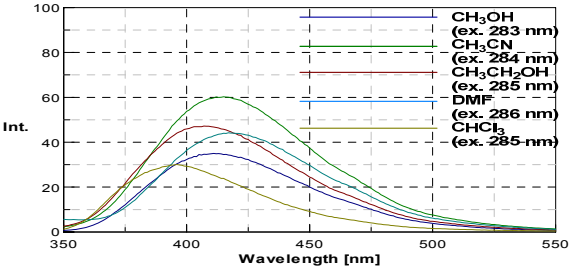
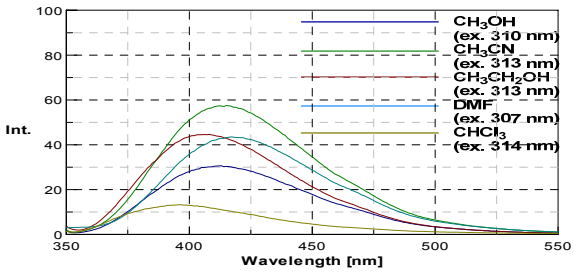
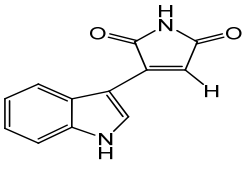

CH3OH
(ex. 283 nm)
CH3CN
(ex. 284 nm)
CH3CH2OH
(ex. 285 nm)
DMF
(ex. 286 nm)
CHCl3
(ex. 285 nm)
Int.
Wavelength [nm]


CH3OH
(ex. 310 nm)
CH3CN
(ex. 313 nm)
CH3CH2OH
(ex. 313 nm)
DMF
(ex. 307 nm)
CHCl3
(ex. 314 nm)
Int.
Wavelength [nm]



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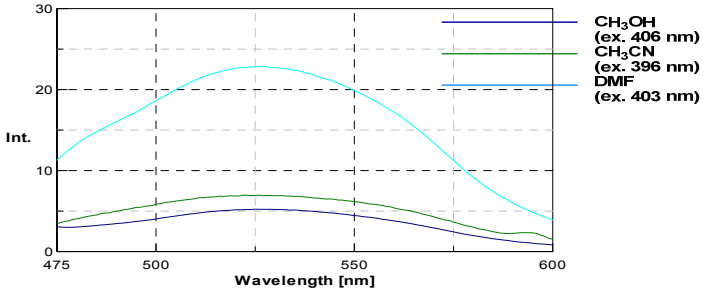
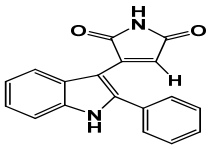

CH3OH
(ex. 406 nm)
CH3CN
(ex. 396 nm)
DMF
(ex. 403 nm)
Int.
Wavelength [nm]



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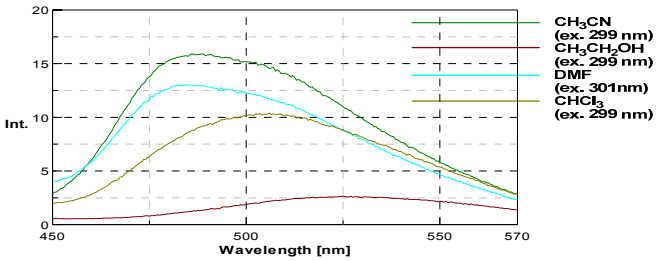
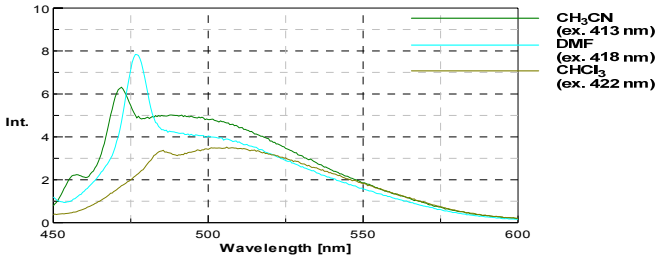
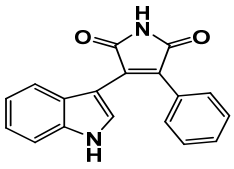

Int.
Wavelength [nm]
CH3CN
(ex. 299 nm)
CH3CH2OH
(ex. 299 nm)
DMF
(ex. 301nm)
CHCl3
(ex. 299 nm)


Int.
Wavelength [nm]
CH3CN
(ex. 413 nm)
DMF
(ex. 418 nm)
CHCl3
(ex. 422 nm)



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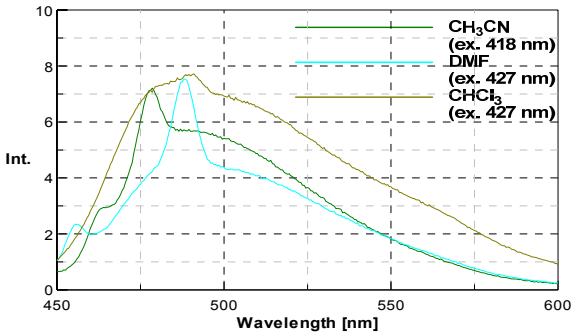
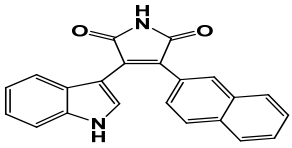

Int.
Wavelength [nm]
CH3CN
(ex. 418 nm)
DMF
(ex. 427 nm)
CHCl3
(ex. 427 nm)



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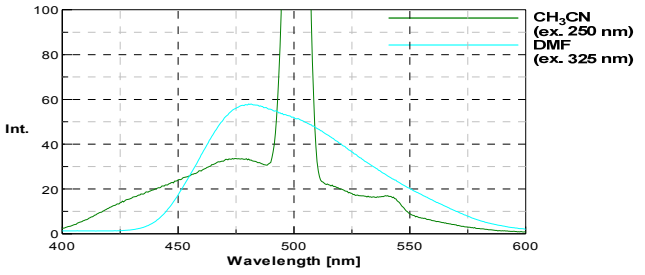
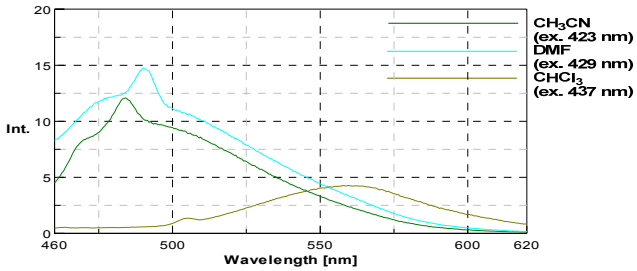

Int.
Wavelength [nm]
CH3CN
(ex. 250 nm)
DMF
(ex. 325 nm)


Int.
Wavelength [nm]
CH3CN
(ex. 423 nm)
DMF
(ex. 429 nm)
CHCl3
(ex. 437 nm)

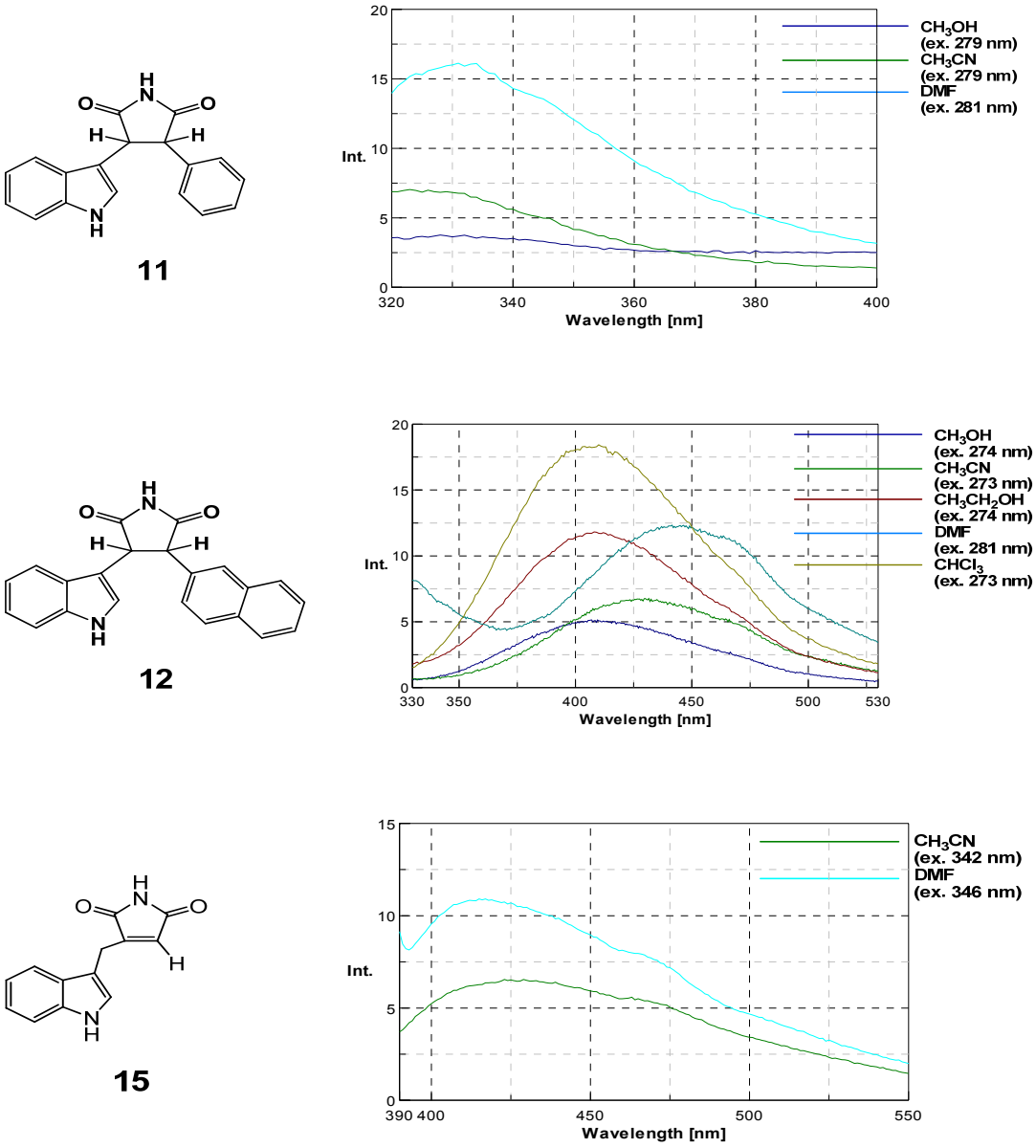
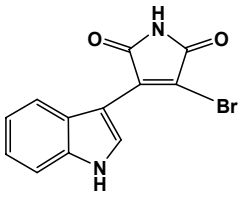
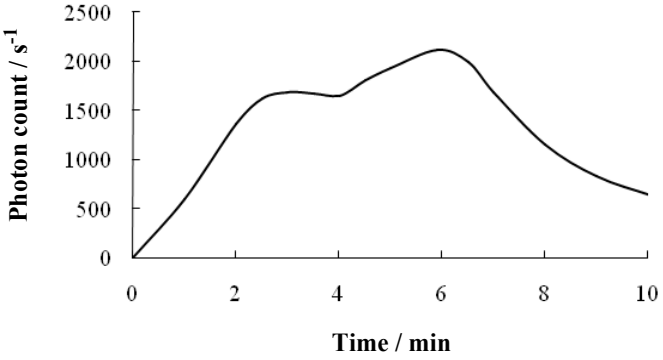


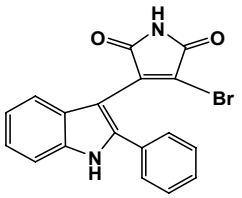
Fig. S2. FL spectra of compounds **1**–**12** and **15**

The concentration of compounds is 0.1 μM except for compounds **1**, **4**, **7**, **11** and **15** (10 μM).

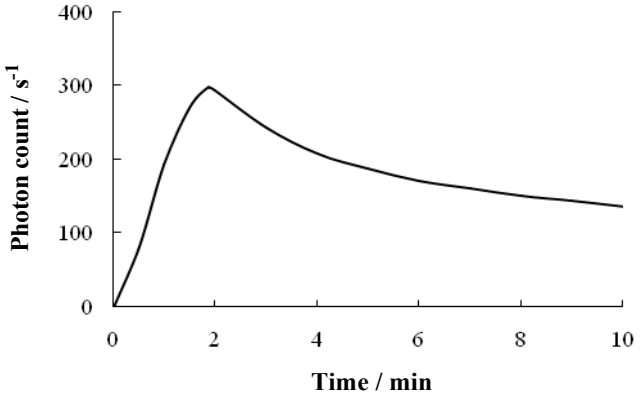

H
N
O
O
Br
N
H

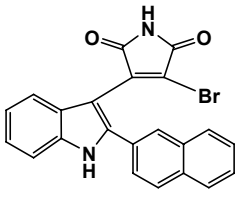
1


Photon count / s-1
2500
2000
1500
1000
500
0
0
2
4
6
8
10
Time / min

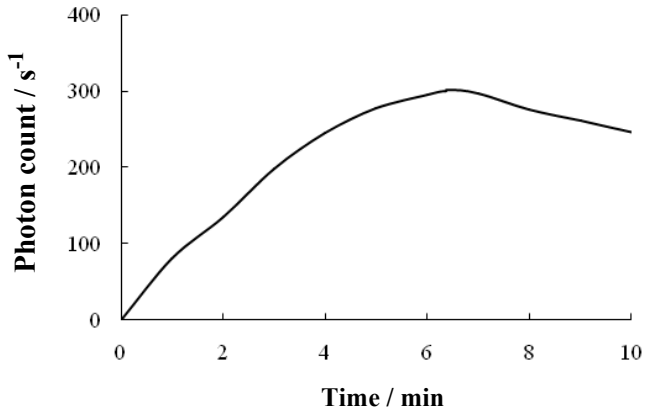

H
N
O
O
Br
N
H

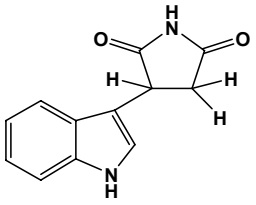
2


Photon count / s-1
400
300
200
100
0
0
2
4
6
8
10
Time / min

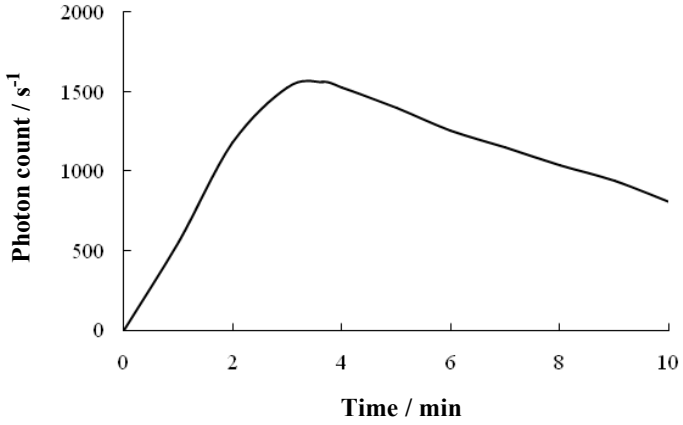

H
N
O
O
Br
N
H

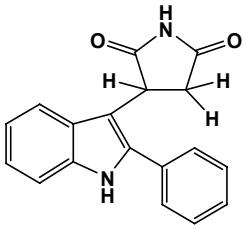
3


Photon count / s-1
400
300
200
100
0
0
2
4
6
8
10
Time / min

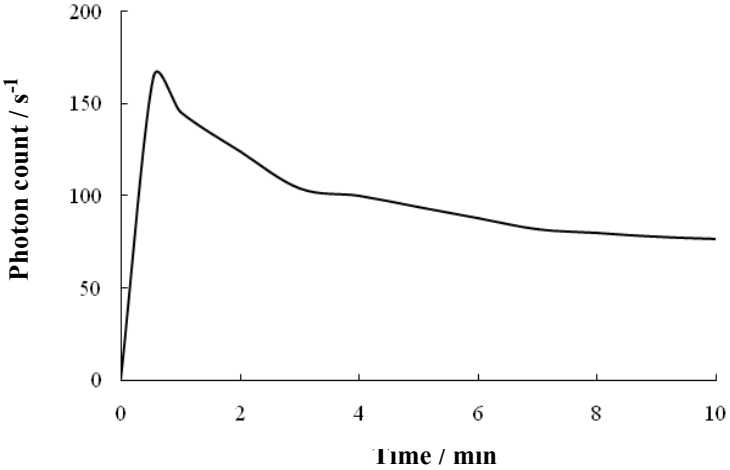

H
N
O
O
H
H
H
N
H

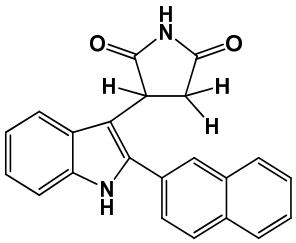
4


Photon count / s-1
2000
1500
1000
500
0
0
2
4
6
8
10
Time / min

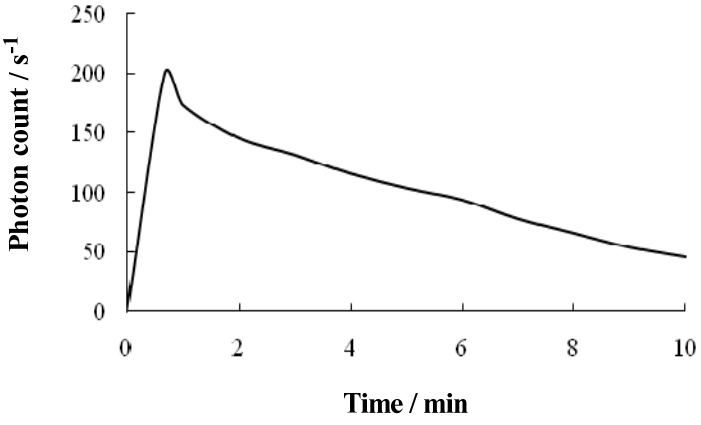

H
N
O
O
H
H
H
N
H

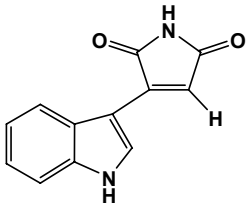
5


Photon count / s-1
200
150
100
50
0
0
2
4
6
8
10
Time / min

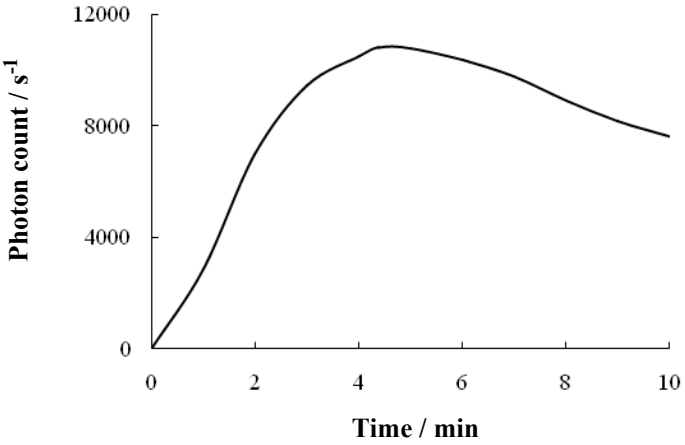

H
N
O
O
H
H
H
N
H

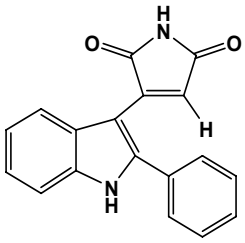
6


Photon count / s-1
250
200
150
100
50
0
0
2
4
6
8
10
Time / min

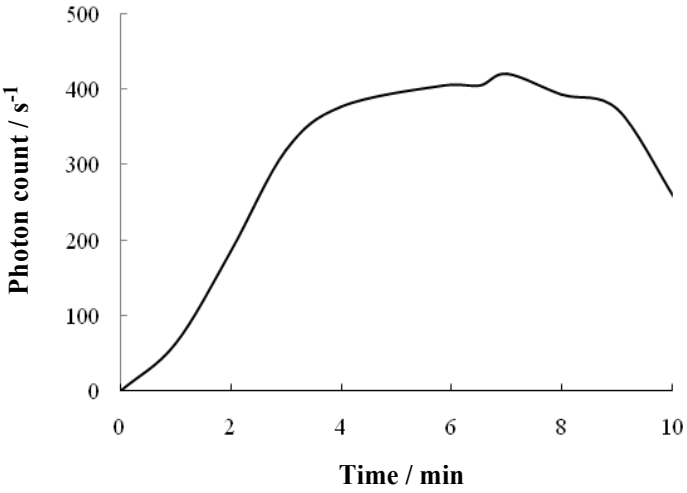


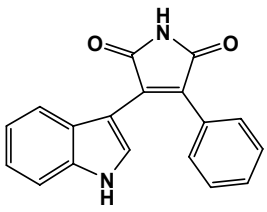
7


Photon count / s-1
12000
8000
4000
0
0
2
4
6
8
10
Time / min

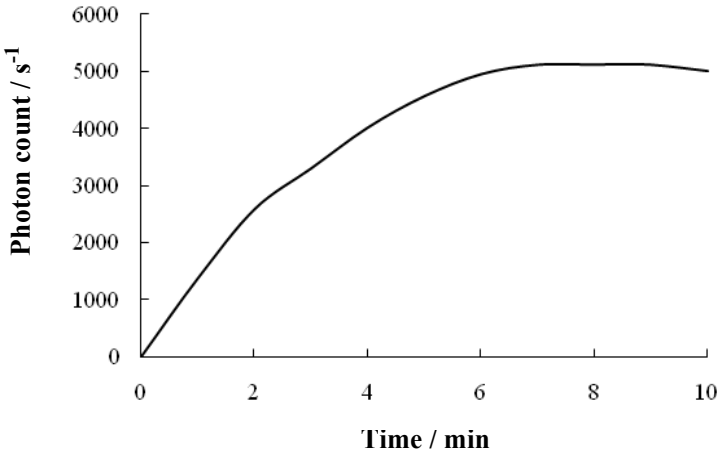


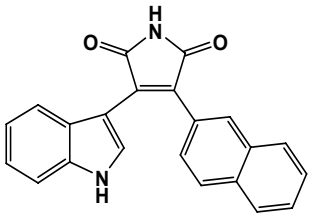
8


Photon count / s-1
500
400
300
200
100
0
0
2
4
6
8
10
Time / min



9


Photon count / s-1
6000
5000
4000
3000
2000
1000
0
0
2
4
6
8
10
Time / min



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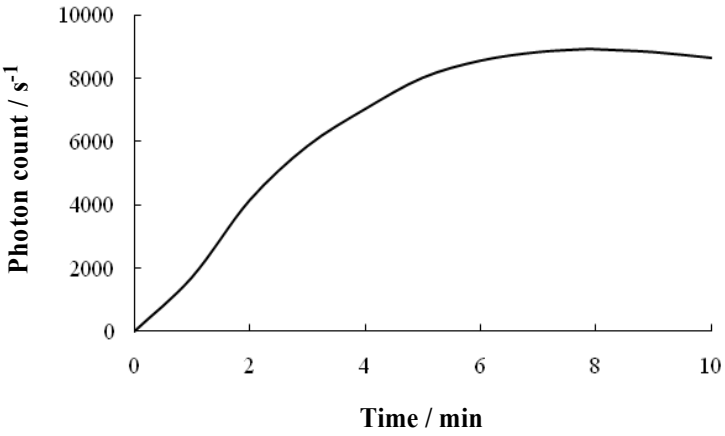
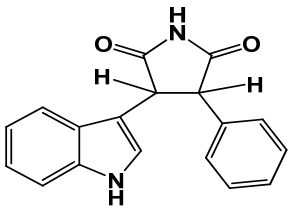
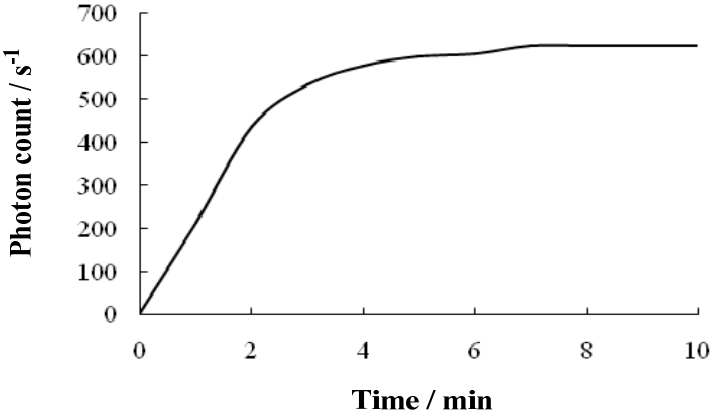
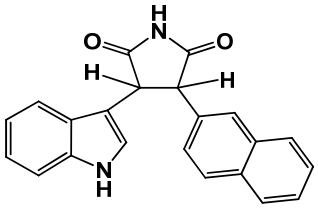

Photon count / s-1
10000
8000
6000
4000
2000
0
0
2
4
6
8
10
Time / min

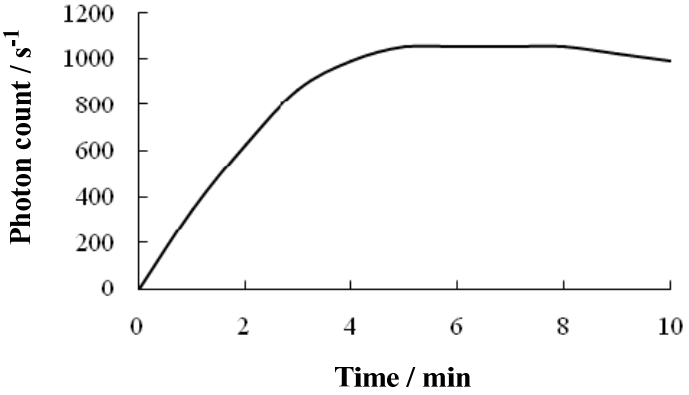


11


Photon count / s-1
700
600
500
400
300
200
100
0
0
2
4
6
8
10
Time / min



12


Photon count / s-1
1200
1000
800
600
400
200
0
0
2
4
6
8
10
Time / min

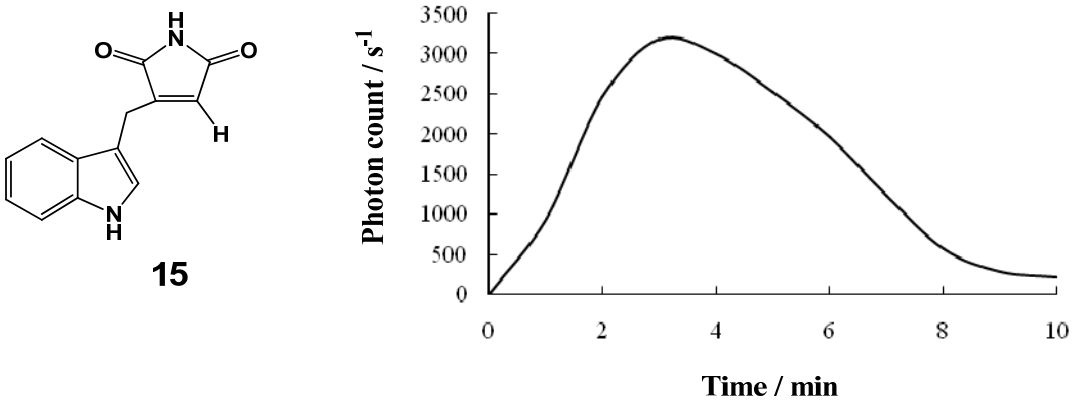


Fig. S3. Time course of CL of compounds **1–12** and **15**

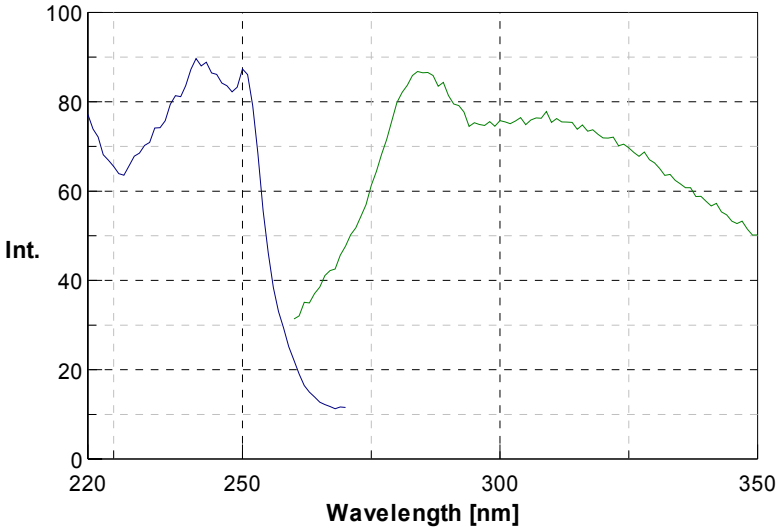
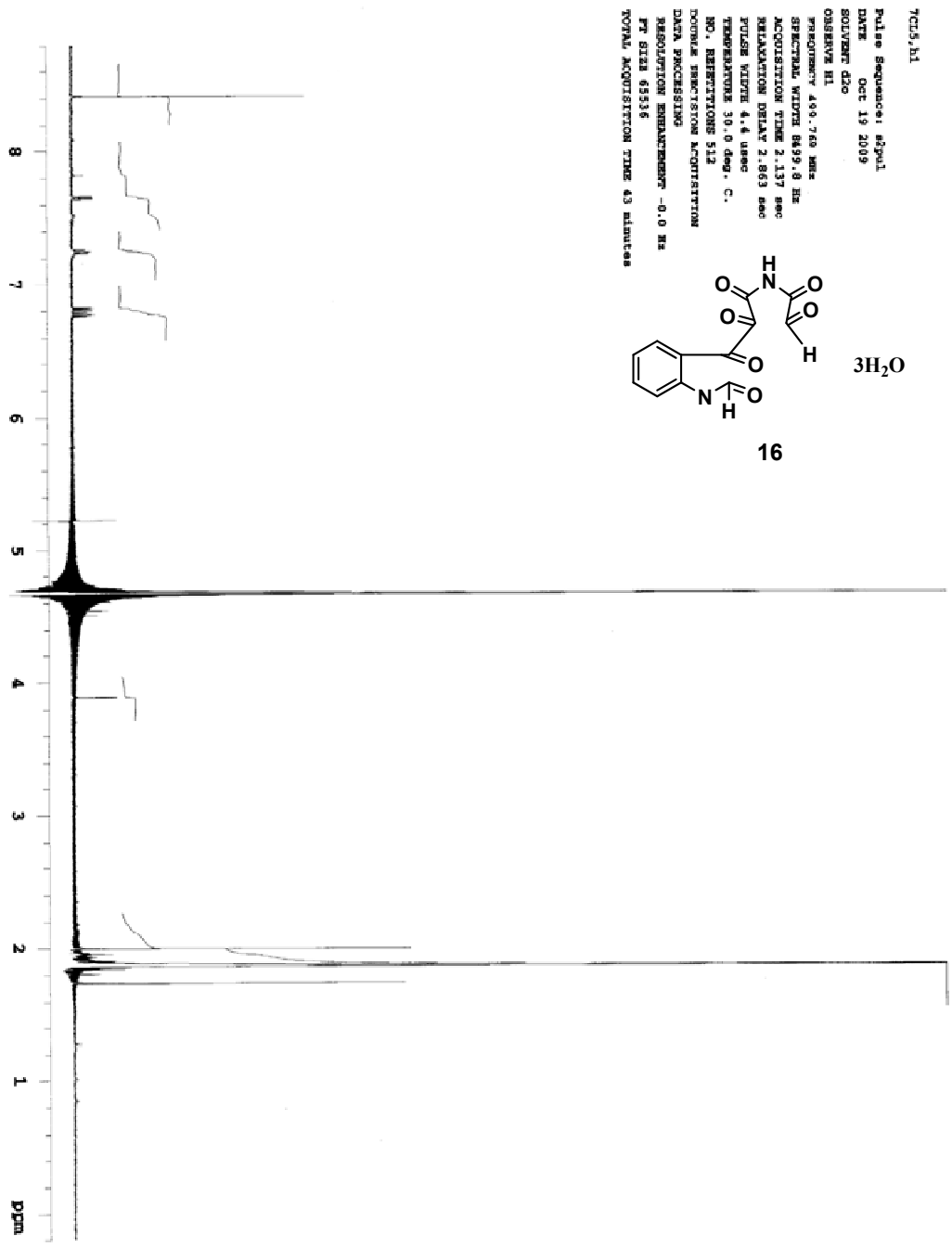
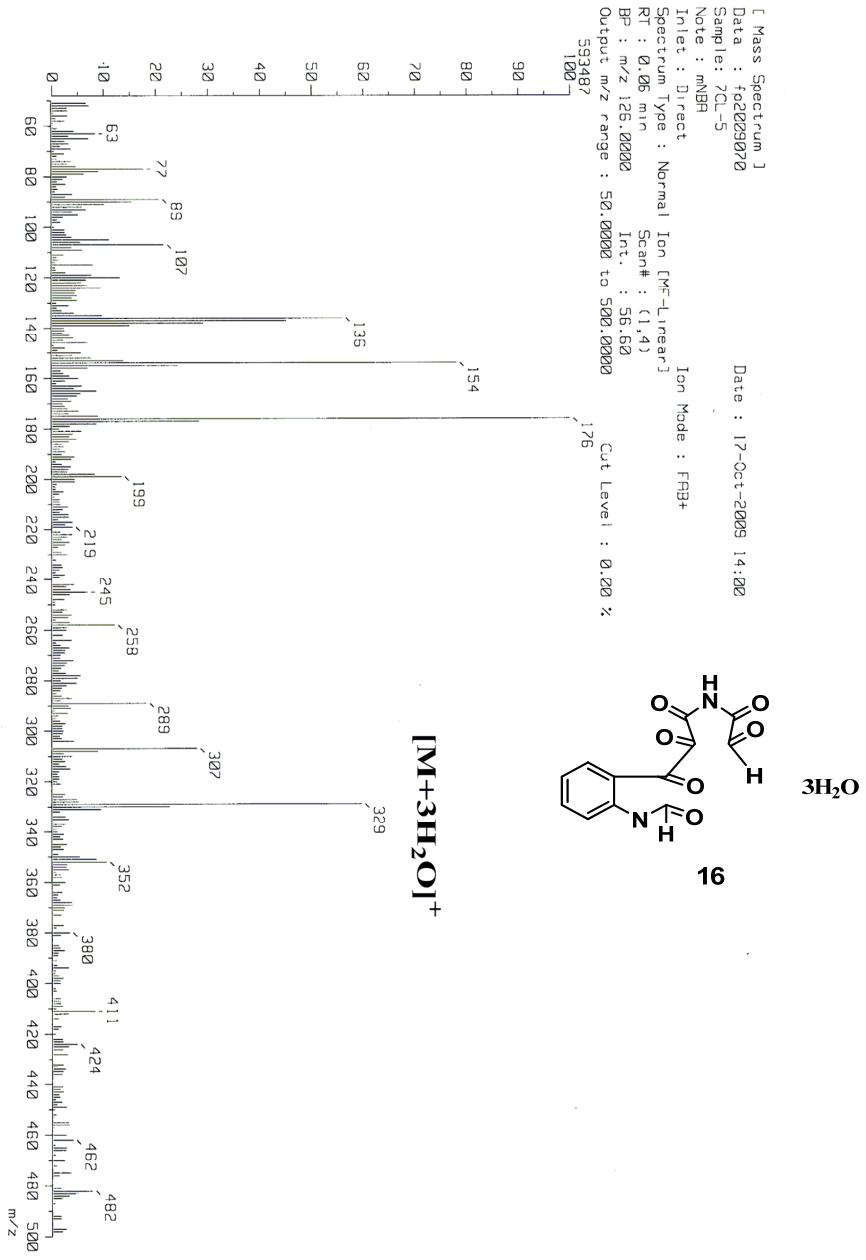


Fig. S4. FL spectrum of compound **16** in H_2O

^{1}H-NMR spectrum of compound **16**



FAB MS of compound **16**



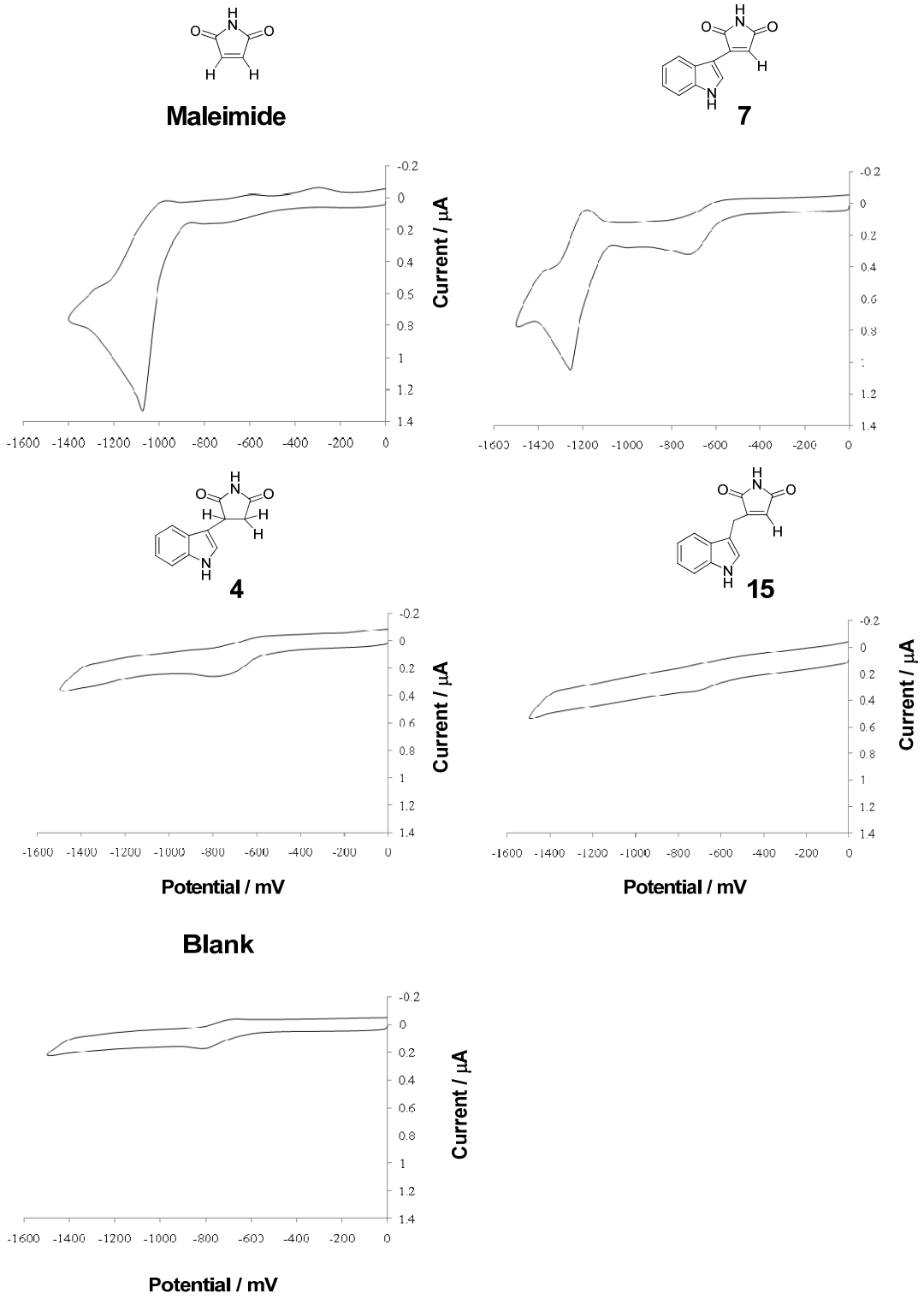


Fig. S5. Cyclic voltammograms of maleimide, compounds **4**, **7** and **15**

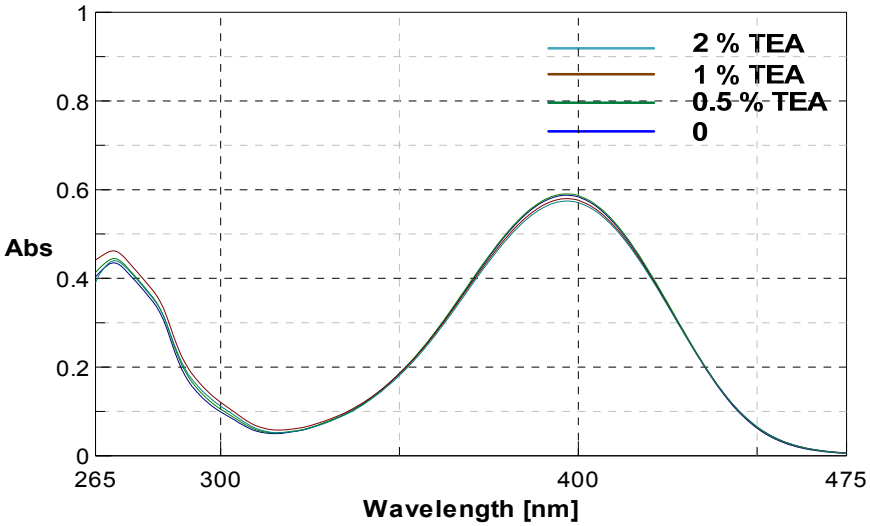


Fig. S6. Absorption spectra of compound **7** (0.05 mM) in 0, 0.5, 1 or 2 % triethylamine-CH_3CN solution

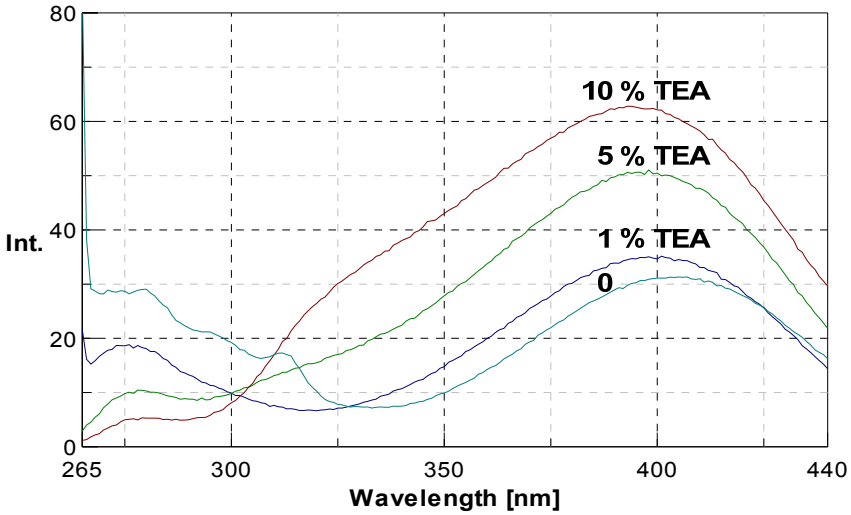


Fig. S7. The FL excitation spectra of compound **7** (10 μM) in 0, 1, 5 or 10 % triethylamine-CH_3CN solution

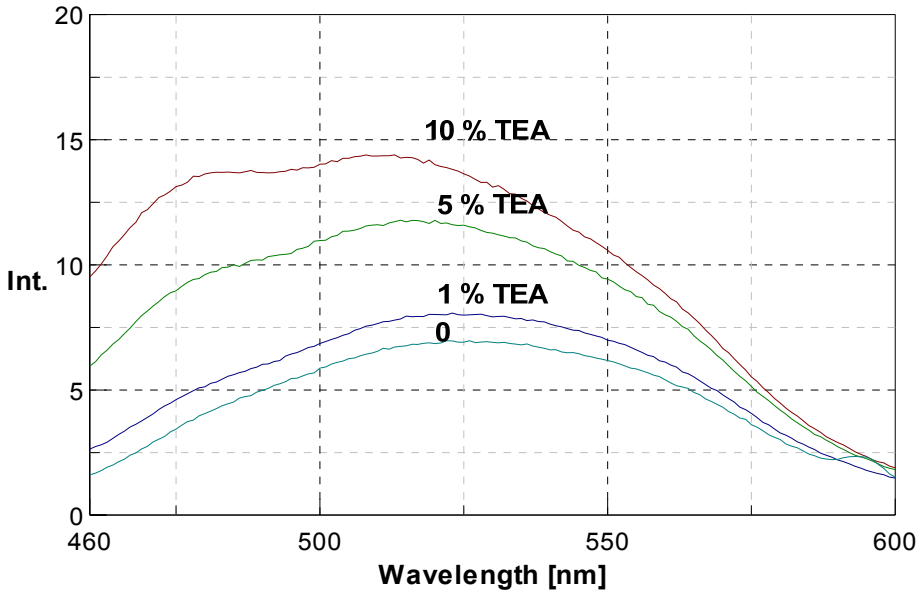


Fig. S8. The FL emission spectra of compound **7** (10 μM) in 0, 1, 5 or 10 % triethylamine-CH_3CN solution (ex. 396 nm)