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Electronic Supplementary Information

For

Four component domino reaction for the synthesis of highly functionalized dimeric tetracyclic dilactam fluorophores: H-bond Aided Self-Assembly

G. Ramachandran,[a,b] A. Raman,[c] S. Easwaramoorthi,[c] R.S. Rathore [d] and K. Sathiyanarayanan[a*]

[a] Chemistry Division, School of Advanced Sciences, VIT University, Vellore, sathiya_kuna@hotmail.com*.

[b] Department of Chemistry, IIT Kanpur, Uttar Pradesh - 208016.

[c] Chemical Laboratory, CSIR-Central Leather Research Institute, Adyar, Chennai – 600020 and Academy of Scientific and Innovative Research, New Delhi – 110001.

[d] Bioinformatics Infrastructure Facility, School of life sciences, University of Hyderabad, Hyderabad-500046, India.

Table of content

General experiment method:

Chemicals were purchased from Aldrich and they were used without further purification. TLC -Thin layer chromatography (Merck, Silica gel 60 F254) was performed on alumina plates (pre-coated silica gel). FT-IR spectra were recorded in the range of 4000-400cm^{-1} on JASCO-4100 spectrometer instrument using KBr pellets. ^{1}H NMR and ^{13}C NMR spectra recorded using a Bruker AMX 400 FT. HRMS analysis was obtained from JEOL GC Mate. The X-ray crystallographic diffractions were determined using a Smart – CCD (Bruker, 2004). The UV-visible absorption spectra were measured using Shimadzu UV-1800 double beam spectrophotometer. Fluorescence spectra were measured using Varian-Cary Eclipse fluorescence spectrophotometer.

Experimental procedure:

Synthesis of tetracyclic quinoline (4a – 4l): A dry 100ml Erlenmeyer flask was charged with α-tetralone (10 mmol); aromatic aldehydes (10 mmol); cyanoacetamide (20 mmol); sodium hydroxide (0.5 mol %) and methanol (15 ml). The reaction mixture was stirred at room temperature for 30-60 min. The reaction was monitored by TLC and after the completion of reaction, the mixture was neutralized using 0.1 N HCl and extracted with DCM (3 X 20 ml). The crude reaction mixture was purified by column chromatography on silica gel using ethyl acetate/hexane as the eluents.

Spectra Data:

4-phenyl-4,4a,5,6-tetrahydro-1H-10b,3-(epiminomethano)benzo[h]quinoline-2,12(3H)-dione (4a): Light yellow powder Solid; mp > 300^{o}C; R_f 0.82 (60% ethyl acetate : hexane); FTIR (KBr) *v*: 3510, 3195, 2939, 1708 cm^{-1}; ^{1}H NMR (400 MHz, DMSO): 1.74-1.87 (td, CH_2, 2H), 2.44-2.48 (t, CH, 1H), 2.97-2.99 (m, CH, 1H), 3.08-3.13 (m, CH_2, 2H), 3.97-3.98 (d, CH, 1H), 6.90-7. 29 (ArH, 9H), 8.72 (s, $CONH_2$, 2H) ppm; ^{13}C NMR (100MHz, DMSO): 29.04, 34.37, 45.52, 50.12, 60.08, 118.24, 128.35, 128.72, 129.62, 130.89, 131.76, 135.86, 160.05, 166.06 ppm; HRMS: calculated for $C_{20}H_{18}N_2O_2$ ([M]$^{+}$) 318.1368, Found 318.1368.

4-phenyl-4,4a,5,6-tetrahydro-1H-10b,3-(epiminomethano)benzo[h]quinoline-2,12(3H)-dione (4a): Light yellow powder Solid; mp > 300^{o}C; R_f 0.82 (60% ethyl acetate : hexane); FTIR (KBr) *v*: 3510, 3195, 2939, 1708 cm^{-1}; ^{1}H NMR (400 MHz, DMSO): 1.74-1.87 (t, CH_2, 2H), 2.44-2.48 (t, CH, 1H), 3.03-3.16 (m, CH_2 & CH, 3H), 3.97-3.98 (d, CH, 1H), 6.90-7. 29 (ArH, 9H), 8.72 (s, $CONH_2$, 2H) ppm; ^{13}C NMR (100MHz, DMSO): 29.04, 34.37, 45.52, 50.12, 60.08, 118.24, 128.35, 128.72, 129.62, 130.89, 131.76, 135.86, 160.05, 166.06 ppm; HRMS: calculated for $C_{20}H_{18}N_2O_2$ ([M]$^{+}$) 318.1368, Found 318.1368.

4-(2-(trifluoromethyl)phenyl)-4,4a,5,6-tetrahydro-1H-10b,3-(epiminomethano)benzo[h] quinoline-2,12(3H)-dione (4b): Light greenish yellow crystalline Solid; mp > 300^{o}C; R_f 0.79 (60% ethyl acetate : hexane); FTIR (KBr) *v*: 3501, 3183, 2916, 1692 cm^{-1}; ^{1}H NMR (400 MHz, DMSO): 1.46-1.49 (d, CH_2, 1H), 1.55-1.58 (dd, CH_2, 1H), 2.41-2.43 (t, CH, 1H), 2.75-2.78 (m, CH & CH_2, 3H), 3.38-3.41 (d, CH, 1H), 6.60-7. 52 (ArH, 8H), 7.63 (s, $CONH_2$, 2H) ppm; ^{13}C NMR (100MHz, DMSO): 30.42, 46.44, 57.33, 60.21, 114.87, 115.37, 122.09, 124.79, 125.42, 128.36, 129.13, 130.42, 137.91, 138.72, 162.22, 163.16 ppm; HRMS: calculated for $C_{21}H_{17}F_3N_2O_2$ ([M]$^{+}$) 386.1242, Found 386.1243.

4-(2-bromophenyl)-4,4a,5,6-tetrahydro-1H-10b,3-(epiminomethano)benzo[h]quinoline-2,12(3H)-dione (4c): Yellow powder Solid; mp > 300^{o}C; R_f 0.68 (60% ethyl acetate : hexane); FTIR (KBr) *v*: 3551, 3184, 2974, 1721 cm^{-1}; ^{1}H NMR (400 MHz, DMSO): 1.73-1.85 (t, CH_2, 2H), 2.58-2.62 (t, CH, 1H), 3.00-3.02 (m, CH_2, 2H), 3.36-3.38 (t, CH, 1H), 3.93-3.94 (d, CH, 1H), 6.87-7. 56 (ArH, 8H), 8.62 (s, $CONH_2$, 2H) ppm; ^{13}C NMR (100MHz, DMSO): 22.39, 29.07, 52.30, 55.28, 66.83, 110.09, 120.54, 126.58, 128.04,

130.16, 133.52, 144.61, 155.63, 175.93 ppm; HRMS: calculated for $C_{20}H_{17}BrN_2O_2$ ([M] $^+$) 396.0473, Found 396.0471.

4-(4-methoxyphenyl)-4,4a,5,6-tetrahydro-1H-10b,3-(epiminomethano)benzo[h]quinoline-2,12(3H)-dione (4d): Light greenish powder Solid; mp > 300^{o}C; R_f 0.71 (60% ethyl acetate : hexane); FTIR (KBr) *v*: 3584, 3141, 2982, 1712 cm^{-1}; ^{1}H NMR (400 MHz, DMSO): 1.71-1.82 (t, CH_2, 2H), 2.23-2.26 (t, CH, 1H), 2.98-3.00 (m, CH, 1H), 3.15-3.20 (t, CH_2, 2H), 3.81 (s, OCH_3, 3H), 4.02-4.04 (d, CH, 1H), 6.91-7. 40 (ArH, 8H), 8.53 (s, $CONH_2$, 2H) ppm; ^{13}C NMR (100MHz, DMSO): 23.06, 27.25, 55.64, 56.33, 69.94, 111.73, 116.15, 120.76, 125.21, 127.08, 129.34, 131.16, 139.29, 155.54, 172.24 ppm; HRMS: calculated for $C_{21}H_{20}N_2O_3$ ([M] $^+$) 348.1474, Found 348.1473.

4-(2-fluorophenyl)-4,4a,5,6-tetrahydro-1H-10b,3-(epiminomethano)benzo[h]quinoline-2,12(3H)-dione (4e): Greenish yellow powder Solid; mp > 300^{o}C; R_f 0.76 (60% ethyl acetate : hexane); FTIR (KBr) *v*: 3500, 3102, 2972, 1718 cm^{-1}; ^{1}H NMR (400 MHz, DMSO): 1.73-1.89 (td, CH_2, 2H), 2.28-2.30 (t, CH, 1H), 2.51-2.54 (m, CH_2, 2H), 3.09-3.11 (t, CH, 1H), 3.95-3.96 (d, CH, 1H), 6.91-7.60 (ArH, 8H), 10.25 (s, $CONH_2$, 2H) ppm; ^{13}C NMR (100MHz, DMSO): 18.98, 32.74, 58.63, 60.03, 117.66, 125.85, 127.10, 129.25, 130.21, 134.24, 140.00, 161.27, 166.48 ppm; HRMS: calculated for $C_{20}H_{17}FN_2O_2$ ([M] $^+$) 336.1274, Found 336.1274.

4-(3-fluorophenyl)-4,4a,5,6-tetrahydro-1H-10b,3-(epiminomethano)benzo[h]quinoline-2,12(3H)-dione (4f): Greenish powder Solid; mp > 300^{o}C; R_f 0.78 (60% ethyl acetate : hexane); FTIR (KBr) *v*: 3472, 3136, 2984, 1692 cm^{-1}; ^{1}H NMR (400 MHz, DMSO): 1.72-1.85 (td, CH_2, 2H), 2.45-2.49 (t, CH, 1H), 2.97-2.99 (m, CH, 1H), 3.09-3.17 (t, CH_2, 2H), 3.78-3.79 (d, CH, 1H), 6.91-7. 22 (ArH, 8H), 9.23 (s, $CONH_2$, 2H) ppm; ^{13}C NMR (100MHz, DMSO): 13.90, 20.61, 30.50, 57.72, 59.94, 114.55, 116.03, 123.03, 129.97, 130.33, 136.57, 160.56, 163.22, 163.48 ppm; HRMS: calculated for $C_{20}H_{17}FN_2O_2$ ([M] $^+$) 336.1274, Found 336.1273.

4-(4-fluorophenyl)-4,4a,5,6-tetrahydro-1H-10b,3-(epiminomethano)benzo[h]quinoline-2,12(3H)-dione (4g): Greenish powder Solid; mp > 300^{o}C; R_f 0.81 (60% ethyl acetate : hexane); FTIR (KBr) *v*: 3518, 3181, 2925, 1671 cm^{-1}; ^{1}H NMR (400 MHz, DMSO): 1.74-1.86 (td, CH_2, 2H), 2.47-2.51 (t, CH, 1H), 2.88-2.89 (m, CH, 1H), 2.95-2.97 (t, CH_2, 2H), 3.98-4.00 (d, CH, 1H), 6.91-7.78 (ArH, 8H), 8.83 (s, $CONH_2$, 2H) ppm; ^{13}C NMR (100MHz, DMSO): 22.33, 26.95, 49.71, 54.72, 62.53, 113.32, 122.21, 123.30, 125.85, 128.98, 137.17, 160.42, 165.70 ppm; HRMS: calculated for $C_{20}H_{17}FN_2O_2$ ([M] $^+$) 336.1274, Found 336.1276.

4-(*o*-tolyl)-4,4a,5,6-tetrahydro-1H-10b,3-(epiminomethano)benzo[h]quinoline-2,12(3H)-dione (4h): Light yellow powder Solid; mp > 300^{o}C; R_f 0.72 (60% ethyl acetate : hexane); FTIR (KBr) *v*: 3486, 3172, 2979, 1709 cm^{-1}; ^{1}H NMR (400 MHz, DMSO): 1.69-1.83 (td, CH_2, 2H), 2.29 (s, CH_3, 3H), 2.33 (CH, 1H), 3.07-3.23 (m, CH_2 & CH, 3H), 3.73-3.75 (d, CH, 1H), 6.95-7.62 (ArH, 8H), 8.82 (s, $CONH_2$, 2H) ppm; ^{13}C NMR (100MHz, DMSO): 23.26, 27.78, 54.68, 63.58, 67.93, 113.23, 123.97, 126.64, 129.83, 138.13, 158.54, 168.96 ppm; HRMS: calculated for $C_{21}H_{20}N_2O_2$ ([M] $^+$) 332.1525, Found 332.1524.

4-(*p*-tolyl)-4,4a,5,6-tetrahydro-1H-10b,3-(epiminomethano)benzo[h]quinoline-2,12(3H)-dione (4i): Light yellow powder Solid; mp > 300^{o}C; R_f 0.75 (60% ethyl acetate : hexane); FTIR (KBr) *v*: 3551, 3162, 2984, 1708 cm^{-1}; ^{1}H NMR (400 MHz, DMSO): 1.71-1.85 (td, CH_2, 2H), 2.08-2.11 (d, CH, 1H), 2.26 (s, CH_3, 3H), 2.99-3.15 (m, CH_2 & CH, 3H), 3.75 (CH, 1H), 7.04-7.60 (ArH, 8H), 8.65 (s, $CONH_2$, 2H) ppm; ^{13}C NMR (100MHz, DMSO): 20.96, 35.52, 38.94, 55.21, 63.29, 117.84, 123.31, 126.80, 129.36, 136.27, 137.43, 163.57, 166.40 ppm; HRMS: calculated for $C_{21}H_{20}N_2O_2$ ([M] $^+$) 332.1525, Found 332.1526.

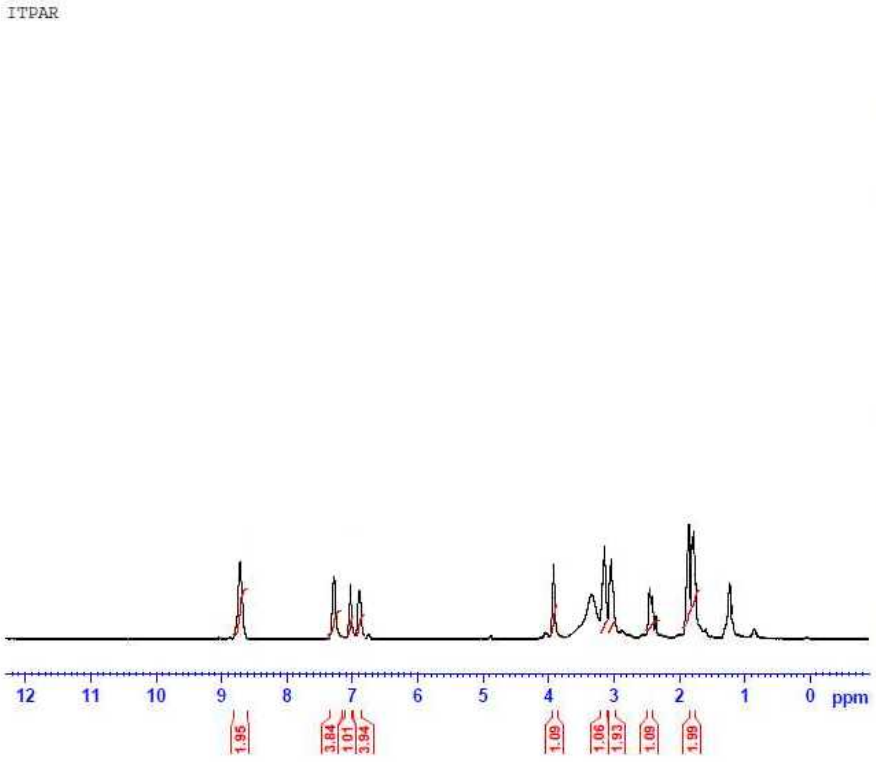
4-(2-chlorophenyl)-4,4a,5,6-tetrahydro-1H-10b,3-(epiminomethano)benzo[h]quinoline-2,12(3H)-dione (4j): Pale yellow powder Solid; mp > 300^{o}C; R_f 0.76 (60% ethyl acetate : hexane); FTIR (KBr) *v*: 3477, 3201, 2891, 1682 cm^{-1}; ^{1}H NMR (400 MHz, DMSO): 1.76-

1.86 (td, CH_2, 2H), 2.12-2.15 (CH_2 & CH, 3H), 2.89-2.92 (d, CH, 1H), 3.84-3.86 (CH, 1H), 7.15-7.73 (ArH, 8H), 9.03 (s, $CONH_2$, 2H) ppm; ^{13}C NMR (100MHz, DMSO): 26.63, 29.41, 41.83, 50.09, 58.79, 69.56, 126.85, 128.09, 129.35, 130.06, 133.76, 137.47, 172.122 ppm; HRMS: calculated for $C_{20}H_{17}ClN_2O_2$ ($[M]^+$) 352.0979, Found 352.0978.

4-(4-chlorophenyl)-4,4a,5,6-tetrahydro-1H-10b,3-(epiminomethano)benzo[h]quinoline-2,12(3H)-dione (4k): Pale greenish yellow powder Solid; mp > 300°C; R_f 0.83 (60% ethyl acetate : hexane); FTIR (KBr) *v*: 3573, 3172, 2974, 1701 cm^{-1}; ^1H NMR (400 MHz, DMSO): 1.89-1.91 (CH_2 & CH , 3H), 3.06-3.18 (CH_2 & CH , 3H), 3.80-3.82 (d, CH, 1H), 6.91-7.36 (ArH, 8H), 9.89 (s, $CONH_2$, 2H) ppm; ^{13}C NMR (100MHz, DMSO): 30.68, 36.68, 46.27, 47.65, 57.89, 116.61, 127.65, 129.12, 130.89, 133.62, 134.43, 163.96, 172.054 ppm; HRMS: calculated for $C_{20}H_{17}ClN_2O_2$ ($[M]^+$) 352.0979, Found 352.0977.

4-(naphthalen-1-yl)-4,4a,5,6-tetrahydro-1H-10b,3-(epiminomethano)benzo[h]quinoline-2,12(3H)-dione (4l): Light brownish yellow powder Solid; mp > 300°C; R_f 0.85 (60% ethyl acetate : hexane); FTIR (KBr) *v*: 3592, 3143, 2948, 1704 cm^{-1}; ^1H NMR (400 MHz, DMSO): 2.16-2.18 (td, CH_2, 2H), 3.46-3.51 (m, CH_2 & CH, 3H), 3.74-3.76 (d, CH, 1H), 3.93-3.94 (d, CH, 1H), 7.43 -8.03 (ArH, 11H), 9.73 (s, $CONH_2$, 2H) ppm; ^{13}C NMR (100MHz, DMSO): 22.19, 32.13, 50.18, 59.94, 68.63, 118.30, 123.52, 125.44, 126.39, 127.47, 128.67, 131.15, 132.70, 133.39, 159.28, 166.29 ppm; HRMS: calculated for $C_{24}H_{20}N_2O_2$ ($[M]^+$) 368.1525, Found 368.1525.

^{1}H & ^{13}C-NMR spectra of 4a

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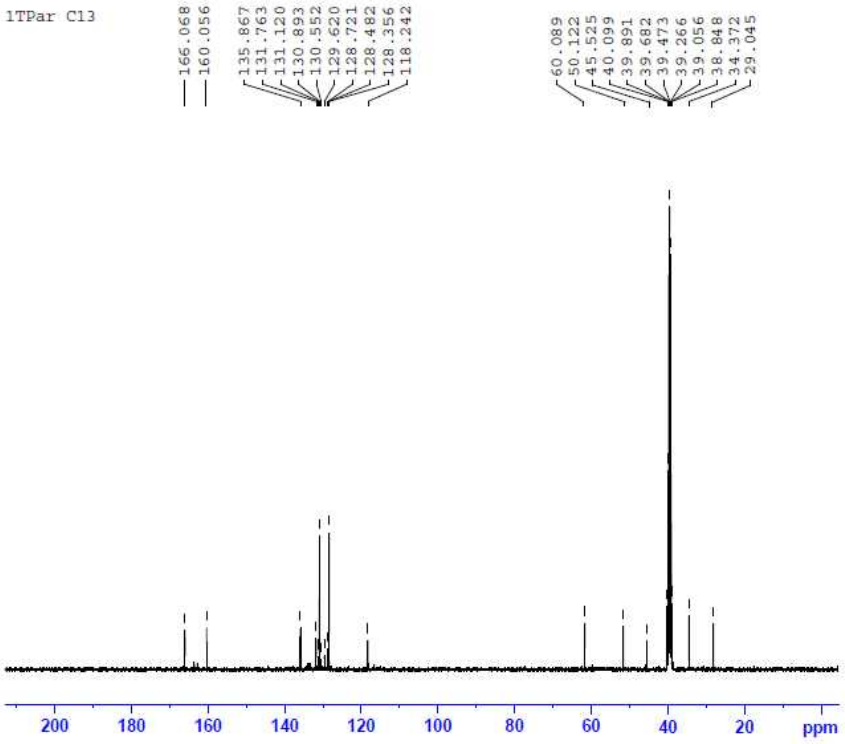


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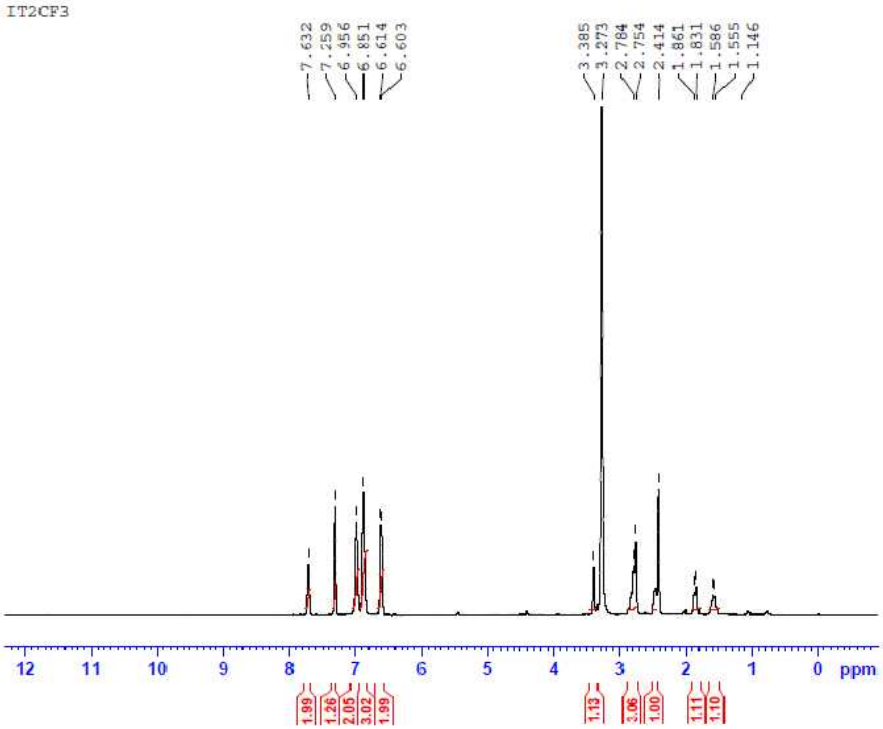
^{1}H & ^{13}C-NMR spectra of 4b

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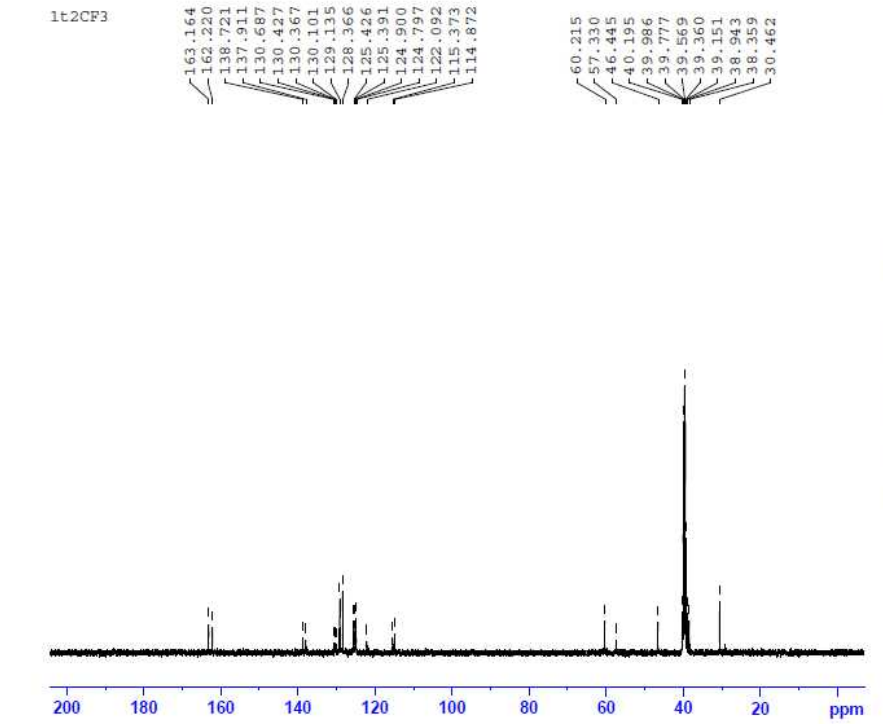


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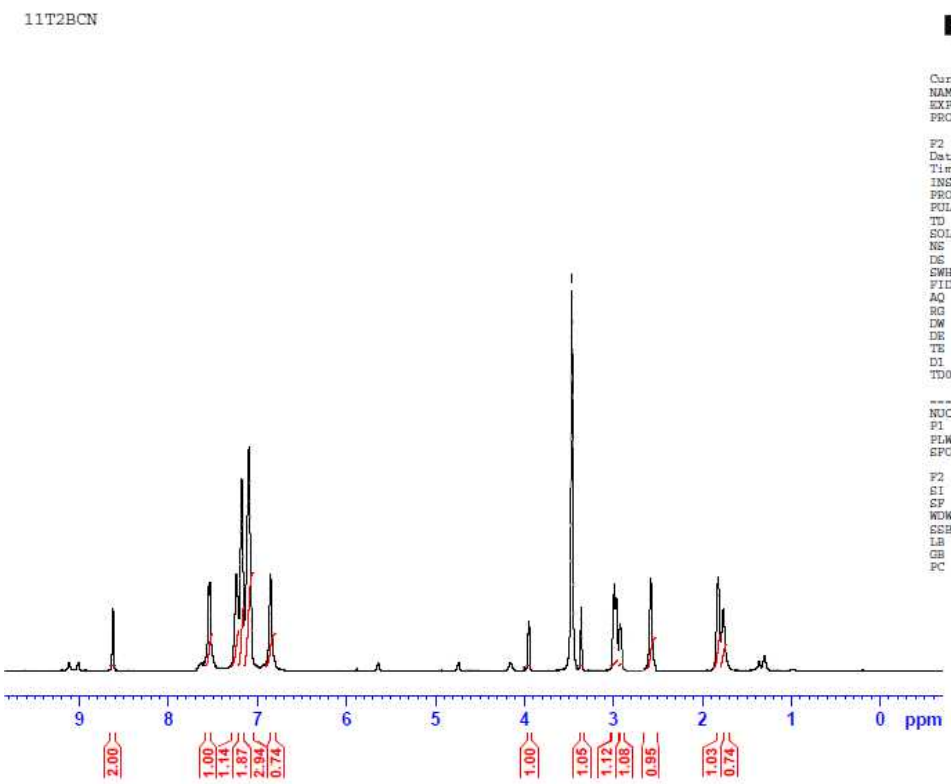
^{1}H & ^{13}C-NMR spectra of 4c

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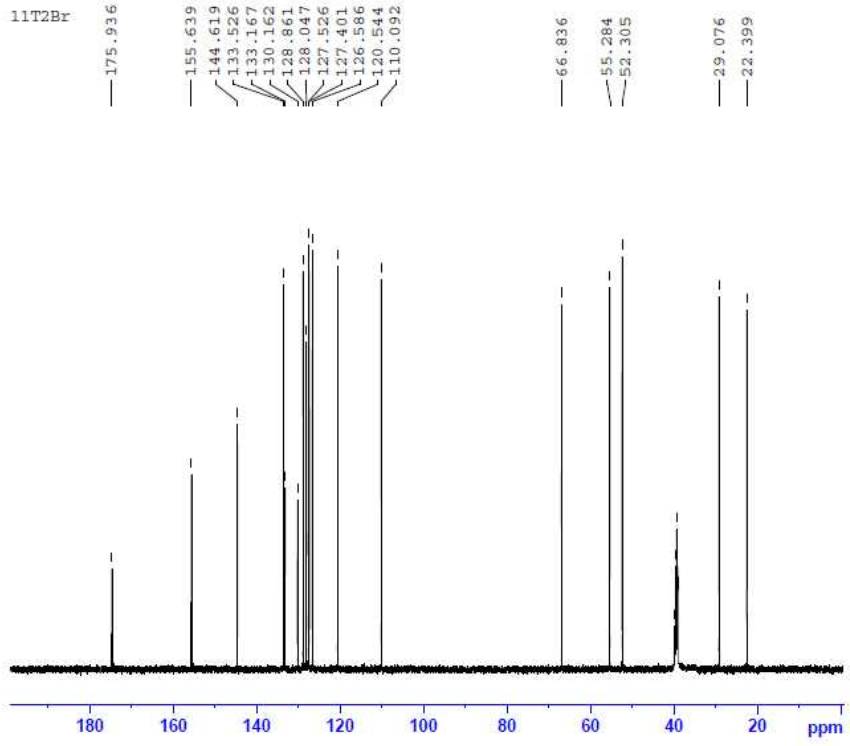


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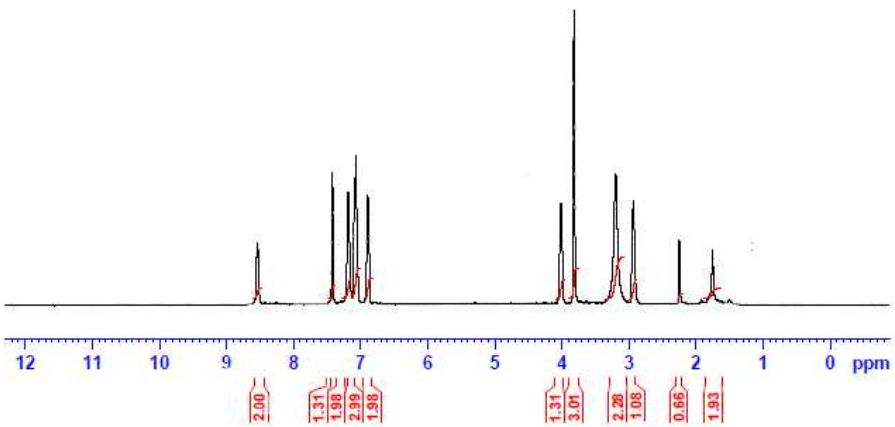
^{1}H & ^{13}C-NMR spectra of 4d

1T40M1

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======== CHANNEL f1 ========
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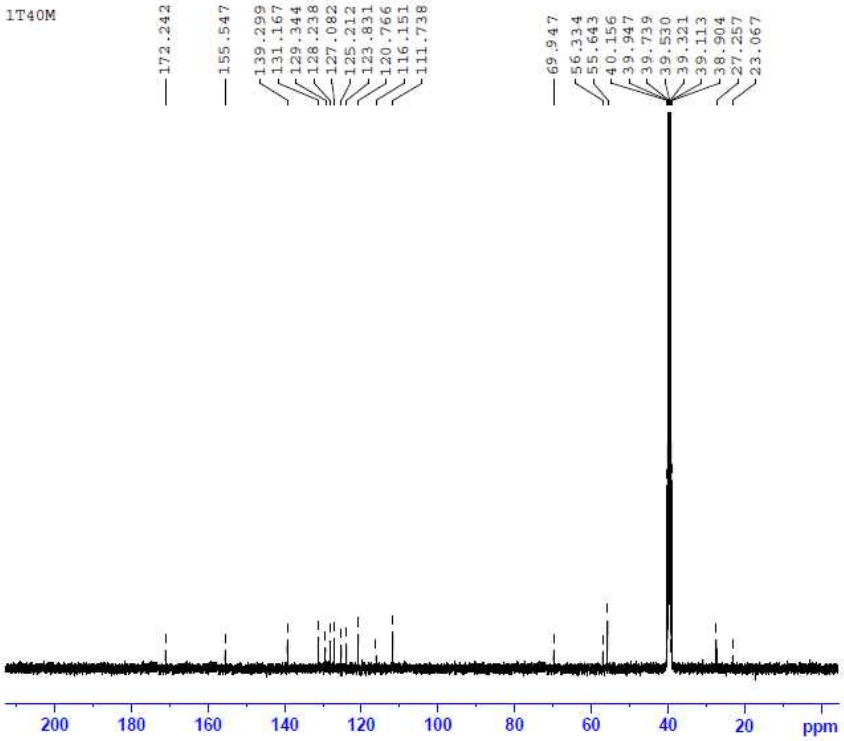
```

1T40M



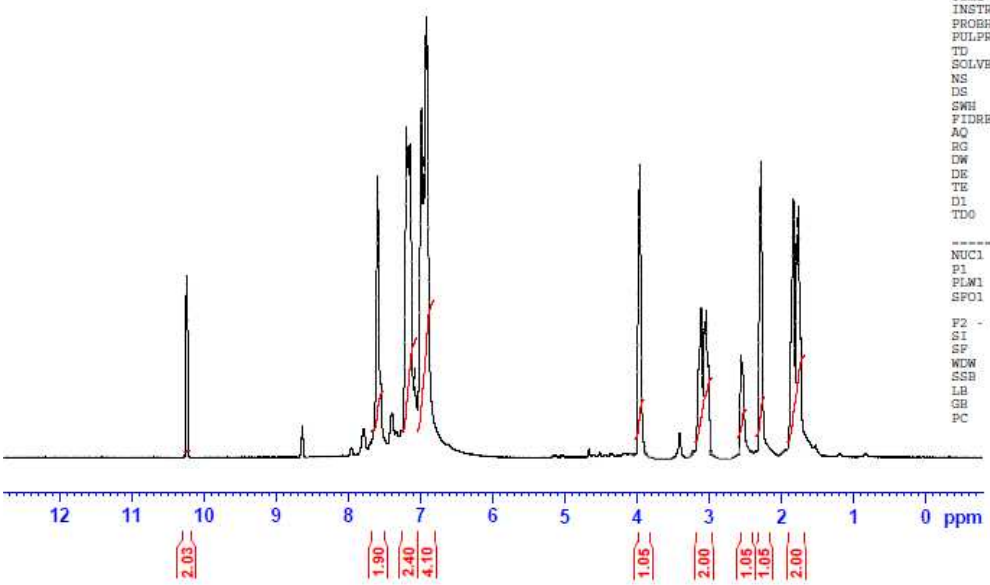

```
Current Data Parameters
NAME                  1T40M
EXPNO                     31
PROCNO                     1

F2 - Acquisition Parameters
Date_               20130215
Time                   18.17
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT                DMSO
NS                       512
DS                         4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                     143.73
DW                     20.800 usec
DE                      6.50 usec
TE                     297.3 K
D1                  2.00000000 sec
d11                 0.03000000 sec
DELTA               1.89999998 sec
TD0                        1
SFO1               100.6550182 MHz
NUC1                      13C
P1                      9.80 usec
PLW1               58.00000000 W
SFO2               400.2596010 MHz
NUC2                      1H
CPDPRG[2                waltz16
PCPD2                  90.00 usec
PLW2               14.00000000 W
PLW12               0.35097000 W
PLW13               0.28428999 W

F2 - Processing parameters
SI                        32768
SF                 100.6450015 MHz
WDW                        EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

^{1}H & ^{13}C-NMR spectra of 4e

IT2FCN



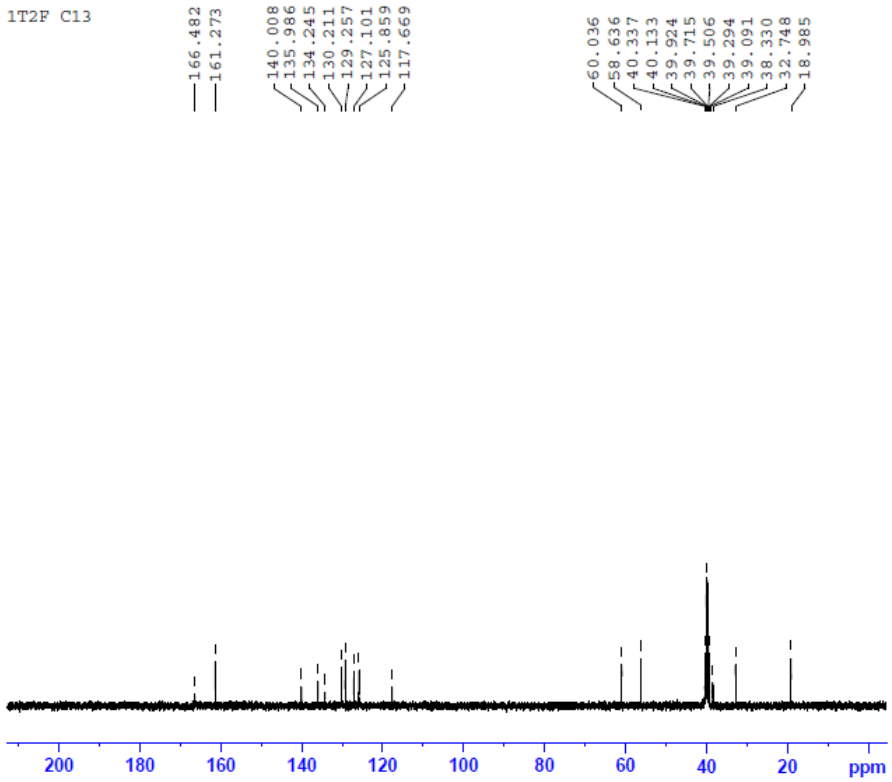

```
Current Data Parameters
NAME                  IT2FCN
EXPNO                     60
PROCNO                     1

F2 - Acquisition Parameters
Date_              20130315
Time                  13.26
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        16
DS                         2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9845889 sec
RG                    71.13
DW                   60.800 usec
DE                    6.50 usec
TE                   296.2 K
D1              1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     14.25 usec
PLW1           14.00000000 W
SFO1           400.2604718 MHz

F2 - Processing parameters
SI                        65536
SF             400.2579917 MHz
WDW                       EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

1T2F C13

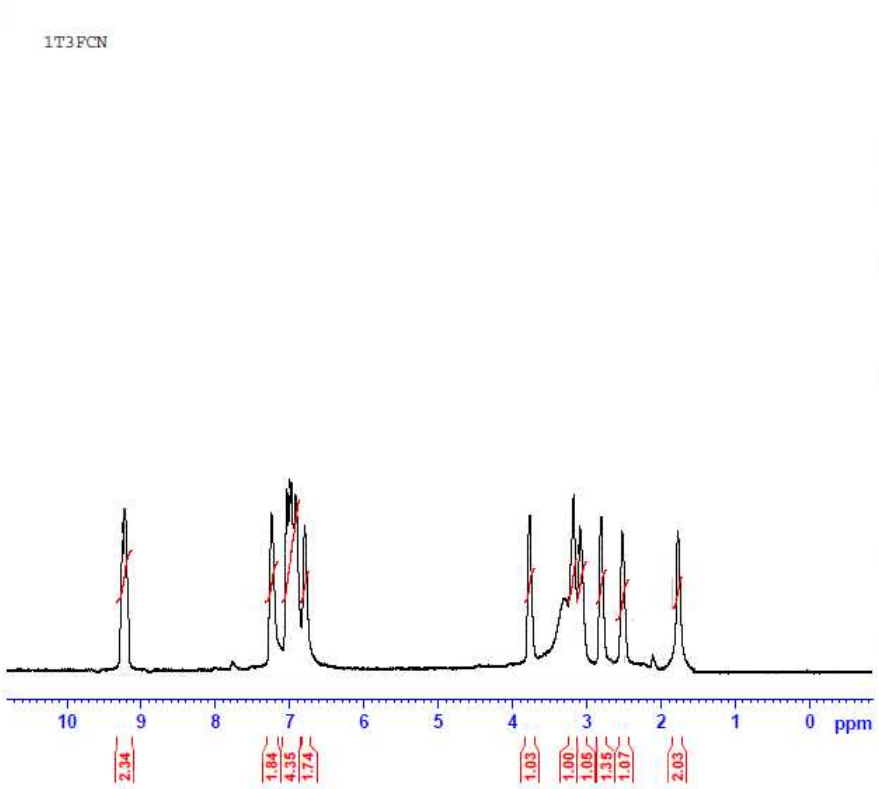



```
Current Data Parameters
NAME                  1T2F C13
EXPNO                       13
PROCNO                       1

F2 - Acquisition Parameters
Date_              20130403
Time                   6.37
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT                DMSO
NS                       512
DS                         4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631488 sec
RG                    175.97
DW                   20.800 usec
DE                    6.50 usec
TE                   295.6 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                        1
SFO1           100.6550182 MHz
NUC1                      13C
P1                     9.80 usec
PLW1           58.00000000 W
SFO2           400.2596010 MHz
NUC2                      1H
CPDPRG[2            waltz16
PCPD2                 90.00 usec
PLW2           14.00000000 W
PLW12           0.35097000 W
PLW13           0.28428999 W

F2 - Processing parameters
SI                        32768
SF             100.6449913 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

^{1}H & ^{13}C-NMR spectra of 4f

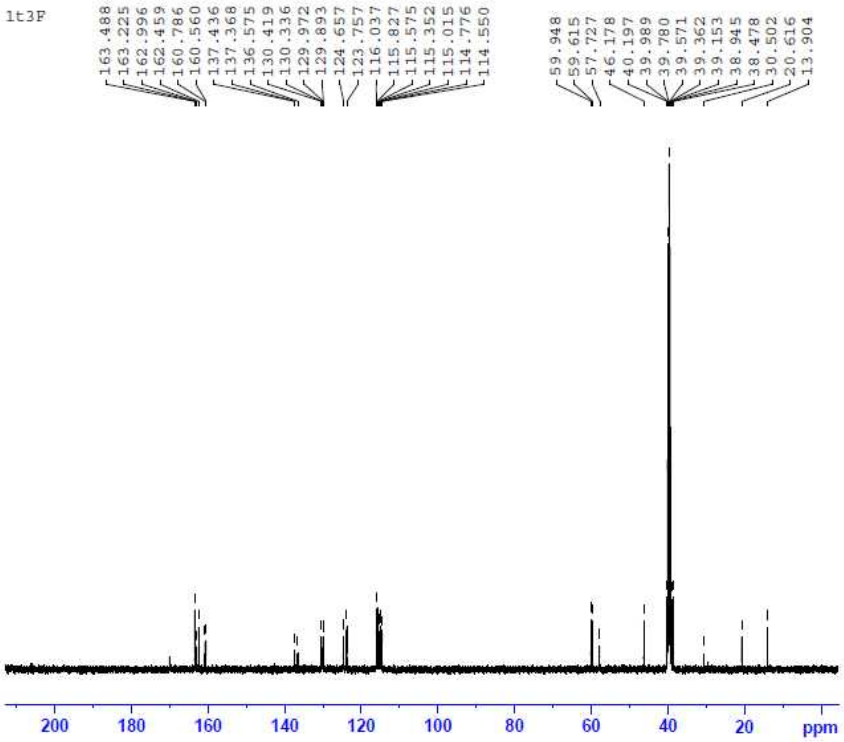



```
Current Data Parameters
NAME                  1T3FCN
EXPNO                     56
PROCNO                     1

F2 - Acquisition Parameters
Date_              20130314
Time                  22.19
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT               DMSO
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9845889 sec
RG                   175.97
DW                   60.800 usec
DE                    6.50 usec
TE                   294.8 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                    14.25 usec
PLW1             14.00000000 W
SFO1            400.2604718 MHz

F2 - Processing parameters
SI                    65536
SF               400.2579968 MHz
WDW                      EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```

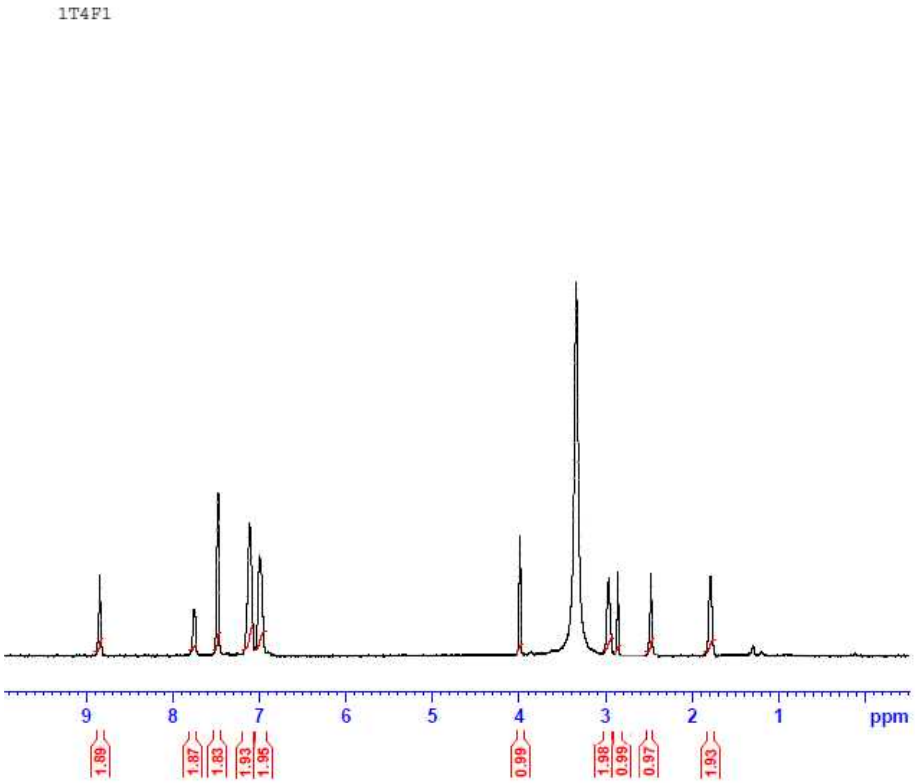



```
Current Data Parameters
NAME                   1t3F
EXPNO                    29
PROCNO                    1

F2 - Acquisition Parameters
Date_              20130404
Time                   5.43
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT               DMSO
NS                     512
DS                       4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631488 sec
RG                   175.97
DW                   20.800 usec
DE                    6.50 usec
TE                   295.2 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                       1
SFO1            100.6550182 MHz
NUC1                    13C
P1                    9.80 usec
PLW1             58.00000000 W
SFO2            400.2596010 MHz
NUC2                    1H
CPDPRG[2            waltz16
PCPD2                90.00 usec
PLW2             14.00000000 W
PLW12             0.35097000 W
PLW13             0.28428999 W

F2 - Processing parameters
SI                    32768
SF              100.6450043 MHz
WDW                      EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

^{1}H & ^{13}C-NMR spectra of 4g



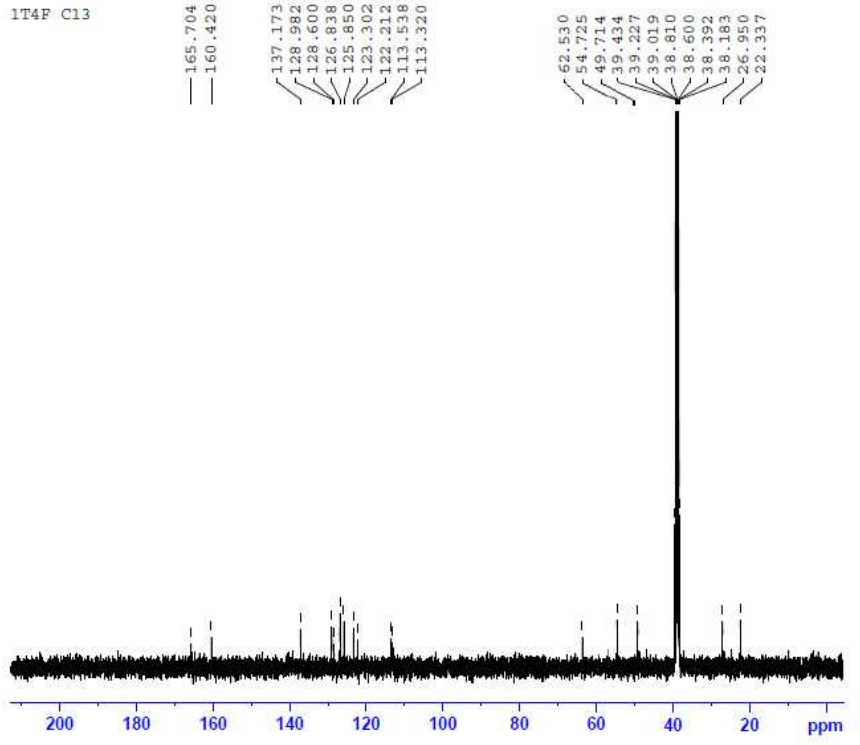
BRUKER

```
Current Data Parameters
NAME                  1T4F1
EXPNO                    45
PROCNO                    1

F2 - Acquisition Parameters
Date_              20130219
Time                   4.10
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9845889 sec
RG                     199.6
DW                    60.800 usec
DE                     6.50 usec
TE                    293.3 K
D1                 1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                    14.25 usec
PLW1           14.00000000 W
SFO1           400.2604718 MHz

F2 - Processing parameters
SI                    65536
SF             400.2598582 MHz
WDW                      EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```



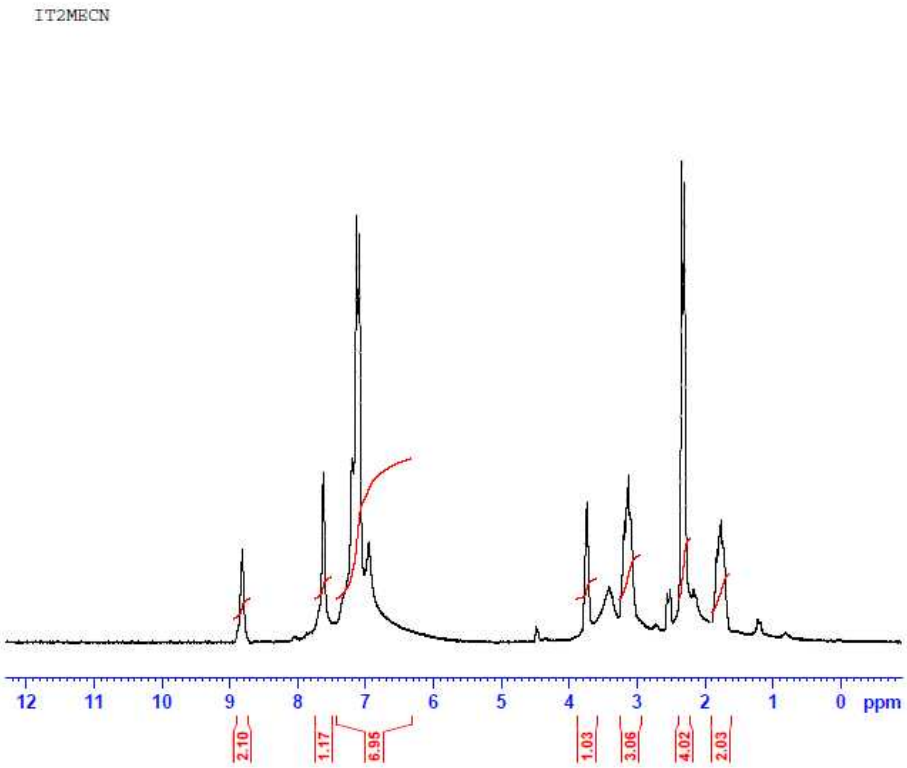
BRUKER

```
Current Data Parameters
NAME                1T4F C13
EXPNO                     44
PROCNO                     1

F2 - Acquisition Parameters
Date_               20130219
Time                    4.05
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                     65536
SOLVENT                DMSO
NS                       512
DS                         4
SWH                24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                     156.91
DW                    20.800 usec
DE                     6.50 usec
TE                    294.1 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                        1
SFO1           100.6550182 MHz
NUC1                     13C
P1                     9.80 usec
PLW1           58.00000000 W
SFO2           400.2596010 MHz
NUC2                     1H
CPDPRG[2           waltz16
PCPD2                 90.00 usec
PLW2           14.00000000 W
PLW12           0.35097000 W
PLW13           0.28428999 W

F2 - Processing parameters
SI                     32768
SF             100.6455634 MHz
WDW                      EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

^{1}H & ^{13}C-NMR spectra of 4h

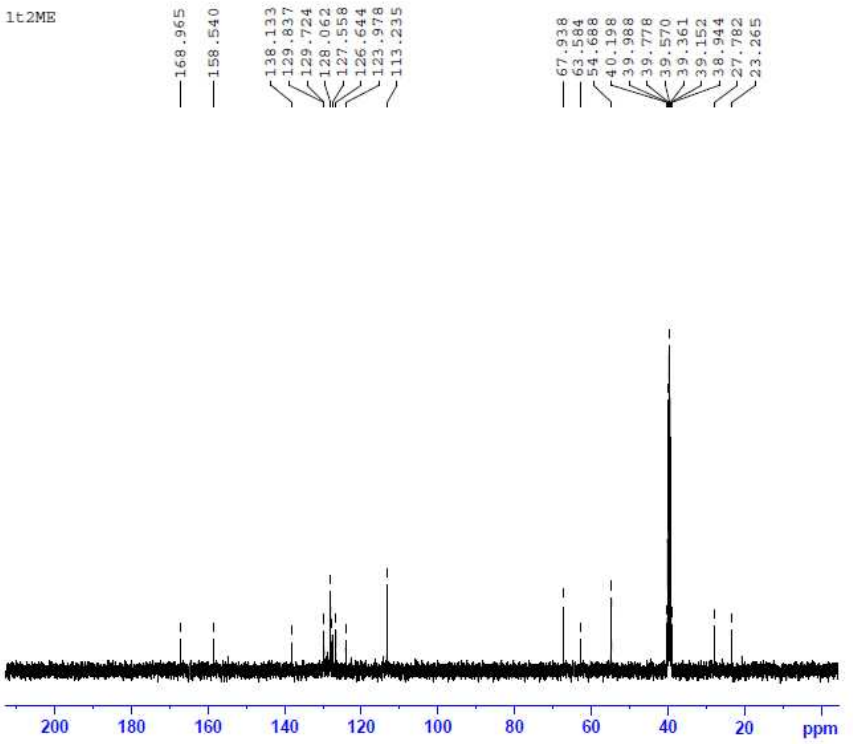



```
Current Data Parameters
NAME                  IT2MECN
EXPNO                      31
PROCNO                      1

F2 - Acquisition Parameters
Date_               20130309
Time                    6.58
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg30
TD                     65536
SOLVENT                 DMSO
NS                         16
DS                          2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                  3.9845889 sec
RG                     127.79
DW                     60.800 usec
DE                      6.50 usec
TE                     292.7 K
D1                  1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      14.25 usec
PLW1           14.00000000 W
SFO1           400.2604718 MHz

F2 - Processing parameters
SI                     65536
SF             400.2580000 MHz
WDW                       EM
SSB         0
LB                      0.30 Hz
GB          0
PC                      1.00
```

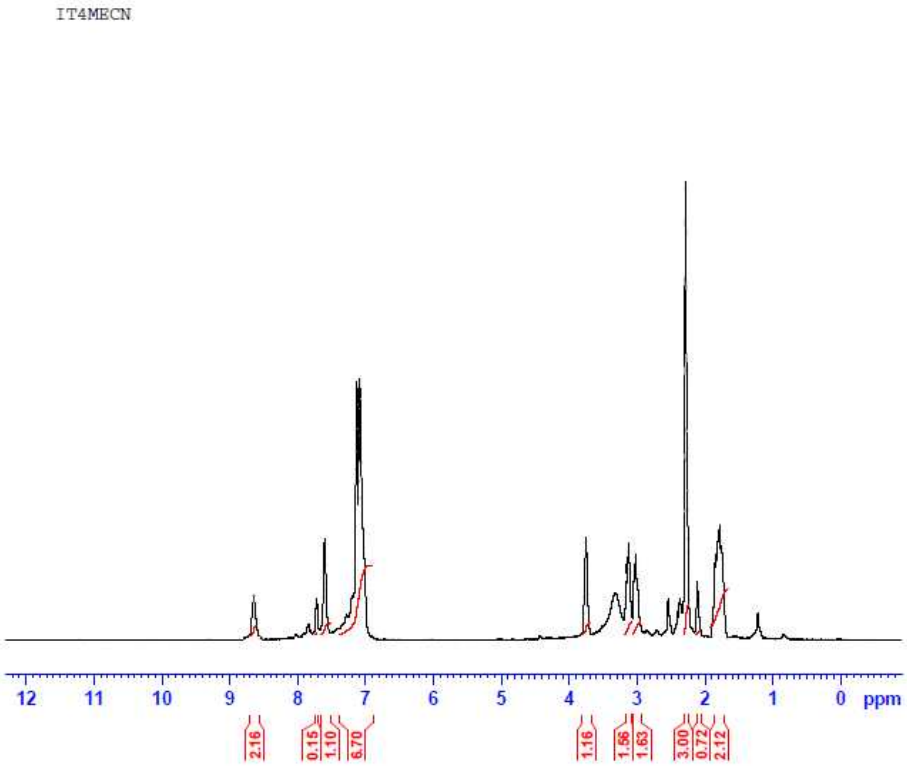



```
Current Data Parameters
NAME                   1t2ME
EXPNO                     42
PROCNO                     1

F2 - Acquisition Parameters
Date_               20130219
Time                    3.30
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zgpg30
TD                     65536
SOLVENT                 DMSO
NS                        512
DS                          4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                     175.97
DW                     20.800 usec
DE                      6.50 usec
TE                     294.3 K
D1                  2.00000000 sec
d11                 0.03000000 sec
DELTA               1.89999998 sec
TD0                         1
SFO1           100.6550182 MHz
NUC1                      13C
P1                      9.80 usec
PLW1           58.00000000 W
SFO2           400.2596010 MHz
NUC2                       1H
CPDPRG[2            waltz16
PCPD2                  90.00 usec
PLW2           14.00000000 W
PLW12           0.35097000 W
PLW13           0.28428999 W

F2 - Processing parameters
SI                     32768
SF             100.6449882 MHz
WDW                       EM
SSB         0
LB                      1.00 Hz
GB          0
PC                      1.40
```

^{1}H & ^{13}C-NMR spectra of 4i

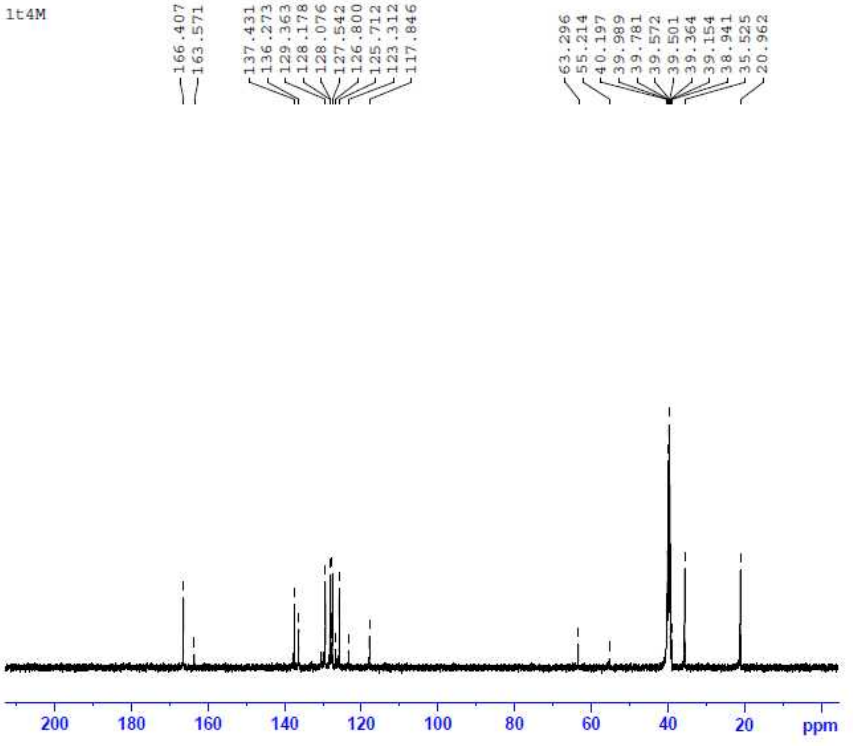



```
Current Data Parameters
NAME                  IT4MECN
EXPNO                      21
PROCNO                      1

F2 - Acquisition Parameters
Date_               20130308
Time                   18.29
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        16
DS                         2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9845889 sec
RG                    127.79
DW                    60.800 usec
DE                     6.50 usec
TE                    296.7 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     14.25 usec
PLW1              14.00000000 W
SFO1              400.2604718 MHz

F2 - Processing parameters
SI                        65536
SF                400.2579922 MHz
WDW                        EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```

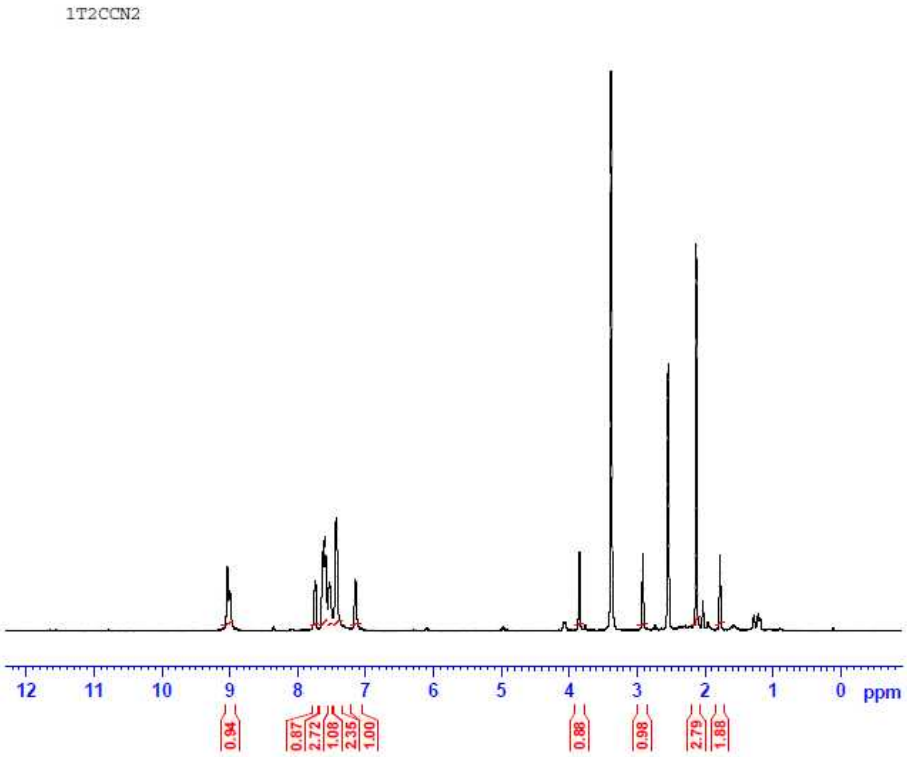



```
Current Data Parameters
NAME                    1t4M
EXPNO                     25
PROCNO                     1

F2 - Acquisition Parameters
Date_               20130404
Time                    4.35
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT                DMSO
NS                       512
DS                         4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                    143.73
DW                    20.800 usec
DE                     6.50 usec
TE                    295.2 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                        1
SFO1              100.6550182 MHz
NUC1                      13C
P1                     9.80 usec
PLW1              58.00000000 W
SFO2              400.2596010 MHz
NUC2                      1H
CPDPRG[2             waltz16
PCPD2                 90.00 usec
PLW2              14.00000000 W
PLW12              0.35097000 W
PLW13              0.28428999 W

F2 - Processing parameters
SI                        32768
SF                100.6450043 MHz
WDW                        EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

^{1}H & ^{13}C-NMR spectra of 4j

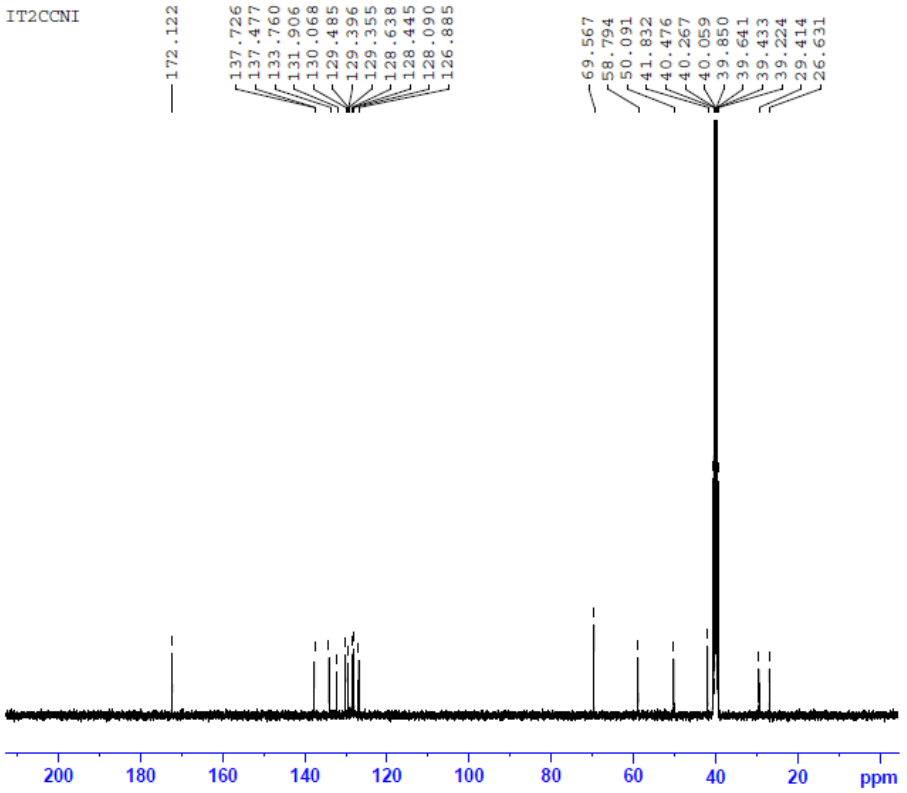



```
Current Data Parameters
NAME                  1T2CCN2
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20130206
Time                  15.25
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT               DMSO
NS                      16
DS                       2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9845889 sec
RG                    156.91
DW                    60.800 usec
DE                     6.50 usec
TE                    295.4 K
D1                 1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      14.25 usec
PLW1              14.00000000 W
SFO1             400.2604718 MHz

F2 - Processing parameters
SI                       65536
SF                400.2579895 MHz
WDW                         EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```

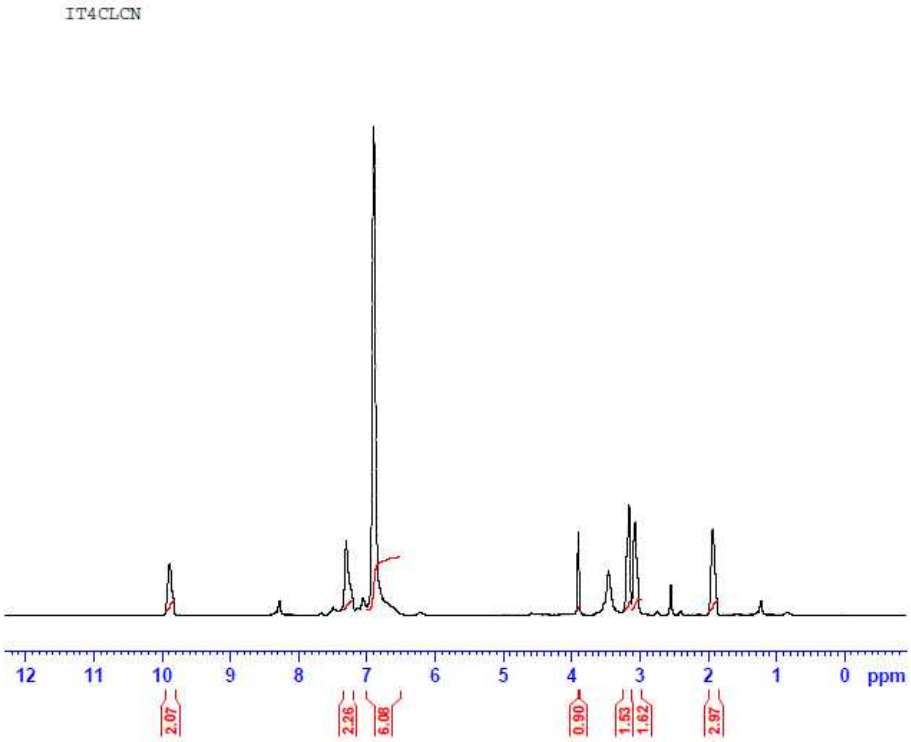



```
Current Data Parameters
NAME                  1T2CCN1
EXPNO                      34
PROCNO                      1

F2 - Acquisition Parameters
Date_              20130103
Time                  17.32
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT               DMSO
NS                    1024
DS                       4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                    143.73
DW                    20.800 usec
DE                     6.50 usec
TE                    295.2 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                         1
SFO1             100.6550182 MHz
NUC1                       13C
P1                      9.80 usec
PLW1              58.00000000 W
SFO2             400.2596010 MHz
NUC2                       1H
CPDPRG[2              waltz16
PCPD2                  90.00 usec
PLW2              14.00000000 W
PLW12              0.35097000 W
PLW13              0.28428999 W

F2 - Processing parameters
SI                       32768
SF                100.6449653 MHz
WDW                         EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

^{1}H & ^{13}C-NMR spectra of 4k

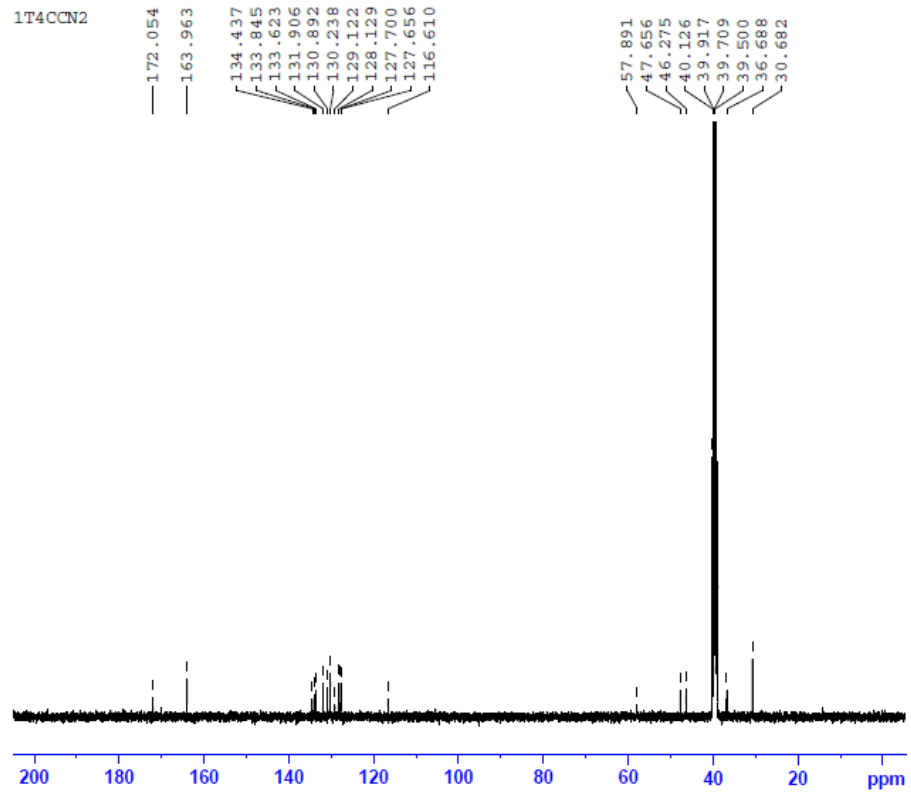



```
Current Data Parameters
NAME                  IT4CLCN
EXPNO                       7
PROCNO                      1

F2 - Acquisition Parameters
Date_               20130308
Time                   18.24
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9845889 sec
RG                    112.69
DW                    60.800 usec
DE                     6.50 usec
TE                    296.7 K
D1                 1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     14.25 usec
PLW1              14.00000000 W
SFO1             400.2604718 MHz

F2 - Processing parameters
SI                    65536
SF               400.2579898 MHz
WDW                      EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

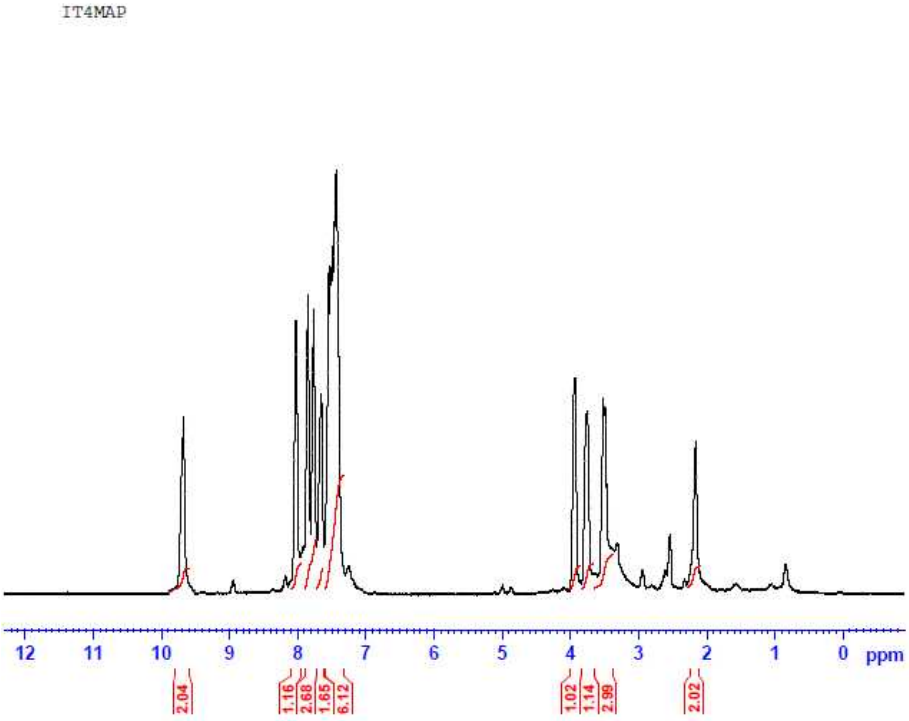



```
Current Data Parameters
NAME                 1T4CCN2
EXPNO                       4
PROCNO                      1

F2 - Acquisition Parameters
Date_               20130206
Time                   16.25
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                    112.69
DW                    20.800 usec
DE                     6.50 usec
TE                    296.9 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                       1
SFO1             100.6550182 MHz
NUC1                     13C
P1                     9.80 usec
PLW1              58.00000000 W
SFO2             400.2596010 MHz
NUC2                      1H
CPDPRG[2             waltz16
PCPD2                 90.00 usec
PLW2              14.00000000 W
PLW12              0.35097000 W
PLW13              0.28428999 W

F2 - Processing parameters
SI                    32768
SF               100.6450037 MHz
WDW                      EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

^{1}H & ^{13}C-NMR spectra of 4l

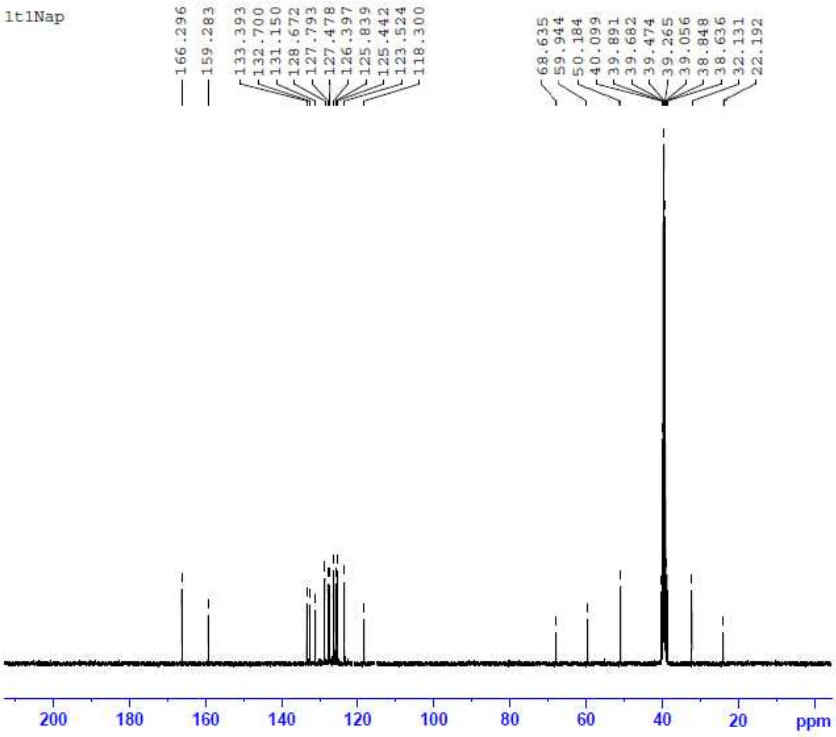



```
Current Data Parameters
NAME                  IT4MAP
EXPNO                     23
PROCNO                     1

F2 - Acquisition Parameters
Date_               20130311
Time                   21.03
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        16
DS                         2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                  3.9845889 sec
RG                     127.79
DW                     60.800 usec
DE                      6.50 usec
TE                     294.1 K
D1                  1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                       1H
P1                      14.25 usec
PLW1               14.00000000 W
SFO1               400.2604718 MHz

F2 - Processing parameters
SI                        65536
SF                 400.2579875 MHz
WDW                        EM
SSB                0
LB                      0.30 Hz
GB                 0
PC                      1.00
```




```
Current Data Parameters
NAME                  1t1Nap
EXPNO                     21
PROCNO                     1

F2 - Acquisition Parameters
Date_               20130403
Time                   13.09
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                       512
DS                         4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                     143.73
DW                     20.800 usec
DE                      6.50 usec
TE                     297.7 K
D1                  2.00000000 sec
d11                 0.03000000 sec
DELTA               1.89999998 sec
TD0                        1
SFO1               100.6550182 MHz
NUC1                      13C
P1                      9.80 usec
PLW1               58.00000000 W
SFO2               400.2596010 MHz
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                  90.00 usec
PLW2               14.00000000 W
PLW12               0.35097000 W
PLW13               0.28428999 W

F2 - Processing parameters
SI                        32768
SF                 100.6450043 MHz
WDW                        EM
SSB                0
LB                      1.00 Hz
GB                 0
PC                      1.40
```

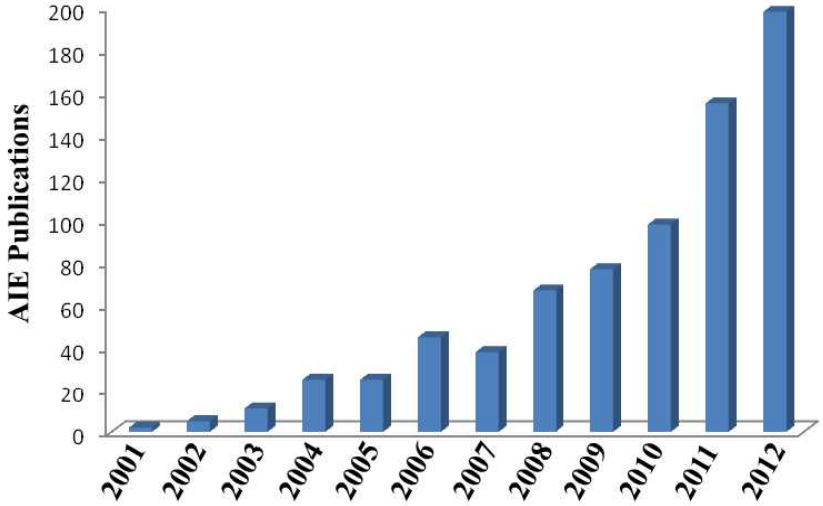
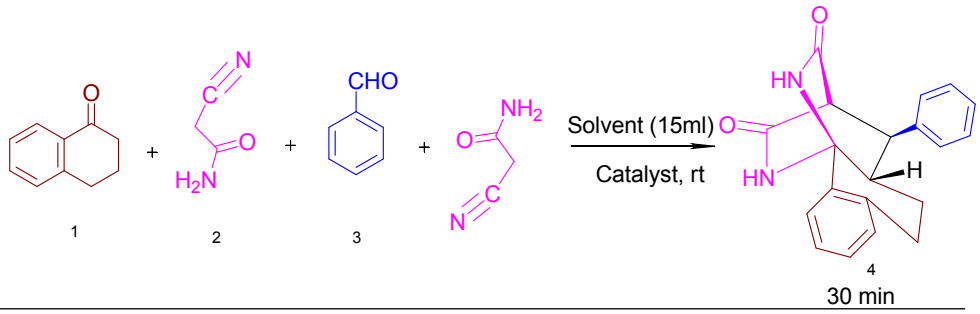


Figure S1. Year wise publication of aggregation induced emission from 2001 (Source Scopus[9])

Table S1. Screening of catalyst and solvent effect on four component domino reaction



Entry	Catalyst (mol %)	Solvent (ml)	Yield (%)[a]
1	None	Methanol	-
2	LiOH (1)	Methanol	24
3	LiOH (0.5)	Methanol	11
4	KOH (1)	Methanol	28
5	KOH (0.5)	Methanol	16
6	NaOH (2)	Methanol	82
7	NaOH (1)	Methanol	82
8	NaOH (0.5)	Methanol	82
9	NaOH (0.25)	Methanol	71
10	NaOH (0.5)	None	-
11	NaOH (0.5)	CH_3CN	-
12	NaOH (0.5)	DCM	-
13	NaOH (0.5)	Ethanol	73
14	NaOH (0.5)	IPA	64

15	NaOH (0.5)	Benzene	-
16	NaOH (0.5)	Hexane	-

[a]Isolated yield, IPA – Isopropyl alcohol, DCM- dichloromethane, CH_3CN – acetonitrile etc.

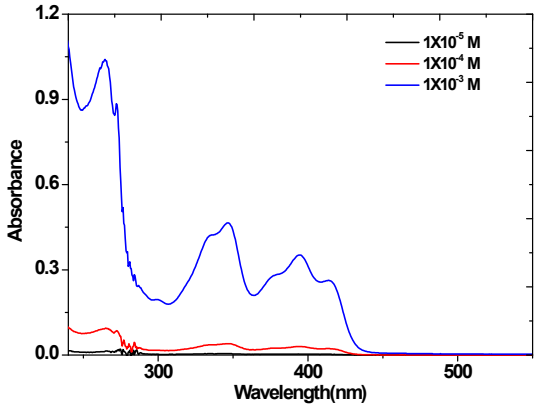


Figure S2: Absorption spectrum of Compound 4h in THF

Table S2: Photophysical data of synthesized compound 4a to 4l

S.No	Code	$\lambda_{Abs.max}$ (nm)	$\lambda_{Flu.max}$ (nm)[a]	Stokes shift (cm^{-1})	HOMO (ev)	LUMO (ev)	Energy gap (ev)
1.	**4a**	393	456	3515	-6.50	-0.79	-5.71
2.	**4b**	383	446	3688	-6.56	-0.84	-5.72
3.	**4c**	391	458	3741	-	-	-
4.	**4k**	394	460	3642	-	-	-
5.	**4d**	393	456	3515	-	-	-
6.	**4e**	395	458	3482	-	-	-
7.	**4f**	395	458	3482	-	-	-
8.	**4g**	394	458	3547	-	-	-
9.	**4h**	392	455	3532	-	-	-
10.	**4i**	393	456	3515	-	-	-
11.	**4j**	394	458	3547	-	-	-
12.	**4l**	393	456	3515	-5.91	-1.06	-4.85

[a]Molecules are excited at respective absorption maximum.

X-ray diffraction

Single crystals of data collection quality for 4b were grown from a mixture of ethanol and THF (1:1) Data were collected on a single-crystal Bruker SMART APEX2 diffractometer. The structure was solved by applying the direct phase-determination technique using SHELXS-97, and refined by full-matrix least square on F^2 using SHLEXL-97 (Sheldrick, 2008). Structural calculations were performed with WinGX suit of programs (version 1.85.05) (Farrugia, 1999). Hydrogens were stereochemically fixed and refined with the riding options. Amide NH and water hydrogens were isotropically refined. The N-H and O-H distance in the final cycle of refinement was 0.91(3)-0.92(3) Å & 0.81(3)-0.82(3) Å, respectively. Distances with rest of the hydrogen atoms are: aromatic/sp^2 C—H = 0.93 Å, methine C—H = 0.98 Å, and Uiso = 1.2 Ueq(parent). Essential crystal data are listed in

Table S3. Crystallographic data for the structures in this paper have been deposited with the Cambridge Crystallographic Data Centre having accession numbers, CCDC 956630. Copies of the data can be obtained, free of charge, on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: +44 (0)1223 336033 or email: deposit@ccdc.cam.ac.uk).

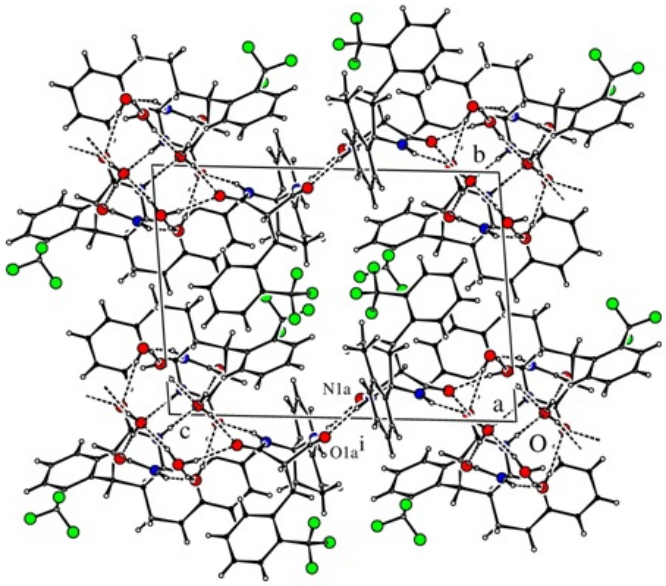


Figure S3. Crystal packing projected along a-axis displaying nanotube structure of 4b occupied with water

Table S3. Crystal data of 4b

	4b
Crystal Data	
Empirical formula	2(C21 H17 F3 N2 O2), 3(H2 O)
Molecular weight	826.78
Morphology	Colorless, block
Crystallizing solvent	CH_3CN : THF (1:1)
Crystal size (mm)	0.20x0.15x0.10
Cell Parameters	
a(Å)	10.0111(6)
b(Å)	11.8131(7)
c(Å)	16.4284(9)
α(°)	84.685(2)
β(°)	84.790(3)
γ(°)	83.889(3)

V (Å^3)	1923.39(19)
Cell measuring reflection	9329
θ-range (º)	2.38-27.93
Crystal system	Triclinic
Space group	P1bar
Z/Z'	4/2
Dx(cal.) (g/cm^3)	1.428
μ (mm^{-1})	0.117
Absorption correction	multi-scan
F(000)	860
Data Collection	
Radiation	MoK_α
Temperature (^0K)	295(2)
θ-range (º)	1.74 – 28.71
Index ranges	-12<=h<=13
	-15<=k<=15
	-21<=l<=20
Scan type	ϕ and ω scans
Independent reflections	9075
Observed [$I > 2\sigma(I)$]	5857
Refinement	
Final R [$F^2 > 2(F^2)$]	0.0504
$wR(F^2)$_all	0.1579
Goodness-of-fit (S)	1.006
$(\Delta/\sigma)_{max}$	0.001
$\Delta\rho_{max}$ and $\Delta\rho_{min}$ (e $Å^{-3}$)	0.26, -0.27
Data/restraints/ parameter	9075/0/556

$w = 1/[\sigma^2(F_0^2) + (aP)^2 + bP]$ where $P = (F_o^2 + 2F_c^2)/3$, parameters a and b are: 0.0793, 0.4756, respectively.

Table S4 inter and intra-molecular interactions observed in 4b

	Donor (D)	H	Acceptor (A)	D-H (Å)	H…A (Å)	D…A (Å)	Angle(D-H…A) (°)
N-H…O	N1A	H1A	O1A^{i}	0.86	2.05	2.886(2)	164
	N1B	H1B	O3W^{ii}	0.86	2.12	2.964(2)	166
	N2A	H2A	O1B^{iii}	0.86	2.03	2.852(2)	161
	N2B	H2B	O2W^{iv}	0.86	2.05	2.874(3)	159
Ow-H…X	O1W	H1W1	O2A	0.89(5)	2.10(5)	2.968(3)	167(4)
	O1W	H1W2	O3W^{v}	0.94(4)	2.00(4)	2.922(3)	166(3)
	O2W	H2W1	O1W^{vi}	0.96(4)	1.91(4)	2.852(3)	167(3)
	O2W	H2W2	O1B^{vii}	0.73(6)	2.22(6)	2.927(3)	165(5)
	O3W	H3W1	O2A^{viii}	0.78(4)	2.18(4)	2.940(2)	166(3)
	O3W	H3W2	O2B	0.92(4)	1.89(4)	2.807(2)	175(4)
C-H…O	C5A	H5A	O1A^{ix}	0.93	2.52	3.160(2)	126
C-H….F	C4A	H4A	F1B^{iii}	0.93	2.52	3.354(3)	150
	C8A	H8A1	F2B	0.97	2.54	3.378(3)	145
	C11A	H11A	F1A	0.98	2.30	3.037(2)	131
	C11A	H11A	F2A	0.98	2.46	3.037(2)	117
	C11B	H11B	F1B	0.98	2.34	2.948(2)	119
	C11B	H11B	F2B	0.98	2.37	3.083(2)	129
	C17A	H17A	F3A	0.93	2.33	2.680(3)	102
	C17B	H17B	F3B	0.93	2.33	2.678(3)	102

Symmetry codes: (i) -x,-y,1-z, (ii) 1-x,2-y,-z, (iii)x,-1+y,z, (iv) x,y,-1+z, (v)1-x,1-y,-z, (vi) 1-x,1-y,1-z, (vii) 1-x,2-y,1-z, (viii)1+x,1+y,z, (ix) 1+x,y,z.